

SAS/STAT® 14.1 User's Guide The GAM Procedure



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SAS/STAT® 14.1 User's Guide

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Chapter 41 The GAM Procedure

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The GAM procedure fits generalized additive models as defined by Hastie and Tibshirani (1990). This procedure provides powerful tools for nonparametric regression and smoothing.

Nonparametric regression relaxes the usual assumption of linearity and enables you to uncover relationships between the independent variables and the dependent variable that might otherwise be missed. SAS provides many procedures for nonparametric regression, such as the LOESS procedure for local regression and the TPSPLINE procedure for thin-plate smoothing splines. The generalized additive models fit by the GAM procedure combine the following:

- an additivity assumption (Stone 1985) that enables relatively many nonparametric relationships to be explored simultaneously
- the distributional flexibility of generalized linear models (Nelder and Wedderburn 1972)

Thus, you can use the GAM procedure when you have multiple independent variables whose effect you want to model nonparametrically, or when the dependent variable is not normally distributed. See the section "Nonparametric Regression" on page 2820 for more details on the form of generalized additive models.

The GAM procedure does the following:

- provides nonparametric estimates for additive models
- supports the use of multidimensional data
- supports multiple SCORE statements
- fits both generalized semiparametric additive models and generalized additive models
- enables you to choose a particular model by specifying the model degrees of freedom or smoothing parameter
- produces graphs with ODS Graphics

Getting Started: GAM Procedure

The following example illustrates the use of the GAM procedure to explore in a nonparametric way how two factors affect a response. The data come from a study of the factors affecting patterns of insulin-dependent diabetes mellitus in children (Sochett et al. 1987). The objective is to investigate the dependence of the level of serum C-peptide on various other factors in order to understand the patterns of residual insulin secretion. The response measurement is the logarithm of C-peptide concentration (pmol/ml) at diagnosis, and the predictor measurements are age and base deficit (a measure of acidity).

```
title 'Patterns of Diabetes';
data diabetes;
  input Age BaseDeficit CPeptide @@;
  logCP = log(CPeptide);
  datalines;
5.2
     -8.1 4.8
              8.8 -16.1 4.1 10.5
                                    -0.9 5.2
10.6
     -7.8 5.5 10.4 -29.0 5.0
                                1.8 -19.2
12.7 -18.9 3.4 15.6 -10.6 4.9
                                5.8
                                     -2.8 5.6
1.9
    -25.0 3.7 2.2 -3.1 3.9
                                4.8
                                     -7.8 4.5
7.9
     -13.9 4.8 5.2
                    -4.5 4.9
                                0.9 -11.6 3.0
     -2.1 4.6
               7.9
11.8
                    -2.0 4.8 11.5
                                    -9.0 5.5
10.6 -11.2 4.5 8.5 -0.2 5.3 11.1 -6.1 4.7
12.8 -1.0 6.6 11.3 -3.6 5.1 1.0 -8.2 3.9
    -0.5 5.7 11.9
14.5
                     -2.0 5.1
                                8.1
                                     -1.6 5.2
13.8 -11.9 3.7 15.5
                     -0.7 4.9
                              9.8
                                    -1.2 4.8
11.0 -14.3 4.4 12.4 -0.8 5.2 11.1 -16.8 5.1
5.1
     -5.1 4.6 4.8 -9.5 3.9 4.2 -17.0 5.1
                     -0.7 6.0
     -3.3 5.1 13.2
6.9
                                9.9
                                    -3.3 4.9
12.5 -13.6 4.1 13.2 -1.9 4.6
                                8.9 -10.0 4.9
10.8 -13.5 5.1
```

The following statements perform the desired analysis. The PROC GAM statement invokes the procedure and specifies the diabetes data set as input. The MODEL statement specifies logCP as the response variable and names Age and BaseDeficit as independent variables with univariate smoothing splines and the default of four degrees of freedom.

```
ods graphics on;
proc gam data=diabetes;
  model logCP = spline(Age) spline(BaseDeficit);
run;
```

The results are shown in Figure 41.1 and Figure 41.2.

Figure 41.1 Summary Statistics

Patterns of Diabetes

The GAM Procedure Dependent Variable: logCP Smoothing Model Component(s): spline(Age) spline(BaseDeficit)

| Summary of Input Data Set | |
|--------------------------------|--|
| Number of Observations 43 | |
| Number of Missing Observations | |
| Distribution Gaussian | |
| Link Function Identity | |

| Iteration Summary and Fit Statistics | | |
|--|--|--|
| Final Number of Backfitting Iterations 5 | | |
| Final Backfitting Criterion 5.542745E | | |
| The Deviance of the Final Estimate 0.418079172 | | |

Regression Model Analysis
Parameter Estimates
Parameter Standard
Parameter Estimate Error t Value Pr > |t|
Intercept 1.48141 0.05120 28.93 <.0001

0.01437

0.00807

0.00437

0.00247

3.28 0.0024

3.27 0.0025

Linear(Age)

Linear(BaseDeficit)

Figure 41.2 Analysis of Model

| Smoothing Model Analysis |
|--------------------------------------|
| Fit Summary for Smoothing Components |

| | Smoothing | | | Num Unique |
|---------------------|-----------|----------|----------|---------------|
| Component | Parameter | DF | GCV | Obs |
| Spline(Age) | 0.995582 | 3.000000 | 0.011675 | 37 |
| Spline(BaseDeficit) | 0.995299 | 3.000000 | 0.012437 | 39 |

| Smoothing Model Analysis Analysis of Deviance | | | | |
|--|---------|----------|------------|------------|
| _ | Sum of | | | |
| Source | DF | Squares | Chi-Square | Pr > ChiSq |
| Spline(Age) | 3.00000 | 0.150761 | 12.2605 | 0.0065 |
| Spline(BaseDeficit) | 3.00000 | 0.081273 | 6.6095 | 0.0854 |

Figure 41.2 displays summary statistics for the model. It consists of three tables. The first is the "Parameter Estimates" table for the parametric part of the model. It indicates that the linear trends for both Age and BaseDeficit are highly significant. The second table is the summary of smoothing components of the nonparametric part of the model. This table presents the smoothing parameter and degrees of freedom (DF) for each component. By default, each smoothing component has approximately 4 DF. For univariate spline components, one DF is taken up by the (parametric) linear part of the model, so the remaining approximate DF is 3. Finally, the third table is the "Analysis of Deviance" table for the nonparametric component of the model.

With ODS Graphics enabled, PROC GAM produces by default a panel of plots of partial prediction curves of smoothing components. In these plots, the partial prediction for a predictor such as Age is its nonparametric contribution to the model, s(Age). For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." For specific information about the graphics available in the GAM procedure, see the section "ODS Graphics" on page 2834.

Plots for both predictors (Figure 41.3) show a strong quadratic pattern, with a possible indication of higher-order behavior. Further investigation is required to determine whether these patterns are real or not.

