

SAS/STAT® 12.1 User's Guide The ORTHOREG Procedure (Chapter)



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Chapter 66

The ORTHOREG Procedure

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Overview: ORTHOREG Procedure	5509
Getting Started: ORTHOREG Procedure	5510
Longley Data	5510
Syntax: ORTHOREG Procedure	5514
PROC ORTHOREG Statement	5514
BY Statement	5515
CLASS Statement	5516
EFFECT Statement	5517
EFFECTPLOT Statement	5519
ESTIMATE Statement	5520
LSMEANS Statement	5521
LSMESTIMATE Statement	5522
MODEL Statement	5523
SLICE Statement	5523
STORE Statement	5523
TEST Statement	5523
WEIGHT Statement	5524
Details: ORTHOREG Procedure	5524
Missing Values	5524
Output Data Set	5524
Displayed Output	5525
ODS Table Names	5525
ODS Graphics	5526
Examples: ORTHOREG Procedure	5526
Example 66.1: Precise Analysis of Variance	5526
Example 66.2: Wampler Data	5530
Example 66.3: Fitting Polynomials	5532
References	5537

Overview: ORTHOREG Procedure

The ORTHOREG procedure fits general linear models by the method of least squares. Other SAS/STAT software procedures, such as the GLM and REG procedures, fit the same types of models, but PROC

ORTHOREG can produce more accurate estimates than other regression procedures when your data are ill-conditioned. Instead of collecting crossproducts, PROC ORTHOREG uses Gentleman-Givens transformations to update and compute the upper triangular matrix **R** of the QR decomposition of the data matrix, with special care for scaling (Gentleman 1972, 1973). This method has the advantage over other orthogonalization methods (for example, Householder transformations) of not requiring the data matrix to be stored in memory.

The standard SAS regression procedures (PROC REG and PROC GLM) are very accurate for most problems. However, if you have very ill-conditioned data, these procedures can produce estimates that yield an error sum of squares very close to the minimum but still different from the exact least squares estimates. Normally, this coincides with estimates that have very high standard errors. In other words, the numerical error is much smaller than the statistical standard error.

PROC ORTHOREG fits models by the method of linear least squares, minimizing the sum of the squared residuals for predicting the responses—that is, the distance between the regression line and the observed Ys. The "ORTHO" in the name of the procedure refers to the orthogonalization approach to solving the least squares equations. In particular, PROC ORTHOREG does *not* perform the modeling method known as "orthogonal regression," which minimizes a different criterion (namely, the distance between the regression line and the X/Y points taken together.)

Getting Started: ORTHOREG Procedure

Longley Data

The labor statistics data set of Longley (1967) is noted for being ill-conditioned. Both the ORTHOREG and GLM procedures are applied for comparison (only portions of the PROC GLM results are shown).

NOTE: The results from this example vary from machine to machine, depending on floating-point configuration.

The following statements read the data into the SAS data set Longley:

```
title 'PROC ORTHOREG used with Longley data';
data Longley;
  input Employment Prices GNP Jobless Military PopSize Year;
   datalines;
60323 83.0 234289 2356 1590 107608 1947
61122 88.5 259426 2325 1456 108632 1948
60171 88.2 258054 3682 1616 109773 1949
61187 89.5 284599 3351 1650 110929 1950
63221 96.2 328975 2099 3099 112075 1951
63639
      98.1 346999 1932 3594 113270 1952
64989 99.0 365385 1870 3547 115094 1953
63761 100.0 363112 3578 3350 116219 1954
66019 101.2 397469 2904 3048 117388 1955
67857 104.6 419180 2822 2857 118734 1956
68169 108.4 442769 2936 2798 120445 1957
66513 110.8 444546 4681 2637 121950 1958
68655 112.6 482704 3813 2552 123366 1959
```

```
69564 114.2 502601 3931 2514 125368 1960 69331 115.7 518173 4806 2572 127852 1961 70551 116.9 554894 4007 2827 130081 1962 ;
```

The data set contains one dependent variable, Employment (total derived employment), and six independent variables: Prices (GNP implicit price deflator normalized to the value 100 in 1954), GNP (gross national product), Jobless (unemployment), Military (size of armed forces), PopSize (noninstitutional population aged 14 and over), and Year (year).

The following statements use the ORTHOREG procedure to model the Longley data by using a quadratic model in each independent variable, without interaction:

Figure 66.1 shows the resulting analysis.

Figure 66.1 PROC ORTHOREG Results

	PROC (ORTHOREG us	ed wit	h Longley data		
	The ORTHOREG Procedure					
	Deper	ndent Varia	ble: E	mployment		
		Su	m of			
Source	DF	Squ	ares	Mean Square	F Value	Pr > F
Model	12	1848645	08.5	15405375.709	320.24	0.0003
Error	3	144317.4	9568	48105.831895		
Corrected Total	15	18500	8826			
		Root MSE	219.	33041717		
		R-Square	0.99	92199426		

Figure 66.1 continued

			Standard		
Parameter	DF	Parameter Estimate	Error	t Value	Pr > t
Intercept	1	186931078.640216	154201839.66	1.21	0.312
Prices	1	1324.50679362506	916.17455832	1.45	0.244
Prices**2	1	-6.61923922845539	4.7891445654	-1.38	0.260
GNP	1	-0.12768642156232	0.0738897784	-1.73	0.182
GNP**2	1	3.1369569286212E-8	8.7167753E-8	0.36	0.742
Jobless	1	-4.35507653558708	1.3851792402	-3.14	0.051
Jobless**2	1	0.00022132944101	0.0001763541	1.26	0.298
Military	1	4.91162014560828	1.826715856	2.69	0.074
Military**2	1	-0.00113707146734	0.0003539971	-3.21	0.048
PopSize	1	-0.0303997234299	5.9272538242	-0.01	0.996
PopSize**2	1	-1.212511414607E-6	0.0000237262	-0.05	0.962
Year	1	-194907.139041839	157739.28757	-1.24	0.304
Year**2	1	50.8067603538501	40.279878943	1.26	0.296

The estimates in Figure 66.1 compare very well with the best estimates available; for additional information, see Longley (1967) and Beaton, Rubin, and Barone (1976).

The following statements request the same analysis from the GLM procedure:

Figure 66.2 contains the overall ANOVA table and the parameter estimates produced by PROC GLM. Notice that the PROC ORTHOREG fit achieves a somewhat smaller root mean square error (RMSE) and also that the GLM procedure detects spurious singularities.

Figure 66.2 Partial PROC GLM Results

PROC ORTHOREG used with Longley data The GLM Procedure Dependent Variable: Employment Sum of Source DF Squares Mean Square F Value Pr > FModel 11 184791061.6 16799187.4 308.58 <.0001 Error 4 217764.4 54441.1 Corrected Total 15 185008826.0 R-Square Coeff Var Root MSE Employment Mean 0.998823 0.357221 233.3262 65317.00 Standard Parameter **Estimate** Error t Value Pr > |t| -3598851.899 B Intercept 1327335.652 -2.710.0535 Prices 523.802 688.979 0.76 0.4894 Prices*Prices -2.326 3.507 -0.66 0.5434 GNP -0.138 0.078 -1.760.1526 GNP*GNP 0.000 0.000 0.24 0.8218 Jobless -4.599 1.459 -3.15 0.0344 Jobless*Jobless 0.000 1.14 0.3183 0.000 Military 4.994 1.942 2.57 0.0619 Military*Military -0.001 0.000 -3.150.0346 -4.246 5.156 -0.82 0.4565 PopSize

NOTE: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.

0.000

0.419

0.81

2.48

0.4655

0.0683

0.000 B

0.000 B 1.038

PopSize*PopSize

Year

Year*Year

Syntax: ORTHOREG Procedure

The following statements are available in the ORTHOREG procedure:

```
PROC ORTHOREG < options>;
    CLASS variables < / option>;
    MODEL dependent-variable = independent-effects < / option>;
    BY variables;
    EFFECT name = effect-type (variables < / options>);
    EFFECTPLOT < plot-type < (plot-definition-options) >> < / options>;
    ESTIMATE < 'label' > estimate-specification < / options>;
    LSMEANS < model-effects > < / options>;
    LSMESTIMATE model-effect lsmestimate-specification < / options>;
    SLICE model-effect < / options>;
    STORE < OUT = > item-store-name < / LABEL = 'label'>;
    TEST < model-effects > < / options>;
    WEIGHT variable;
```

The BY, CLASS, MODEL, and WEIGHT statements are described in full after the PROC ORTHOREG statement in alphabetical order. The EFFECT, EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements are common to many procedures. Summary descriptions of functionality and syntax for these statements are also given after the PROC ORTHOREG statement in alphabetical order, and full documentation about them is available in Chapter 19, "Shared Concepts and Topics."

PROC ORTHOREG Statement

PROC ORTHOREG < options > ;

The PROC ORTHOREG statement invokes the ORTHOREG procedure. Table 66.1 summarizes the options available in the PROC ORTHOREG statement.

Table 66.1 PROC ORTHOREG Statement Options

Option	Description
DATA=	Specifies the input SAS data set
NOPRINT	Suppresses the normal display of results
ORDER=	Specifies the order in which to sort class levels
OUTEST=	Produces an output data set
SINGULAR=	Specifies the singularity criterion

The PROC ORTHOREG statement has the following options:

DATA=SAS-data-set

specifies the input SAS data set to use. By default, the procedure uses the most recently created SAS data set. The data set specified cannot be a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set.

NOPRINT

suppresses the normal display of results. This option temporarily disables the Output Delivery System (ODS); see Chapter 20, "Using the Output Delivery System" for more information.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the classification variables (which are specified in the CLASS statement). This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option may be useful when you use ESTIMATE statement. This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

OUTEST=SAS-data-set

produces an output data set that contains the parameter estimates, the BY variables, and the special variables _TYPE_ (value "PARMS"), _NAME_ (blank), and _RMSE_ (root mean squared error).

SINGULAR=s

specifies a singularity criterion ($s \ge 0$) for the inversion of the triangular matrix **R**. By default, SINGULAR=1E-12.

BY Statement

BY variables;

You can specify a BY statement with PROC ORTHOREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the ORTHOREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in SAS Language Reference: Concepts. For more information about the DATASETS procedure, see the discussion in the Base SAS Procedures Guide.

CLASS Statement

CLASS variable < (REF= option) > . . . < variable < (REF= option) > > < / global-options > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC ORTHOREG statement. You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

REF='level' | FIRST | LAST

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ORTHOREG's singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the REF= *global-option* after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

REF=FIRST | LAST

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ORTHOREG's singular parameterization. Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use REF= options for individual variables.

TRUNCATE

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

EFFECT Statement

EFFECT name=effect-type (variables < / options >);

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section "GLM Parameterization of Classification Variables and Effects" on page 383 in Chapter 19, "Shared Concepts and Topics."