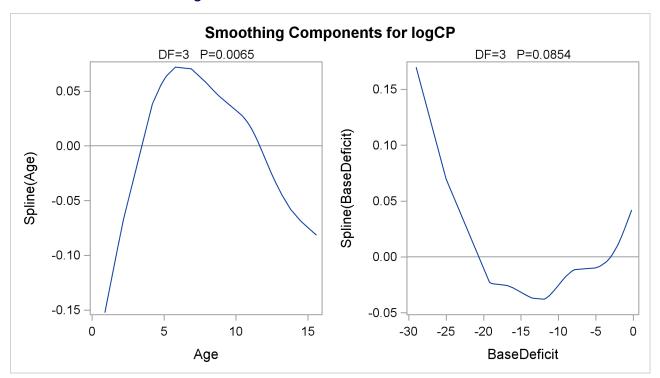


Figure 41.3 Partial Predictions for Each Predictor

Syntax: GAM Procedure

The following statements are available in the GAM procedure:

```
PROC GAM < options>;
    CLASS variable < (options) > < variable < (options) > ... > </ options>;
    MODEL dependent < (options) > = < PARAM(effects) > < smoothing-effects > </ options>;
    SCORE DATA= SAS-data-set OUT= SAS-data-set;
    OUTPUT OUT= SAS-data-set < keyword< = prefix > ... keyword< = prefix > ... keyword< = prefix > ;
    BY variables;
    FREQ variable;
```

The syntax of the GAM procedure is similar to that of other regression procedures in the SAS System. The PROC GAM and MODEL statements are required. The CLASS statement, if specified, must precede the MODEL statement. The CLASS and SCORE statements can appear multiple times; all other statements must appear only once.

The syntax for PROC GAM is described in the following sections in alphabetical order after the description of the PROC GAM statement.

PROC GAM Statement

PROC GAM < options > ;

The PROC GAM statement invokes the procedure. Table 41.1 summarizes the *options* available in the PROC GAM statement.

OptionDescriptionDATA=Specifies the input SAS data setDESCENDINGReverses the sort order of all CLASS variablesORDER=Specifies the sort order for CLASS variablesPLOTSControls plots produced through ODS Graphics

Table 41.1 PROC GAM Statement Options

You can specify the following options.

DATA=SAS-data-set

specifies the SAS data set to be read by PROC GAM. The default value is the most recently created data set.

DESCENDING

DESC

reverses the sort order of all classification variables (specified in the CLASS statement). If both the DESCENDING and ORDER= options are specified, PROC GAM orders the categories according to the ORDER= option and then reverses that order. This option has the same effect as the classification variable option DESCENDING in the CLASS statement and the response variable option DESCENDING in the MODEL statement.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of all classification variables (specified in the CLASS statement). This ordering determines which parameters in the model correspond to each level in the data. Note that the ORDER= option in the CLASS statement and the ORDER= response variable option in the MODEL statement override the ORDER= option in the PROC GAM statement.

PLOTS < (global-plot-options) > <= plot-request < (options) >>

PLOTS < (*global-plot-options*) > <=(*plot-request* < (*options*) > < ... *plot-request* < (*options*) > >) > controls the plots produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. Here are some examples:

```
plots=all
plots=components(commonaxes)
plots(unpack)=components(commonaxes clm)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc gam data=test plots(unpack)=components(commonaxes clm);
   model z=spline(x) spline(y);
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 609 in Chapter 21, "Statistical Graphics Using ODS."

With ODS Graphics enabled, PROC GAM produces by default a panel of plots of partial prediction curves of smoothing components.

Global Plot Options

The *global-plot-options* apply to all plots generated by the GAM procedure, unless altered by a *specific-plot-option*.

UNPACK

separately displays the smoothing component plots that are by default presented in panels. Use this option if you want to access individual smoothing component plots within the panel.

Specific Plot Options

The following listing describes the specific plots and their options.

ALL

requests that all plots be produced.

NONE

suppresses all plots.

COMPONENTS | COMPONENT < (components-options) >

displays a panel of smoothing component plots. The following components-options are available:

ADDITIVE

produces the additive component plots for spline and loess effects. The additive component plots combine the linear trend and the nonparametric prediction for each spline or loess effect.

CLM

includes confidence limits in the smoothing component plots. By default, 95% confidence limits are produced, but you can change the significance level by specifying the ALPHA= option in the MODEL statement. Note that producing these limits can be computationally intensive for large data sets.

COMMONAXES

specifies that smoothing component plots use a common vertical axis. This enables you to visually judge relative effect size.

UNPACK

displays the smoothing components individually.

BY Statement

BY variables;

You can specify a BY statement with PROC GAM 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 GAM 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 < (options) > < variable < (options) > ... > < / options > ;

The CLASS statement names the classification variables to be used in the analysis. The CLASS statement must precede the MODEL statement. You can specify various *options* for each variable by enclosing them in parentheses after the variable name. You can also specify global *options* for the CLASS statement by placing them after a slash (/). Global *options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the global *options* specified on any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the global *options*.

DESCENDING

DESC

reverses the sort order of the classification variable. If both the DESCENDING and ORDER= options are specified, PROC GAM orders the categories according to the ORDER= option and then reverses that order.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the categories of categorical variables. This ordering determines which parameters in the model correspond to each level in the data. When the default ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. The following table shows how PROC GAM interprets values of the ORDER= option.

| 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 observa- tions come first in the order |
| INTERNAL | Unformatted value |

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

REF='level' | keyword

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 linear estimates with a singular parameterization.

For an individual variable REF= option (but not for a global REF= option), you can specify the *level* of the variable to use as the reference level. Specify the formatted value of the variable if a format is assigned. For a global or individual variable REF= option, you can use one of the following *keywords*. The default is REF=LAST.

FIRST designates the first ordered level as reference.

LAST designates the last ordered level as reference.

TRUNCATE<=n>

specifies the length n of CLASS variable values to use in determining CLASS variable levels. If you specify TRUNCATE without the length n, the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases previous to SAS 9. The default is to use the full formatted length of the CLASS variable. The TRUNCATE option is available only as a global option.

FREQ Statement

FREQ variable;

The FREQ statement names a variable that provides frequencies for each observation in the DATA= data set. Specifically, if n is the value of the FREQ variable for a given observation, then that observation is used n times.

The analysis produced by using a FREQ statement reflects the expanded number of observations. You can produce the same analysis (without the FREQ statement) by first creating a new data set that contains the expanded number of observations. For example, if the value of the FREQ variable is 5 for the first observation, the first five observations in the new data set are identical. Each observation in the old data set is replicated n_i times in the new data set, where n_i is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

The FREQ statement is not available when a loess smoother is included in the model.

MODEL Statement