You can specify the following effect-types:

COLLECTION	is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.
LAG	is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.
MULTIMEMBER MM	is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.
POLYNOMIAL POLY	is a multivariate polynomial effect in the specified numeric variables.
SPLINE	is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables.

Table 66.2 summarizes the *options* available in the EFFECT statement.

Table 66.2 EFFECT Statement Options

Option	Description	
Collection Effects	Options	
DETAILS	Displays the constituents of the collection effect	

Table 66.2 continued

Option	Description
Lag Effects Options	
DESIGNROLE=	Names a variable that controls to which lag design an observation is assigned
DETAILS	Displays the lag design of the lag effect
NLAG=	Specifies the number of periods in the lag
PERIOD=	Names the variable that defines the period
WITHIN=	Names the variable or variables that define the group within which each period is defined
Multimember Effects C	Options
NOEFFECT	Specifies that observations with all missing levels for the multi- member variables should have zero values in the corresponding design matrix columns
WEIGHT=	Specifies the weight variable for the contributions of each of the classification effects
Polynomial Effects Opt	ions
DEGREE=	Specifies the degree of the polynomial
MDEGREE=	Specifies the maximum degree of any variable in a term of the polynomial
STANDARDIZE=	Specifies centering and scaling suboptions for the variables that define the polynomial
Spline Effects Options	
BASIS=	Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion
DEGREE=	Specifies the degree of the spline transformation
KNOTMETHOD=	Specifies how to construct the knots for spline effects

For more information about the syntax of these effect-types and how columns of constructed effects are computed, see the section "EFFECT Statement" on page 393 in Chapter 19, "Shared Concepts and Topics."

EFFECTPLOT Statement

EFFECTPLOT < plot-type < (plot-definition-options) >> </ options>;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 66.3 describes the available *plot-types* and their *plot-definition-options*.

 Table 66.3
 Plot-Types and Plot-Definition-Options

Plot-Type and Description	Plot-Definition-Options
BOX	
Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the INTERACTION <i>plot-type</i> .	PLOTBY= variable or CLASS effect X= CLASS variable or effect
CONTOUR	
Displays a contour plot of predicted values against two continuous covariates.	PLOTBY= variable or CLASS effect X= continuous variable Y= continuous variable
FIT	
Displays a curve of predicted values versus a continuous variable.	PLOTBY= variable or CLASS effect X= continuous variable
INTERACTION	
Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.	PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= CLASS variable or effect
SLICEFIT	
Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.	PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= continuous variable

For full details about the syntax and options of the EFFECTPLOT statement, see the section "EFFECTPLOT Statement" on page 411 in Chapter 19, "Shared Concepts and Topics."

ESTIMATE Statement

```
ESTIMATE < 'label' > estimate-specification < (divisor=n) >
           <, ... < 'label' > estimate-specification < (divisor=n) >>
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form $L\beta$. You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 66.4 summarizes the options available in the ESTIMATE statement.

Table 66.4 ESTIMATE Statement Options

Option	Description	
Construction and Com	putation of Estimable Functions	
DIVISOR=	Specifies a list of values to divide the coefficients	
NOFILL	Suppresses the automatic fill-in of coefficients for higher-order ef-	
	fects	
SINGULAR=	Tunes the estimability checking difference	
Degrees of Freedom an	nd p-values	
ADJUST=	Determines the method for multiple comparison adjustment of es-	
	timates	
ALPHA= α	Determines the confidence level $(1 - \alpha)$	
LOWER	Performs one-sided, lower-tailed inference	
STEPDOWN	Adjusts multiplicity-corrected p-values further in a step-down	
	fashion	
TESTVALUE=	Specifies values under the null hypothesis for tests	
UPPER	Performs one-sided, upper-tailed inference	
Statistical Output		
CL	Constructs confidence limits	
CORR	Displays the correlation matrix of estimates	
COV	Displays the covariance matrix of estimates	
E	Prints the L matrix	
JOINT	Produces a joint F or chi-square test for the estimable functions	
SEED=	Specifies the seed for computations that depend on random	
	numbers	

For details about the syntax of the ESTIMATE statement, see the section "ESTIMATE Statement" on page 437 in Chapter 19, "Shared Concepts and Topics."

LSMEANS Statement

LSMEANS < model-effects > </ options > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 66.5 summarizes the options available in the LSMEANS statement.

Table 66.5 LSMEANS Statement Options

Option	Description
Construction and Com	putation of LS-Means
AT	Modifies the covariate value in computing LS-means
BYLEVEL	Computes separate margins
DIFF	Requests differences of LS-means
OM=	Specifies the weighting scheme for LS-means computation as de-
	termined by the input data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom an	d p-values
ADJUST=	Determines the method for multiple-comparison adjustment of LS-
	means differences
$ALPHA=\alpha$	Determines the confidence level $(1 - \alpha)$
STEPDOWN	Adjusts multiple-comparison p-values further in a step-down
	fashion
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
Е	Prints the L matrix
LINES	Produces a "Lines" display for pairwise LS-means differences
MEANS	Prints the LS-means
PLOTS=	Requests graphs of means and mean comparisons
SEED=	Specifies the seed for computations that depend on random
	numbers

For details about the syntax of the LSMEANS statement, see the section "LSMEANS Statement" on page 453 in Chapter 19, "Shared Concepts and Topics."

LSMESTIMATE Statement

```
LSMESTIMATE model-effect < 'label' > values < divisor=n > < , ... < 'label' > values < divisor=n > > < / options > ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 66.6 summarizes the options available in the LSMESTIMATE statement.

Table 66.6 LSMESTIMATE Statement Options

Option	Description
Construction and C	omputation of LS-Means
AT	Modifies covariate values in computing LS-means
BYLEVEL	Computes separate margins
DIVISOR=	Specifies a list of values to divide the coefficients
OM=	Specifies the weighting scheme for LS-means computation as determined by a data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom	and p-values
ADJUST=	Determines the method for multiple-comparison adjustment of LS-
	means differences
$ALPHA=\alpha$	Determines the confidence level $(1 - \alpha)$
LOWER	Performs one-sided, lower-tailed inference
STEPDOWN	Adjusts multiple-comparison p-values further in a step-down fash-
	ion
TESTVALUE=	Specifies values under the null hypothesis for tests
UPPER	Performs one-sided, upper-tailed inference
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
ELSM	Prints the K matrix
JOINT	Produces a joint F or chi-square test for the LS-means and LS-
	means differences
SEED=	Specifies the seed for computations that depend on random
	numbers

For details about the syntax of the LSMESTIMATE statement, see the section "LSMESTIMATE Statement" on page 470 in Chapter 19, "Shared Concepts and Topics."

MODEL Statement

MODEL dependent-variable = independent-effects < / option > ;

The MODEL statement names the dependent variable and the independent effects. Only one MODEL statement is allowed. The specification of effects and the parameterization of the linear model are the same as in the GLM procedure; see Chapter 42, "The GLM Procedure" for further details.

The following option can be used in the MODEL statement:

NOINT

omits the intercept term from the model. Often, this omission also changes the total sum of squares in the ANOVA and the value of R square to forms of these statistics that are not corrected for the mean. However, if the model is determined to contain an implicit intercept, in the sense that the all-ones intercept vector is in the column space of the design, then the usual mean-corrected forms of these statistics are used.

SLICE Statement

SLICE model-effect < / options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section "SLICE Statement" on page 498 in Chapter 19, "Shared Concepts and Topics."

STORE Statement

STORE < OUT = > item-store-name < / LABEL = 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section "STORE Statement" on page 501 in Chapter 19, "Shared Concepts and Topics."

TEST Statement

TEST < model-effects > </ options > ;

The TEST statement enables you to perform *F* tests for model effects that test Type I, Type II, or Type III hypotheses. See Chapter 15, "The Four Types of Estimable Functions," for details about the construction of Type I, II, and III estimable functions.

Table 66.7 summarizes the options available in the TEST statement.

Option	Description
CHISQ	Requests chi-square tests
DDF=	Specifies denominator degrees of freedom for fixed effects
E	Requests Type I, Type II, and Type III coefficients
E1	Requests Type I coefficients
E2	Requests Type II coefficients
E3	Requests Type III coefficients
HTYPE=	Indicates the type of hypothesis test to perform
INTERCEPT	Adds a row that corresponds to the overall intercept

Table 66.7 TEST Statement Options

For details about the syntax of the TEST statement, see the section "TEST Statement" on page 502 in Chapter 19, "Shared Concepts and Topics."

WEIGHT Statement

WEIGHT variable;

A WEIGHT statement names a variable in the input data set whose values are relative weights for a weighted least squares regression. If the weight value is proportional to the reciprocal of the variance for each observation, the weighted estimates are the best linear unbiased estimates (BLUE). For a more complete description of the WEIGHT statement, see the section "WEIGHT Statement" on page 3323 in the GLM procedure.

Details: ORTHOREG Procedure

Missing Values

If there is a missing value for any model variable in an observation, the entire observation is dropped from the analysis.

Output Data Set

The OUTEST= option produces a TYPE=EST output SAS data set that contains the BY variables, parameter estimates, and four special variables. For each new value of the BY variables, PROC ORTHOREG outputs an observation to the OUTEST= data set. The variables in the data set are as follows:

- parameter estimates for all variables listed in the MODEL statement
- BY variables
- _TYPE_, which is a character variable with the value PARMS for every observation

- NAME, which is a character variable left blank for every observation
- _RMSE_, which is the root mean square error (the estimate of the standard deviation of the true errors)
- Intercept, which is the estimated intercept. This variable does not exist in the OUTEST= data set if the NOINT option is specified.

Displayed Output

PROC ORTHOREG displays the parameter estimates and associated statistics. These include the following:

- overall model analysis of variance, including the error mean square, which is an estimate of σ^2 (the variance of the true errors), and the overall F test for a model effect.
- root mean square error, which is an estimate of the standard deviation of the true errors. It is calculated as the square root of the mean squared error.
- R square (R²) measures how much variation in the dependent variable can be accounted for by the model. R square, which can range from 0 to 1, is the ratio of the sum of squares for the model to the corrected total sum of squares. In general, the larger the value of R square, the better the model's fit.
- estimates for the parameters in the linear model

The table of parameter estimates consists of the following:

- the terms used as regressors, including the intercept.
- degrees of freedom (DF) for the variable. There is one degree of freedom for each parameter being estimated unless the model is not full rank.
- estimated linear coefficients.
- estimates of the standard errors of the parameter estimates.
- the critical *t* values for testing whether the parameters are This is computed as the parameter estimate divided by its standard error.
- the two-sided *p*-value for the *t* test, which is the probability that a *t* statistic would obtain a greater absolute value than that observed given that the true parameter is zero.