```
MODEL dependent < (options) > = < PARAM(effects) > < smoothing-effects > < / options > ;
MODEL event/trials = < PARAM(effects) > < smoothing-effects > < / options > ;
```

The MODEL statement specifies the dependent variable and the independent effects you want to use in the model. Specify the independent parametric variables inside the parentheses of PARAM(). The parametric variables can be either classification variables or continuous variables. Classification variables must be declared in a CLASS statement. Interactions between variables can also be included as parametric effects. Multiple PARAM() specifications are allowed in the MODEL statement. The syntax for the specification of effects is the same as for the GLM procedure (Chapter 46, "The GLM Procedure").

Only continuous variables can be specified in *smoothing-effects*. Any number of *smoothing-effects* can be specified, as follows:

| Smoothing Effect | Meaning |
|---|--|
| SPLINE (variable < , DF =number >) | Fits a smoothing spline with the variable and with DF= <i>number</i> |
| LOESS (variable < , DF =number >) | Fits a local regression with the variable and with DF= <i>number</i> |
| SPLINE2 (variable1, variable2 < , DF =number >) | Fits a bivariate thin-plate smoothing spline with <i>variable1</i> and <i>variable2</i> and with DF= <i>number</i> |

The number specified in the DF= option must be positive. If you specify neither the DF= option nor the METHOD=GCV in the MODEL statement, then the default is DF=4. Note that for univariate spline and loess components, a degree of freedom is used by default to account for the linear portion of the model, so the value displayed in the "Fit Summary" and "Analysis of Deviance" tables will be one less than the value you specify.

Both parametric effects and smoothing effects are optional. If none are specified, a model that contains only an intercept is fitted.

If only parametric variables are present, PROC GAM fits a parametric linear model by using the terms inside the parentheses of PARAM(). If only smoothing effects are present, PROC GAM fits a nonparametric additive model. If both types of effect are present, PROC GAM fits a semiparametric model by using the parametric effects as the linear part of the model.

Table 41.2 shows how to specify various models for a dependent variable y and independent variables x, x1, and x2. $s_i()$, i = 1, 2 are nonparametric smooth functions.

Table 41.2 Syntax for Common GAM Models

| Type of Model | Syntax for model | Mathematical Form |
|-------------------|-------------------------|--|
| Parametric | y=param(x1 x2) | $E(Y X = x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ |
| Nonparametric | y=spline(x) | $E(Y X=x) = \beta_0 + \beta_1 x + s(x)$ |
| Nonparametric | y=loess(x) | $E(Y X=x) = \beta_0 + \beta_1 x + s(x)$ |
| Semiparametric | y=spline(x1) param(x2) | $E(Y X = x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + s(x_1)$ |
| Additive | y=spline(x1) spline(x2) | $E(Y X = x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + s_1(x_1) + s_2(x_2)$ |
| Thin-plate spline | y=spline2(x1,x2) | $E(Y X = x) = \beta_0 + s(x_1, x_2)$ |

Table 41.3 summarizes the *options* available in the MODEL statement.

 Table 41.3
 MODEL Statement Options

| Option | Description |
|----------------------|--|
| Response Variable | e Options |
| DESCENDING | Reverses the order of the response categories |
| EVENT= | Specifies the event category for the binary response model |
| ORDER= | Specifies the sort order for the response variable |
| REFERENCE= | Specifies the reference category for the binary response model |
| Model Options | |
| ALPHA= | Specifies the significance level |
| ANODEV= | Specifies the method used to analyze smoothing effects |
| DIST= | Specifies the distribution family |
| EPSILON= | Specifies the convergence criterion for the backfitting algorithm |
| EPSSCORE= | Specifies the convergence criterion for the local scoring algorithm |
| ITPRINT | Produces an iteration summary table for the smoothing effects |
| MAXITER= | Specifies the maximum number of iterations for the backfitting algorithm |
| MAXITSCORE= | Specifies the maximum number of iterations for the local scoring algorithm |
| METHOD= | Specifies the method for selecting the value of the smoothing parameter |
| OFFSET= | Specifies an offset for the linear predictor |

Response Variable Options

Response variable options determine how the GAM procedure models probabilities for binary data.

You can specify the following *options* by enclosing them in parentheses after the response variable. See the section "CLASS Statement" on page 2812 for more detail.

DESCENDING

DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC GAM orders the response categories according to the ORDER= option and then reverses that order.

EVENT='category' | keyword

specifies the event category for the binary response model. PROC GAM models the probability of the event category. You can specify the value (formatted, if a format is applied) of the event category in quotes, or you can specify one of the following *keywords*. The default is EVENT=FIRST.

FIRST

designates the first ordered category as the event.

LAST

designates the last ordered category as the event.

One of the most common sets of response levels is $\{0, 1\}$, with 1 representing the event for which the probability is to be modeled. Consider the example where Y takes the value 1 and 0 for event and nonevent, respectively, and X is the explanatory variable. By default, PROC GAM models the probability that Y = 0. To model the probability that Y = 1, specify the following MODEL statement:

$$model Y (event='1') = X;$$

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the response variable. By default, ORDER=FORMATTED. When ORDER=FORMATTED, the values of numeric variables for which you have supplied no explicit format (that is, for which there is no corresponding FORMAT statement in the current PROC GAM run or in the DATA step that created the data set), are ordered by their internal (numeric) value. If you specify the ORDER= option in the MODEL statement and the ORDER= option in the CLASS statement, the former takes precedence. The following table shows the interpretation of the ORDER= 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 observa- tions come first in the order | |
| INTERNAL | Unformatted value | |

For the FORMATTED and INTERNAL values, 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*.

REFERENCE='category' | keyword

REF='category' | keyword

specifies the reference category for the binary response model. Specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify the value (formatted if a format is applied) of the reference category in quotes, or you can specify one of the following *keywords*:

FIRST designates the first ordered category as the reference.

LAST designates the last ordered category as the reference. This is the default.

The REFERENCE= option is ignored when the EVENT= option is present.

Model Options

ALPHA=number

specifies the significance level α of the confidence limits on the final nonparametric component estimates when you request confidence limits to be included in the output data set. Specify *number* as a value between 0 and 1. The default value is 0.05. See the section "OUTPUT Statement" on page 2818 for more information about the OUTPUT statement.

ANODEV=type

specifies the *type* of method to be used to produce the "Analysis of Deviance" table for smoothing effects. The available choices are as follows:

REFIT specifies that PROC GAM perform χ^2 tests by fitting nested GAM models. This

is the default choice if you do not specify the ANODEV= option. This choice requires fitting separate GAM models where one smoothing term is omitted from

each model.

NOREFIT specifies that PROC GAM perform approximate tests of smoothing effects. To test

each smoothing effect, a weighted least squares model is fitted to the remaining parametric part of the model while keeping other nonlinear smoothers fixed. For details, see Hastie (1991). This choice requires only a single GAM fitting to be

performed, which reduces the time of the procedure.

NONE requests that the procedure not produce the "Analysis of Deviance" table for smooth-

ing effects.

DIST=distribution-id

LINK=distribution-id

specifies the distribution family used in the model. The choices for *distribution-id* are displayed in Table 41.4. See "Distribution Family and Canonical Link" on page 2830 for more information.

| DIST= | Distribution | Link Function | Response Data Type |
|-------------------------|-------------------|---------------------|--------------------------------|
| GAUSSIAN GAUS NORM | Normal (Gaussian) | Identity | Continuous variables |
| BINOMIAL LOGI BIN | Binomial | Logit | Binary variables |
| POISSON POIS LOGL | Poisson | Log | Nonnegative discrete variables |
| GAMMA GAMM | Gamma | Negative reciprocal | Positive continuous variables |
| IGAUSSIAN IGAU INVG | Inverse Gaussian | Squared reciprocal | Positive continuous variables |

Table 41.4 Distribution Families for GAM Models

Canonical link functions are used with those distributions. Although alternative links are possible theoretically, the final fit of nonparametric regression models is relatively insensitive to the precise choice of link functions. Therefore, only the canonical link for each distribution family is implemented in PROC GAM. The loess smoother is not available for DIST=BINOMIAL when the number of trials is greater than 1.

EPSILON=number

specifies the convergence criterion for the backfitting algorithm. The default value is 1E–8.

EPSSCORE=number

specifies the convergence criterion for the local scoring algorithm. The default value is 1E-8.

ITPRINT

produces an iteration summary table for the smoothing effects when doing backfitting and local scoring.

MAXITER=number

specifies the maximum number of iterations for the backfitting algorithm. The default value is 50.

MAXITSCORE=number

specifies the maximum number of iterations for the local scoring algorithm. The default value is 100.

METHOD=GCV

specifies that the value of the smoothing parameter should be selected by generalized cross validation. If you specify both METHOD=GCV and the DF= option for some smoothing effects, the user-specified DF values are used for those effects in which the DF= option is specified. The GCV criterion is used for determining smoothness of the remaining effects. See the section "Selection of Smoothing Parameters" on page 2827 for more details on the GCV method.