ODS Table Names

PROC ORTHOREG assigns a name to each table it creates. You can use these names to reference the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 66.8. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

Each of the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements also creates tables, which are not listed in Table 66.8. For information about these tables, see the corresponding sections of Chapter 19, "Shared Concepts and Topics."

ODS Table Name	Description	Statement
ANOVA	Analysis of variance	Default
FitStatistics	Overall statistics for fit	Default
Levels	Table of class levels	CLASS statement
ParameterEstimates	Parameter estimates	Default

Table 66.8 ODS Tables Produced by PROC ORTHOREG

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, "Statistical Graphics Using ODS."

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 600 in Chapter 21, "Statistical Graphics Using ODS."

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section "A Primer on ODS Statistical Graphics" on page 599 in Chapter 21, "Statistical Graphics Using ODS."

When ODS Graphics is enabled, then each of the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, "Shared Concepts and Topics."

Examples: ORTHOREG Procedure

Example 66.1: Precise Analysis of Variance

The data for the following example are from Powell, Murphy, and Gramlich (1982). In order to calibrate an instrument for measuring atomic weight, 24 replicate measurements of the atomic weight of silver (chemical symbol Ag) are made with the new instrument and with a reference instrument.

NOTE: The results from this example vary from machine to machine, depending on floating-point configuration.

The following statements read the measurements for the two instruments into the SAS data set AgWeight:

```
title 'Atomic Weight of Silver by Two Different Instruments';
data AgWeight;
  input Instrument AgWeight @@;
  datalines;
1 107.8681568
            1 107.8681465
                       1 107.8681572
                                     1 107.8681785
1 107.8681494
1 107.8681616
            1 107.8681587 1 107.8681519
                                     1 107.8681486
1 107.8681419
            1 107.8681569 1 107.8681508
                                     1 107.8681672
1 107.8681424
1 107.8681477
2 107.8681197
2 107.8681604 2 107.8681385 2 107.8681642 2 107.8681365
2 107.8681151 2 107.8681082 2 107.8681517 2 107.8681448
2 107.8681198 2 107.8681482 2 107.8681334
2 107.8681101 2 107.8681512 2 107.8681469
                                    2 107.8681609
                                     2 107.8681360
2 107.8681254
            2 107.8681261 2 107.8681450
                                     2 107.8681368
```

Notice that the variation in the atomic weight measurements is several orders of magnitude less than their mean. This is a situation that can be difficult for standard, regression-based analysis-of-variance procedures to handle correctly.

The following statements invoke the ORTHOREG procedure to perform a simple one-way analysis of variance, testing for differences between the two instruments:

```
proc orthoreg data=AgWeight;
  class Instrument;
  model AgWeight = Instrument;
run;
```

Output 66.1.1 shows the resulting analysis.

Output 66.1.1 PROC ORTHOREG Results for Atomic Weight Example

```
Atomic Weight of Silver by Two Different Instruments

The ORTHOREG Procedure

Class Level Information
Factor Levels -Values-

Instrument 2 1 2
```

Output 66.1.1 continued

Atom	ic Wei	ght of Sil	ver by Two	Different Inst	ruments	
		The O	RTHOREG Pr	ocedure		
		Dependent	Variable:	AgWeight		
			Sum of			
Source		DF	Squares	Mean Square	F Value	Pr > F
Model		1 3.63	83419E-9	3.6383419E-9	15.95	0.0002
Error		46 1.04	95173E-8	2.281559E-10		
Corrected Total		47 1.41	33515E-8			
		Root M	ISE 0.00	00151048		
		R-Squa	re 0.25	74265445		
				Standard		
Parameter	DF	Parameter	Estimate	Error	t Value	Pr > t
Intercept	1	107.868	136354166	3.0832608E-6	3.499E7	<.0001
(Instrument='1')	1	0.00001	741249999	4.3603893E-6	3.99	0.0002
(Instrument='2')	0		0			

The mean difference between instruments is about 1.74×10^{-5} (the value of the (Instrument='1') parameter in the parameter estimates table), whereas the level of background variation in the measurements is about 1.51×10^{-5} (the value of the root mean square error). At this level of error, the difference is significant, with a *p*-value of 0.0002.

The National Institute of Standards and Technology (1998) has provided certified ANOVA values for this data set. The following statements use ODS to examine the ANOVA values produced by both the ORTHOREG and GLM procedures more precisely for comparison with the NIST-certified values:

```
ods listing close;
proc orthoreg data=AgWeight;
   class Instrument;
  model AgWeight = Instrument;
   ods output ANOVA
                      = OrthoregANOVA
              FitStatistics = OrthoregFitStat;
run;
proc glm data=AgWeight;
   class Instrument;
  model AgWeight = Instrument;
   ods output OverallANOVA = GLMANOVA
              FitStatistics = GLMFitStat;
run;
ods listing;
data _null_;
   set OrthoregANOVA (in=inANOVA)
       OrthoregFitStat(in=inFitStat);
   if (inANOVA) then do;
      if (Source = 'Model') then put "Model SS: " ss e20.;
      if (Source = 'Error') then put "Error SS: " ss e20.;
   end;
   if (inFitStat) then do;
      if (Statistic = 'Root MSE') then
                            put "Root MSE: " nValue1 e20.;
      if (Statistic = 'R-Square') then
                         put "R-Square: " nValue1 best20.;
   end;
run;
data _null_;
   set GLMANOVA (in=inANOVA)
       GLMFitStat(in=inFitStat);
   if (inANOVA) then do;
      if (Source = 'Model') then put "Model SS: " ss e20.;
      if (Source = 'Error') then put "Error SS: " ss e20.;
   end;
   if (inFitStat) then
                            put "Root MSE: " RootMSE e20.;
   if (inFitStat) then put "R-Square: " RSquare best20.;
run:
```

In SAS/STAT software prior to SAS 8, PROC GLM gave much less accurate results than PROC ORTHOREG. Table 66.9 and Table 66.10 compare the ANOVA values certified by NIST with those produced by the two procedures.