OFFSET=variable

specifies an offset for the linear predictor. An offset plays the role of a predictor whose coefficient is known to be 1. For example, you can use an offset in a Poisson model when counts have been obtained in time intervals of different lengths. With a log link function, you can model the counts as Poisson variables with the logarithm of the time interval as the offset variable. The offset variable cannot appear in the CLASS statement or elsewhere in the MODEL statement.

OUTPUT Statement

OUTPUT OUT= SAS-data-set < keyword< = prefix > . . . keyword< = prefix > > ;

The OUTPUT statement creates a new SAS data set that contains diagnostic measures calculated after fitting the model.

All the variables in the original data set are included in the new data set, along with new variables that are created with *keywords* specified in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If no *keywords* are present, the OUT= data set contains only the original data set and predicted values. The predicted values include the linear predictor for the response and the prediction for each smoothing term in the model. When you specify a distribution family with the DIST= or LINK= option in the MODEL statement, predicted response values after applying the inverse link function are also included. Predicted values are computed for observations that have missing response values, nonmissing values in the explanatory variables, and values of the smoothing variables that are within the smoothing ranges of the fitted model.

You can specify the following *options* in the OUTPUT statement:

all statistics in this list

OUT=SAS-data-set

specifies the name of the new data set to contain the diagnostic measures. This option is required.

keyword < =prefix >

ALL

specifies the statistics to include in the output data set. The *keywords* and the statistics they represent are as follows:

| PREDICTED | predicted values for each smoothing component and overall predicted values on the response scale at design points. The prediction for each spline or loess term is only for the nonlinear component of each smoother. |
|-----------|---|
| LINP | linear prediction values on the link scale at design points |
| UCLM | upper confidence limits for each predicted smoothing component |
| LCLM | lower confidence limits for each predicted smoothing component |
| ADIAG | diagonal element of the hat matrix associated with the observation for each smoothing spline component |
| RESIDUAL | residual standardized by its weights |
| STD | standard deviation of the prediction for each smoothing component |

The names of the new variables that contain the statistics are formed by concatenating a *prefix* and the corresponding variable names. If you do not specify a *prefix*, the names are formed by using default prefixes listed in the following table:

| Keyword | Prefix |
|---------|---------------------------|
| PRED | P_ |
| LINP | LINP_ |
| UCLM | UCLM_ |
| LCLM | LCLM_ |
| ADIAG | ADIAG_ |
| RESID | R_ |
| STD | STD _ (for spline) |
| | STDP_(for loess) |

For example, suppose that you have a dependent variable y and an independent smoothing variable x. If you specify the keywords PRED=MyP_ and ADIAG=MyA_, the new variables in the output SAS data set are MyP_y, MyP_x, and MyA_x. If you specify the keywords PRED and ADIAG without prefixes, the new variables are P_y, P_x, and ADIAG_x.

SCORE Statement

SCORE DATA= SAS-data-set **OUT=** SAS-data-set;

The SCORE statement calculates predicted values for a new data set. All the variables in the DATA= data set are included in the OUT= data set, along with the predicted values. The predicted values consist of predicted responses after the inverse link function transformation, predicted values of all smoothing terms, and predicted values on the link scale. Predicted values are computed for observations with missing response values whose values of the specified explanatory variables are nonmissing, and whose values of the specified smoothing variables are within the smoothing ranges of the fitted model. The predicted variables use the same naming convention as the OUTPUT statement. If you have multiple data sets to score, you can specify multiple SCORE statements.

The following *options* must be specified in the SCORE statement:

DATA=SAS-data-set

specifies an input SAS data set containing all the variables included in independent effects in the MODEL statement. The predicted response is computed for each observation in the SCORE DATA= data set.

OUT=SAS-data-set

specifies the name of the SAS data set to contain the predictions.

Details: GAM Procedure

Missing Values

When fitting a model, PROC GAM excludes any observation with missing values for an explanatory variable, offset variable, or dependent variable. However, if only the response is missing, predicted values can be computed and output to a data set by using the OUTPUT or SCORE statement.

Nonparametric Regression

Nonparametric regression relaxes the usual assumption of linearity and enables you to explore the data more flexibly, uncovering structure in the data that might otherwise be missed.

However, many forms of nonparametric regression do not perform well when the number of independent variables in the model is large. The sparseness of data in this setting causes the variances of the estimates to

be unacceptably large unless the sample size is extremely large. The problem of rapidly increasing variance for increasing dimensionality is sometimes referred to as the "curse of dimensionality." Interpretability is another problem with nonparametric regression based on kernel and smoothing spline estimates. These estimates contain information about the relationship between the dependent and independent variables, and the information is often difficult to comprehend.

To overcome these difficulties, additive models were proposed by some researchers, for example, Stone (1985). These models estimate an additive approximation to the multivariate regression function. The benefits of an additive approximation are at least twofold. First, since each of the individual additive terms is estimated by using a univariate smoother, the curse of dimensionality is avoided, at the cost of not being able to approximate universally. Second, estimates of the individual terms explain how the dependent variable changes with the corresponding independent variables.

To extend the additive model to a wide range of distribution families, Hastie and Tibshirani (1990) proposed generalized additive models. These models enable the mean of the dependent variable to depend on an additive predictor through a nonlinear link function. The models permit the response probability distribution to be any member of the exponential family of distributions. Many widely used statistical models belong to this general class; they include additive models for Gaussian data, nonparametric logistic models for binary data, and nonparametric log-linear models for Poisson data.

Additive Models and Generalized Additive Models

This section describes the methodology and the fitting procedure behind generalized additive models.

Let Y be a response random variable and X_1, X_2, \dots, X_p be a set of predictor variables. A regression procedure can be viewed as a method for estimating the expected value of Y given the values of X_1, X_2, \dots, X_p . The standard linear regression model assumes a linear form for the dependency of *Y* on *X*:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

where $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$. Given a sample, estimates of $\beta_0, \beta_1, \dots, \beta_p$ are usually obtained by the least squares method.

The additive model generalizes the linear model by modeling the dependency as

$$Y = s_0 + s_1(X_1) + s_2(X_2) + \dots + s_n(X_n) + \epsilon$$

where $s_j(X)$, j = 1, 2, ..., p, are smooth functions, $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$.

In order to be estimable, the smooth functions s_i have to satisfy standardized conditions such as $E\left(s_i(X_i)\right) =$ 0. These functions are not given a parametric form but instead are estimated in a nonparametric fashion.

While traditional linear models and additive models can be used in most statistical data analysis, there are types of problems for which they are not appropriate. For example, the normal distribution might not be adequate for modeling discrete responses such as counts or bounded responses such as proportions.

Generalized additive models address these difficulties, extending additive models to many other distributions besides just the normal. Thus, generalized additive models can be applied to a much wider range of data analysis problems.

Like generalized linear models, generalized additive models consist of a random component, an additive component, and a link function relating the two components. The response *Y*, the random component, is assumed to have exponential family density

$$f_Y(y; \theta, \phi) = \exp\left\{\frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)\right\}$$

where θ is called the natural parameter and ϕ is the scale parameter. The mean of the response variable μ is related to the set of covariates X_1, X_2, \ldots, X_p by a link function g. The quantity

$$\eta = s_0 + \sum_{j=1}^p s_j(X_j)$$

defines the additive component, where $s_1(), \ldots, s_p()$ are smooth functions, and the relationship between μ and η is defined by $g(\mu) = \eta$. The most commonly used link function is the canonical link, for which $\eta = \theta$.

Generalized additive models and generalized linear models can be applied in similar situations, but they serve different analytic purposes. Generalized linear models emphasize estimation and inference for the parameters of the model, while generalized additive models focus on exploring data nonparametrically. Generalized additive models are more suitable for exploring the data and visualizing the relationship between the dependent variable and the independent variables.

Forms of Additive Models

Suppose that y is a continuous variable and x1 and x2 are two explanatory variables of interest. To fit an additive model, you can use a MODEL statement similar to that used in many regression procedures in the SAS System:

```
model y = spline(x1) spline(x2);
```

This model statement requires the procedure to fit the following model:

$$\eta(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + s_1(x_1) + s_2(x_2)$$

where the $s_i()$ terms denote nonparametric spline functions of the respective explanatory variables.

The GAM procedure can fit semiparametric models. The following MODEL statement assumes a linear relation with x1 and an unknown functional relation with x2:

```
model y = param(x1) spline(x2);
```

If you want to fit a model containing a functional two-way interaction between x1 and x2, you can use the following MODEL statement:

```
model y = spline2(x1, x2);
```

In this case, the GAM procedure fits a model equivalent to that of PROC TPSPLINE.

Estimates from PROC GAM

PROC GAM provides the capability to fit both nonparametric and semiparametric models. So that you can better understand the underlying trend of any given factor, PROC GAM separates the linear trend from any general nonparametric trend during the fitting as well as in the final report. This makes it easy to determine whether the significance of a smoothing variable is associated with a simple linear trend or a more complicated pattern.

For example, suppose you want to fit a semiparametric model as

$$y = \alpha_0 + \alpha_1 z + f_1(x_1) + f_2(x_2)$$

The GAM estimate for this model is

$$y = \widehat{\alpha_0} + \widehat{\alpha_1}z + \widehat{\beta_1}x_1 + \widehat{\beta_2}x_2 + \widehat{s_1}(x_1) + \widehat{s_2}(x_2)$$

where $\widehat{s_1}$ and $\widehat{s_2}$ are linear-adjusted nonparametric estimates of the f_1 and f_2 effects. The p-values for $\widehat{\alpha_0}$, $\widehat{\alpha_1}$, $\widehat{\beta_1}$, and $\widehat{\beta_2}$ are reported in the parameter estimates table. $\widehat{\beta_1}$ and $\widehat{\beta_2}$ are the estimates labeled Linear(x1) and Linear(x2) in the table. The p-values for $\widehat{s_1}$ and $\widehat{s_2}$ are reported in the analysis of deviance table.

Only $\hat{s_1}$, $\hat{s_2}$, and \hat{y} are output to the output data set, with the corresponding variable names P_x1, P_x2, and P_y. For Gaussian data, the complete marginal prediction for variable x1 is:

$$\widehat{\beta_1}x_1 + P_x_1$$

If the additive component plots are requested by the ADDITIVE suboption, the additive component for variable x2 is computed as:

$$\widehat{\beta_2}(x_2 - \bar{x}_2) + P_- x_2$$

where \bar{x}_2 is the mean for variable x2.

Backfitting and Local Scoring Algorithms

Much of the development and notation in this section follows Hastie and Tibshirani (1986).

Additive Models

Consider the estimation of the smoothing terms $s_0, s_1(), \dots, s_p()$ in the additive model

$$\eta(X) = s_0 + \sum_{j=1}^{p} s_j(X_j)$$

where $E(s_j(X_j)) = 0$ for every j. Since the algorithm for additive models is the basis for fitting generalized additive models, the algorithm for additive models is discussed first.

Many ways are available to approach the formulation and estimation of additive models. The backfitting algorithm is a general algorithm that can fit an additive model with any regression-type fitting mechanisms.

Define the kth set of partial residuals as

$$R_k = Y - s_0 - \sum_{j \neq k} s_j(X_j)$$

then $E(R_k|X_k) = s_k(X_k)$. This observation provides a way to estimate each smoothing function $s_k()$ given estimates $\{\hat{s}_j(), j \neq k\}$ for all the others. The resulting iterative procedure is known as the backfitting algorithm (Friedman and Stuetzle 1981). The following formulation is taken from Hastie and Tibshirani (1986).

The Backfitting Algorithm

The unweighted form of the backfitting algorithm is as follows:

1. **Initialization:**
$$s_0 = E(Y), s_1^{(1)} = s_2^{(1)} = \dots = s_p^{(1)} = 0, m = 0$$

2. Iterate:

$$\begin{split} m &= m+1; \\ \text{for } j &= 1 \text{ to } p \text{ do:} \\ R_j &= Y - s_0 - \sum_{k=1}^{j-1} s_k^{(m)}(X_k) - \sum_{k=j+1}^p s_k^{(m-1)}(X_k); \\ s_j^{(m)} &= E(R_j|X_j); \end{split}$$

3. Until:

RSS =
$$\frac{1}{n} \| Y - s_0 - \sum_{j=1}^{p} s_j^{(m)}(X_j) \|^2$$
 fails to decrease, or satisfies the convergence criterion.

In the preceding notation, $s_j^{(m)}()$ denotes the estimate of $s_j()$ at the *m*th iteration. It can be shown that with many smoothers (including linear regression, univariate and bivariate splines, and combinations of these), RSS never increases at any step. This implies that the algorithm always converges (Hastie and Tibshirani 1986). Note, however, that for distributions other than Gaussian, numerical instabilities with weights can cause convergence problems. Even when the algorithm converges, the individual functions need not be unique, since dependence among the covariates can lead to more than one representation for the same fitted surface.

A weighted backfitting algorithm has the same form as for the unweighted case, except that the smoothers are weighted. In PROC GAM, weights are used with non-Gaussian data in the local scoring procedure described later in this section.

The GAM procedure uses the following condition as the convergence criterion for the backfitting algorithm:

$$\frac{\sum_{i=1}^{n} \sum_{j=1}^{p} \left(s_{j}^{(m-1)}(\mathbf{X}_{ij}) - s_{j}^{(m)}(\mathbf{X}_{ij}) \right)^{2}}{1 + \sum_{i=1}^{n} \sum_{j=1}^{p} \left(s_{j}^{(m-1)}(\mathbf{X}_{ij}) \right)^{2}} \le \epsilon$$

where $\epsilon = 10^{-8}$ by default; you can change this with the EPSILON= option in the MODEL statement.

Generalized Additive Models

The algorithm described so far fits only additive models. The algorithm for generalized additive models is a little more complicated. Generalized additive models extend generalized linear models in the same manner that additive models extend linear regression models—that is, by replacing the form $\alpha + \sum_j \beta_j \mathbf{x}_j$ with the additive form $\alpha + \sum_j f_j(\mathbf{x}_j)$. See "Generalized Linear Models Theory" on page 3069 in Chapter 44, "The GENMOD Procedure," for more information.

PROC GAM fits generalized additive models by using a modified form of adjusted dependent variable regression, as described for generalized linear models in McCullagh and Nelder (1989), with the additive predictor taking the role of the linear predictor. Hastie and Tibshirani (1986) call this the *local scoring algorithm*. Important components of this algorithm depend on the link function for each distribution, as shown in the following table.