Table 66.9 Accuracy Comparison for Sums of Squares

Values	Model SS	Error SS
NIST-certified ORTHOREG		1.0495172916667E-08 1.0495172916797E-08

Values Model SS Error SS 1.0495172916797E-08 GLM, since SAS 8 3.6383418747907E-09 GLM, before SAS 8 0 1.0331496763990E-08

Table 66.9 continued

Table 66.10 Accuracy Comparison for Fit Statistics

Values	Root MSE	R Square
NIST-certified	1.5104831444641E-05	0.25742654453832
ORTHOREG	1.5104831444735E-05	0.25742654452494
GLM, since SAS 8	1.5104831444735E-05	0.25742654452494
GLM, before SAS 8	1.4986585859992E-05	0

Although the PROC ORTHOREG values and the PROC GLM values for the current version are quite close to the certified ones, the PROC GLM values for releases prior to SAS 8 are not. In fact, since the model sum of squares is so small, in prior releases the GLM procedure set it (and consequently R square) to zero.

Example 66.2: Wampler Data

This example applies the ORTHOREG procedure to a collection of data sets noted for being ill-conditioned. The OUTEST= data set is used to collect the results for comparison with values certified to be correct by the National Institute of Standards and Technology (1998).

NOTE: The results from this example vary from machine to machine, depending on floating-point configuration.

The data are from Wampler (1970). The independent variates for all five data sets are x^i , i = 1, ... 5, for $x = 0, 1, \dots, 20$. Two of the five dependent variables are exact linear functions of the independent terms:

$$y_1 = 1 + x + x^2 + x^3 + x^4 + x^5$$

 $y_2 = 1 + 0.1x + 0.01x^2 + 0.001x^3 + 0.0001x^4 + 0.00001x^5$

The other three dependent variables have the same mean value as y_1 , but with nonzero errors:

$$y_3 = y_1 + e$$

 $y_4 = y_1 + 100e$
 $y_5 = y_1 + 10000e$

where e is a vector of values with standard deviation \sim 2044, chosen to be orthogonal to the mean model for y_1 .

The following statements create a SAS data set Wampler that contains the Wampler data, run a SAS macro program that uses PROC ORTHOREG to fit a fifth-order polynomial in *x* to each of the Wampler dependent variables, and collect the results in a data set named ParmEst:

```
data Wampler;
  do x=0 to 20;
     input e @@;
     v1 = 1 +
                    x
                                   x**2 +
                                               x**3
                    x**4 +
                                   x**5;
     y2 = 1 + .1 *x + .01
                                 *x**2 + .001*x**3
             + .0001*x**4 + .00001*x**5;
     y3 = y1 +
                     e;
     y4 = y1 +
                 100*e;
     y5 = y1 + 10000*e;
      output;
  end;
   datalines;
759 -2048 2048 -2048 2523 -2048 2048 -2048 1838 -2048 2048
-2048 1838 -2048 2048 -2048 2523 -2048 2048 -2048 759
%macro WTest;
  data ParmEst; if (0); run;
  %do i = 1 %to 5;
     proc orthoreg data=Wampler outest=ParmEst&i noprint;
         model y\&i = x x*x x*x*x x*x*x x*x*x*x;
     data ParmEst&i; set ParmEst&i; Dep = "y&i";
      data ParmEst; set ParmEst ParmEst&i;
         label Col1='x' Col2='x**2' Col3='x**3'
              Col4='x**4' Col5='x**5';
      run;
   %end;
%mend:
%WTest;
```

Instead of displaying the raw values of the RMSE and parameter estimates, use an additional DATA step as follows to compute the deviations from the values certified to be correct by the National Institute of Standards and Technology (1998):

```
Intercept = Intercept - 1.00000000000000;
     = Co12
                      - 1.00000000000000;
     Col2
    Col3 = Col3 - 1.0000000000000;
Col4 = Col4 - 1.0000000000000;
Col5 = Col5 - 1.00000000000000;
  end;
  else do;
     Intercept = Intercept - 1.0000000000000;
     = Co12
     Col2
                      - 0.100000000000000e-1;
    end;
run;
proc print data=ParmEst label noobs;
  title 'Wampler data: Deviations from Certified Values';
  format _RMSE_ Intercept Col1-Col5 e9.;
  var Dep _RMSE_ Intercept Col1-Col5;
run;
```

The results, shown in Output 66.2.1, indicate that the values computed by PROC ORTHOREG are quite close to the NIST-certified values.

Output 66.2.1 Wampler Data: Deviations from Certified Values

Wampler data: Deviations from Certified Values									
Dep	_RMSE_	Intercept	x	x**2	x **3	x**4	x **5		
y1	0.00E+00	5.46E-12	-9.82E-11	1.55E-11	-5.68E-13	3.55E-14	-6.66E-16		
y2	0.00E+00	8.88E-16	-3.19E-15	1.24E-15	-1.88E-16	1.20E-17	-2.57E-19		
у3	-2.09E-11	-7.73E-11	1.46E-11	-2.09E-11	2.50E-12	-1.28E-13	2.66E-15		
y4	-4.07E-10	-5.38E-10	8.99E-10	-3.29E-10	4.23E-11	-2.27E-12	4.35E-14		
y5	-3.35E-08	-4.10E-08	8.07E-08	-2.77E-08	3.54E-09	-1.90E-10	3.64E-12		

Example 66.3: Fitting Polynomials

The extra accuracy of the regression algorithm used by PROC ORTHOREG is most useful when the model contains near-singularities that you want to be able to distinguish from true singularities. This example demonstrates this usefulness in the context of fitting polynomials of high degree.

NOTE: The results from this example vary from machine to machine, depending on floating-point configuration.

The following DATA step computes a response y as an exact ninth-degree polynomial function of a predictor x evaluated at 0, 0.01, 0.02, ..., 1.

```
title 'Polynomial Data';
data Polynomial;
  do i = 1 to 101;
    x = (i-1)/(101-1);
    y = 10**(9/2);
    do j = 0 to 8;
        y = y * (x - j/8);
    end;
    output;
end;
run;
```

The polynomial is constructed in such a way that its zeros lie at x = i/8 for i = 0, ..., 8. The following statements use the EFFECT statement to fit a ninth-degree polynomial to this data with PROC ORTHOREG. The EFFECT statement makes it easy to specify complicated polynomial models.

```
ods graphics on;
proc orthoreg data=Polynomial;
  effect xMod = polynomial(x / degree=9);
  model y = xMod;
  effectplot fit / obs;
  store OStore;
run;
ods graphics off;
```

The effect xMod defined by the EFFECT statement refers to all nine degrees of freedom in the ninth-degree polynomial (excluding the intercept term). The resulting output is shown in Output 66.3.1. Note that the R square for the fit is 1, indicating that the ninth-degree polynomial has been correctly fit.

Output 66.3.1 PROC ORTHOREG Results for Ninth-Degree Polynomial

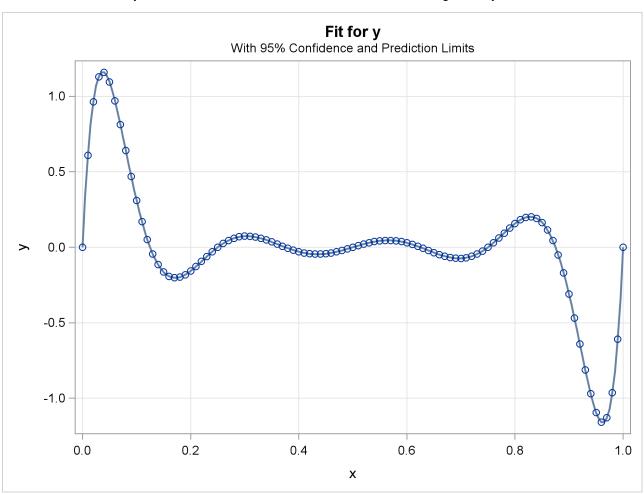
```
Polynomial Data
                            The ORTHOREG Procedure
                           Dependent Variable: y
                                   Sum of
Source
                      DF
                                  Squares
                                             Mean Square
                                                            F Value
                                                                       Pr > F
                                                            1.65E22
                             15.527180055
                                            1.7252422284
                                                                        <.0001
Model
                       9
                                            1.043584E-22
                      91
                             9.496616E-21
Error
Corrected Total
                      100
                             15.527180055
                           Root MSE
                                      1.02156E-11
                           R-Square
```

Output 66.3.1 continued

			Standard		
Parameter	DF	Parameter Estimate	Error	t Value	Pr > t
Intercept	1	-3.24572035915E-11	8.114115E-12	-4.00	0.0001
x	1	75.9977312440678	4.898326E-10	1.55E11	<.0001
x^2	1	-1652.40781362191	9.5027919E-9	-174E9	<.0001
x^ 3	1	14249.4539769783	8.3110512E-8	1.71E11	<.0001
x^4	1	-64932.461575205	3.8997072E-7	-167E9	<.0001
x^5	1	173315.359360779	1.066611E-6	1.62E11	<.0001
x^6	1	-280158.03646002	1.7523078E-6	-16E10	<.0001
x^7	1	269781.812887653	1.7021134E-6	1.58E11	<.0001
x^8	1	-142302.494710055	9.0027891E-7	-158E9	<.0001
x^9	1	31622.7766022468	1.997493E-7	1.58E11	<.0001

The fit plot produced by the EFFECTPLOT statement, Output 66.3.2, also demonstrates the perfect fit.

Output 66.3.2 PROC ORTHOREG Fit Plot for Ninth-Degree Polynomial



Finally, you can use the PLM procedure with the fit model saved by the STORE statement in the item store

OStore to check the predicted values for the known zeros of the polynomial, as shown in the following statements:

```
data Zeros(keep=x);
  do j = 0 to 8;
    x = j/8;
    output;
  end;
run;

proc plm restore=OStore noprint;
  score data=Zeros out=OZeros pred=OPred;
run;

proc print noobs;
run;
```

The predicted values of the zeros, shown in Output 66.3.3, are again all miniscule.