| Distribution | Link | Adjusted Dependent (z) | Weights (w) |
|------------------|--------------------------------------|----------------------------------|---------------|
| Normal | μ | у | 1 |
| Binomial | $\log\left(\frac{\mu}{n-\mu}\right)$ | $\eta + (y - \mu)/n\mu(1 - \mu)$ | $n\mu(1-\mu)$ |
| Gamma | $-1/\mu$ | $\eta + (y - \mu)/\mu^2$ | μ^2 |
| Poisson | $\log(\mu)$ | $\eta + (y - \mu)/\mu$ | μ |
| Inverse Gaussian | $1/\mu^2$ | $\eta - 2(y - \mu)/\mu^3$ | $\mu^3/4$ |

Once the distribution and hence these quantities are defined, the local scoring algorithm proceeds as follows.

The General Local Scoring Algorithm

1. Initialization:

$$s_i = g(E(y)), s_1^0 = s_2^0 = \dots = s_p^0 = 0, m = 0$$

2. Iterate:

$$m = m + 1;$$

Form the predictor η , mean μ , weights w, and adjusted dependent variable z based on their corresponding values from the previous iteration:

$$\eta_{i}^{(m-1)} = s_{0} + \sum_{j=1}^{p} s_{j}^{(m-1)}(x_{ij})
\mu_{i}^{(m-1)} = g^{-1} \left(\eta_{i}^{(m-1)} \right)
w_{i} = \left(V_{i}^{(m-1)} \right)^{-1} \cdot \left[\left(\frac{\partial \mu}{\partial \eta} \right)_{i}^{(m-1)} \right]^{2}
z_{i} = \eta_{i}^{(m-1)} + \left(y_{i} - \mu_{i}^{(m-1)} \right) \cdot \left(\frac{\partial \eta}{\partial \mu} \right)_{i}^{(m-1)}$$

where $V_i^{(m-1)}$ is the variance of Y at $\mu_i^{(m-1)}$. Fit an additive model to z by using the backfitting algorithm with weights w to obtain estimated functions $s_i^{(m)}(), j = 1, ..., p$;

3. Until:

The convergence criterion is satisfied or the deviance fails to decrease. The deviance is an extension to generalized linear models of the RSS; see "Goodness of Fit" on page 3076 in Chapter 44, "The GENMOD Procedure," for a definition.

The GAM procedure uses the following condition as the convergence criterion for local scoring:

$$\frac{\sum_{i=1}^{n} w_{i} \sum_{j=1}^{p} \left(s_{j}^{(m-1)}(\mathbf{X}_{ij}) - s_{j}^{(m)}(\mathbf{X}_{ij}) \right)^{2}}{\sum_{i=1}^{n} w_{i} \left(1 + \sum_{j=1}^{p} \left(s_{j}^{(m-1)}(\mathbf{X}_{ij}) \right)^{2} \right)} \le \epsilon^{s}$$

where $\epsilon^s = 10^{-8}$ by default; you can change this with the EPSSCORE= option in the MODEL statement.

The estimating procedure for generalized additive models consists of two loops. Inside each step of the local scoring algorithm (outer loop), a weighted backfitting algorithm (inner loop) is used until convergence or until the RSS fails to decrease. Then, based on the estimates from this weighted backfitting algorithm, a new set of weights is calculated and the next iteration of the scoring algorithm starts. The scoring algorithm stops when the convergence criterion is satisfied or the deviance of the estimates stops decreasing.

Smoothers

You can specify three types of smoothers in the MODEL statement:

- SPLINE(x) specifies a cubic smoothing spline term for variable x
- LOESS(x) specifies a loess term for variable x
- SPLINE2(x1, x2) specifies a thin-plate smoothing spline term for variables x1 and x2

A smoother is a tool for summarizing the trend of a response measurement Y as a function of one or more predictor measurements X_1, \ldots, X_p . It produces an estimate of the trend that is less variable than Y itself. An important property of a smoother is its nonparametric nature. It does not assume a rigid form for the dependence of Y on X_1, \ldots, X_p . This section gives a brief overview of the smoothers that can be used with the GAM procedure.

Cubic Smoothing Spline

A smoothing spline is the solution to the following optimization problem: among all functions $\eta(x)$ with two continuous derivatives, find one that minimizes the penalized least square

$$\sum_{i=1}^{n} (y_i - \eta(x_i))^2 + \lambda \int_a^b (\eta''(t))^2 dt$$

where λ is a fixed constant and $a \le x_1 \le \cdots \le x_n \le b$. The first term measures closeness to the data while the second term penalizes curvature in the function. It can be shown that there exists an explicit, unique minimizer, and that minimizer is a natural cubic spline with knots at the unique values of x_i .

The value $\lambda/(1+\lambda)$ is the *smoothing parameter*. When λ is large, the smoothing parameter is close to 1, producing a smoother curve; small values of λ , corresponding to smoothing parameters near 0, are apt to produce rougher curves, more nearly interpolating the data.

Local Regression

Local regression was proposed by Cleveland, Devlin, and Grosse (1988). The idea of local regression is that at a predictor x, the regression function $\eta(x)$ can be locally approximated by the value of a function in some specified parametric class. Such a local approximation is obtained by fitting a regression surface to the data points within a chosen neighborhood of the point x. A weighted least squares algorithm is used to fit linear functions of the predictors at the centers of neighborhoods. The radius of each neighborhood is chosen so that the neighborhood contains a specified percentage of the data points. The smoothing parameter for the local regression procedure, which controls the smoothness of the estimated curve, is the fraction of the data in each local neighborhood. Data points in a given local neighborhood are weighted by a smooth decreasing function of their distance from the center of the neighborhood. See Chapter 71, "The LOESS Procedure," for more details.

Thin-Plate Smoothing Spline

The thin-plate smoothing spline is a multivariate version of the cubic smoothing spline. The theoretical foundations for the thin-plate smoothing spline are described in Duchon (1976, 1977); Meinguet (1979). The smoothing parameter for the thin-plate smoothing spline smoother is the parameter that controls the smoothness penalty. When the smoothing parameter is close to 0, the fit is close to an interpolation. When the smoothing parameter is very large, the fit is a smooth surface. Further results and applications are given in Wahba and Wendelberger (1980). See Chapter 116, "The TPSPLINE Procedure," for more details.

Selection of Smoothing Parameters

CV and GCV