Output 66.3.3 Predicted Zeros for Ninth-Degree Polynomial

Po	ynomial Data	
х	OPred	
0.00	-3.2457E-11	
0.12	-2.1262E-11	
0.2	-9.5867E-12	
0.3	-2.2895E-11	
0.50	-5.2154E-11	
0.62	-1.2329E-10	
0.79	-2.5329E-10	
0.8	-3.9836E-10	
1.00	-5.9663E-10	

To compare these results with those from a least squares fit produced by an alternative algorithm, consider fitting a polynomial to this data using the GLM procedure. PROC GLM does not have an EFFECT statement, but the familiar bar notation can still be used to specify a ninth-degree polynomial fairly succinctly, as shown in the following statements:

```
proc glm data=Polynomial;
  model y = x|x|x|x|x|x|x|x;
  store GStore;
run;
```

Partial results are shown in Output 66.3.4. In this case, the R square for the fit is only about 0.83, indicating that the full ninth-degree polynomial was not correctly fit.

Output 66.3.4 PROC GLM for Ninth-Degree Polynomial

Polynomial Data The GLM Procedure							
Dependent Variable: y							
Source	DF	Sum Squa	of res	Mean	Square	F Value	Pr > F
Model	8	12.91166	643	1.61	.395830	56.77	<.0001
Error	92	2.61551	363	0.02	842950		
Corrected Total	100	15.52718	006				
R-Square	Coeff	Var	Root I	MSE	уМ	l ean	
0.831553	-6.669	1E17	0.168	610	-0.000	0000	

The following statements, which use the PLM procedure to compute predictions based on the GLM fit at the true zeros of the polynomial, also confirm that PROC GLM is not able to correctly fit a polynomial of this degree, as shown in Output 66.3.5.

```
proc plm restore=GStore noprint;
   score data=Zeros out=GZeros pred=GPred;
run;
data Zeros;
   merge OZeros GZeros;
run;
proc print noobs;
run;
```

Output 66.3.5 Predicted Zeros for Ninth-Degree Polynomial

	Polynomial Dat	a
x	OPred	GPred
0.000	-3.2457E-11	0.44896
0.125	-2.1262E-11	0.22087
0.250	-9.5867E-12	-0.19037
0.375	-2.2895E-11	0.12710
0.500	-5.2154E-11	0.00000
0.625	-1.2329E-10	-0.12710
0.750	-2.5329E-10	0.19037
0.875	-3.9836E-10	-0.22087
1.000	-5.9663E-10	-0.44896

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Subject Index

```
Gentleman-Givens computational method, 5510
GLM procedure
    compared to other procedures, 5510
ill-conditioned data
    ORTHOREG procedure, 5510
Longley data set, 5510
ODS examples
    ORTHOREG procedure, 5528
options summary
    EFFECT statement, 5517
    ESTIMATE statement, 5520
ORTHOREG procedure
    compared to other procedures, 5510
    input data sets, 5514
    introductory example, 5510
    missing values, 5524
    ODS graphics, 5526
    ODS table names, 5525
    output data sets, 5515, 5524
ORTHOREG procedure
    ordering of effects, 5515
REG procedure
    compared to other procedures, 5510
regression
    ill-conditioned data, 5510
    ORTHOREG procedure, 5510
Wampler data set, 5530
```

Syntax Index

BY statement	ORTHOREG procedure, ESTIMATE statement, 552
ORTHOREG procedure, 5515	ORTHOREG procedure, LSMEANS statement, 552
1 /	ORTHOREG procedure, LSMESTIMATE statement
CLASS statement	5522
ORTHOREG procedure, 5516	ORTHOREG procedure, PROC ORTHOREG
•	statement
DATA= option	ORDER= option, 5515
PROC ORTHOREG statement, 5514	ORTHOREG procedure, SLICE statement, 5523
	ORTHOREG procedure, STORE statement, 5523
EFFECT statement	
ORTHOREG procedure, 5517	ORTHOREG procedure, TEST statement, 5523
EFFECTPLOT statement	OUTEST= option
ORTHOREG procedure, 5519	PROC ORTHOREG statement, 5515
ESTIMATE statement	DDGG ODTHODEG
ORTHOREG procedure, 5520	PROC ORTHOREG statement, see ORTHOREG
F, F	procedure
LSMEANS statement	DEE .:
ORTHOREG procedure, 5521	REF= option
LSMESTIMATE statement	CLASS statement (ORTHOREG), 5516, 5517
ORTHOREG procedure, 5522	CDICHT AD
0111101120 p10 00 0110, 00 22	SINGULAR= option
MODEL statement	PROC ORTHOREG statement, 5515
ORTHOREG procedure, 5523	SLICE statement
F, F	ORTHOREG procedure, 5523
NOINT option	STORE statement
MODEL statement (ORTHOREG), 5523	ORTHOREG procedure, 5523
NOPRINT option	
PROC ORTHOREG statement, 5515	TEST statement
TROC ORTHORES statement, 3313	ORTHOREG procedure, 5523
ORDER= option	TRUNCATE option
PROC ORTHOREG statement, 5515	CLASS statement (ORTHOREG), 5517
ORTHOREG procedure	•
syntax, 5514	WEIGHT statement
ORTHOREG procedure, BY statement, 5515	ORTHOREG procedure, 5524
ORTHOREG procedure, MODEL statement, 5523	•
NOINT option, 5523	
ORTHOREG procedure, PROC ORTHOREG	
statement, 5514	
DATA= option, 5514	
NOPRINT option, 5515	
OUTEST= option, 5515	
SINGULAR= option, 5515	
ORTHOREG procedure, WEIGHT statement, 5524	
ORTHOREG procedure, CLASS statement, 5516	
REF= option, 5517	
REF= variable option, 5516	
TRUNCATE option, 5517	
ORTHOREG procedure, EFFECT statement, 5517	
ORTHOREG procedure, EFFECTPLOT statement,	
5519	

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