The smoothers discussed here have a single smoothing parameter. In choosing the smoothing parameter, cross validation can be used. Cross validation works by leaving points (x_i, y_i) out one at a time, estimating the squared residual for smooth function at x_i based on the remaining n-1 data points, and choosing the smoother to minimize the sum of those squared residuals. This mimics the use of training and test samples for prediction. The cross validation function is defined as

$$CV(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \hat{\eta}_{\lambda}^{(-i)}(x_i) \right)^2$$

where $\hat{\eta}_{\lambda}^{(-i)}(x_i)$ indicates the fit at x_i , computed by leaving out the *i*th data point. The quantity $n\text{CV}(\lambda)$ is sometimes called the prediction sum of squares, or PRESS (Allen 1974).

All of the smoothers fit by the GAM procedure can be formulated as a linear combination of the sample responses

$$\hat{\eta}(x) = \mathbf{A}(\lambda)\mathbf{y}$$

for some matrix $A(\lambda)$, which depends on λ . (The matrix $A(\lambda)$ depends on x and the sample data as well, but this dependence is suppressed in the preceding equation.) Let a_{ii} be the *i*th diagonal element of $A(\lambda)$. Then the CV function can be expressed as

$$CV(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{(y_i - \hat{\eta}_{\lambda}(x_i))}{1 - a_{ii}} \right)^2$$

In most cases, it is very time-consuming to compute the quantity a_{ii} individually. To solve this computational problem, Wahba (1990) has proposed the generalized cross validation function (GCV) that can be used to solve a wide variety of problems involving selection of a parameter to minimize the prediction risk.

The GCV function is defined as

$$GCV(\lambda) = \frac{n \sum_{i=1}^{n} (y_i - \hat{\eta}_{\lambda}(x_i))^2}{(n - \text{Trace}(\mathbf{A}(\lambda)))^2}$$

The GCV formula simply replaces the a_{ii} with $\text{Trace}(\mathbf{A}(\lambda))/n$. Therefore, it can be viewed as a weighted version of CV. In most of the cases of interest, GCV is closely related to CV but much easier to compute. Specify the METHOD=GCV option in the MODEL statement in order to use the GCV function to choose the smoothing parameters.

Degrees of Freedom

The estimated GAM model can be expressed as

$$\hat{\eta}(X) = \hat{s}_0 + \sum_{j=1}^p \mathbf{A}_j(\lambda_j) Y$$

Because the weights are calculated based on previous iteration during the local scoring iteration, the matrices A_j might depend on Y for non-Gaussian data. However, for the final iteration, the A_j matrix for the spline smoothers has the same role as the projection matrix in linear regression; therefore, nonparametric degrees of freedom (DF) for the jth spline smoother can be defined as

$$DF(j \text{ th spline smoother}) = Trace(\mathbf{A}_j(\lambda_j))$$

For loess smoothers A_i is not symmetric and so is not a projection matrix. In this case PROC GAM uses

$$DF(j \text{ th loess smoother}) = Trace(\mathbf{A}_j(\lambda_j)' \mathbf{A}_j(\lambda_j))$$

The GAM procedure gives you the option of specifying the degrees of freedom for each individual smoothing component. If you choose a particular value for the degrees of freedom, then during every local scoring iteration the procedure will search for a corresponding smoothing parameter lambda that yields the specified value or comes as close as possible. The final estimate for the smoother during this local scoring iteration will be based on this lambda. Note that for univariate spline and loess components, an additional degree of freedom is used by default to account for the linear portion of the model, so the value displayed in the "Fit Summary" and "Analysis of Deviance" tables will be one less than the value you specify.

Confidence Intervals for Smoothers

Buja, Hastie, and Tibshirani (1989) showed that each smoothing function estimate from the backfitting algorithm is the result of a linear mapping applied to the working response, if the backfitting algorithm converges.

The smoothing function estimate can be expressed as

$$\hat{s}_j(\mathbf{x}_j) = \mathbf{H}_j \mathbf{z}$$

where \mathbf{x}_j is the *j*th covariate and \mathbf{z} is the adjusted dependent variable that is formed in the local scoring algorithm. If the errors are independent and identically distributed, then

$$Cov(\hat{s}_j) = \sigma^2 \mathbf{H}_j \mathbf{H}'_j$$

where $\sigma^2 = \text{Var}(\mathbf{z})$.

However, direct computation of \mathbf{H}_j is formidable within the backfitting framework. Hastie and Tibshirani (1990) proposed using each individual smoothing matrix $\mathbf{A}_j(\lambda_j)$ as a substitute for the linear operator \mathbf{H}_j when computing confidence intervals. In the GAM procedure, curvewise confidence intervals for smoothing splines and pointwise confidence intervals for loess are provided in the output data set.

Curvewise Confidence Interval for Smoothing Spline Smoothers

Viewing the spline model as a Bayesian model, Wahba (1983) proposes Bayesian confidence intervals for smoothing spline estimates as:

$$\hat{s}_{\lambda}(x_i) \pm z_{\alpha/2} \sqrt{\hat{\mathbf{V}}_{ii}(\lambda)}$$

where $\hat{\mathbf{V}}_{ii}(\lambda)$ is the *i*th diagonal element of the Bayesian posterior covariance matrix $\hat{\mathbf{V}}$ and $z_{\alpha/2}$ is the $1-\alpha/2$ quantile of the standard normal distribution. The confidence intervals are interpreted as intervals "across the function" as opposed to pointwise intervals.

Suppose that you fit a spline estimate to experimental data that consist of a true function f and a random error term ϵ_i . In repeated experiments, it is likely that about $100(1-\alpha)\%$ of the confidence intervals cover the corresponding true values, although some values are covered every time and other values are not covered by the confidence intervals most of the time. This effect is more pronounced when the true response curve or surface has small regions of particularly rapid change.

In the GAM procedure, let the smoothing matrix for the nonlinear part of the *j*th spline term be $\tilde{\mathbf{A}}_j$ after the linear part is separated out from $\mathbf{A}_j(\lambda)$. The Bayesian posterior variance for the nonlinear part is computed as

$$\hat{\mathbf{V}}_j = \hat{\boldsymbol{\phi}} \tilde{\mathbf{A}}_j \mathbf{W}^{-1}$$

where $\hat{\phi}$ is the dispersion parameter estimate and **W** is the weight matrix from the final local scoring iteration. If you specify UCLM, LCLM, ADIAG, and STD options in the OUTPUT statement, the statistics are derived based on $\hat{\mathbf{V}}_i$.

When you request both the ADDITIVE and CLM suboptions in the PLOTS=COMPONENTS option, each of the smoothing component plots displays a confidence band for the total contribution of each smoothing spline smoother. The confidence band is derived from the total variance that is contributed by both linear and nonlinear parts by the *j*th term

$$\hat{\phi}\left(\mathbf{x}_{j}'(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{x}_{j}+\tilde{\mathbf{A}}_{j}\mathbf{W}^{-1}\right)$$

As shown in Cleveland, Devlin, and Grosse (1988), the smoothing matrix $A(\lambda)$ for a loess smoother is asymmetric. The confidence intervals are computed as follows:

$$\hat{s}_{\lambda}(x_i) \pm z_{\alpha/2} \sqrt{\hat{\mathbf{V}}_{ii}(\lambda)}$$

where $\hat{\mathbf{V}}_{ii}(\lambda)$ is the *i*th diagonal element of the covariance matrix $\hat{\mathbf{V}}$ and $z_{\alpha/2}$ is the $1 - \alpha/2$ quantile of the standard normal distribution.

In the GAM procedure, let the smoothing matrix for the nonlinear part of the *j*th loess term be $\tilde{\mathbf{A}}_j$ after the linear part is separated out from $\mathbf{A}_j(\lambda)$. The covariance matrix for the nonlinear part is then

$$\hat{\mathbf{V}}_j = \hat{\boldsymbol{\phi}} \tilde{\mathbf{A}}_j \mathbf{W}^{-1} \tilde{\mathbf{A}}_j'$$

where $\hat{\phi}$ is the dispersion parameter estimate and **W** is the weight matrix from the final local scoring iteration. If you specify UCLM, LCLM, and STD options in the OUTPUT statement, the statistics are derived based on $\hat{\mathbf{V}}_i$.

When you request both the ADDITVE and CLM suboptions in the PLOTS=COMPONENTS option, each of the smoothing component plots displays confidence intervals for total prediction of each loess smoother. The confidence intervals are derived from the total variance that is contributed by both the linear and nonlinear parts by the *j*th term

$$\hat{\phi}\left(\mathbf{x}_{j}'(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{x}_{j} + \tilde{\mathbf{A}}_{j}\mathbf{W}^{-1}\tilde{\mathbf{A}}_{j}'\right)$$

Distribution Family and Canonical Link

In general, there is not just one reasonable link function for a given response variable distribution. For parametric models, the choice of link function can lead to substantively different estimates and tests. However, the inherent flexibility of nonparametric models makes them less likely to be sensitive to the precise choice of link function. Thus, for simplicity and computational efficiency, the GAM procedure uses only the canonical link for each distribution, as discussed in the following sections.

The Gaussian Model

For a Gaussian model, the link function is the identity function, and the generalized additive model is the same as the additive model. The Gaussian model is selected by default or when you specify the DIST=GAUSSIAN option in the MODEL statement.

The Binomial Model

The binomial model is selected by specifying the DIST=BINOMIAL option in the MODEL statement. A binomial response model assumes that the proportion of successes Y is such that Y has a Bi(n, p(x)) distribution. Bi(n, p(x)) refers to the binomial distribution with the parameters n and p(x). Often the data are binary, in which case n = 1. The canonical link is

$$g(p) = \log \frac{p}{n - p} = \eta$$

By default, PROC GAM models the probability of the response level with the *lower ordered value*. Ordered values are assigned to response levels in ascending sorted order and are displayed in the "Response Profiles" table. For binary data, if your event category has a higher Ordered Value, then by default the nonevent is modeled. The effect of modeling the nonevent is to change the signs of the estimated coefficients for linear terms in the model for the event. You can change which probability is modeled by specifying the EVENT=, DESCENDING, or ORDER= response variable options in the MODEL statement.

The Poisson Model

The Poisson model is selected by specifying the DIST=POISSON option in the MODEL statement. The link function for the Poisson model is the log function. Assuming that the mean of the Poisson distribution is $\mu(x)$, the dependence of $\mu(x)$ and independent variables x_1, \ldots, x_k is

$$g(\mu) = \log(\mu) = \eta$$

The Gamma Model

The gamma model is selected by specifying the DIST=GAMMA option in the MODEL statement. Let the mean of the gamma distribution be $\mu(x)$. The canonical link function for the gamma distribution is $-1/\mu(x)$. Note that this link function is the negative of the default link function in PROC GENMOD for a gamma model. The relationship between $\mu(x)$ and the independent variables x_1, \ldots, x_k is

$$g(\mu) = -\frac{1}{\mu} = \eta$$

The Inverse Gaussian Model

The inverse Gaussian model is selected by specifying the DIST=IGAUSSIAN option in the MODEL statement. Let the mean of the inverse Gaussian distribution be $\mu(x)$. The canonical link function for inverse Gaussian distribution is $1/\mu^2$. Therefore, the relationship between $\mu(x)$ and the independent variables x_1, \ldots, x_k is

$$g(\mu) = \frac{1}{\mu^2} = \eta$$

Dispersion Parameter

Continuous distributions in the exponential family (Gaussian, gamma, and inverse Gaussian) have a dispersion parameter that can be estimated by the scaled deviance. For these continuous response distributions, PROC GAM incorporates this dispersion parameter estimate into standard errors of the parameter estimates, prediction standard errors of spline and loess components, and chi-square statistics. The discrete distributions used in GAM (binomial and Poisson) do not have a dispersion parameter. For more details on the distributions, dispersion parameter, and deviance, see "Generalized Linear Models Theory" on page 3069 in Chapter 44, "The GENMOD Procedure."

Since PROC GAM implements a doubly iterative method (inner backfitting iterations within each local scoring iteration), data are accessed multiple times in performing a fit. To expedite the data access, PROC GAM keeps the data used in the analysis in memory.

Let

n = number of observations used in the analysis

 p_r = number of parametric variables

 p_s = number of univariate spline smoothers

 p_I = number of loess smoothers

 p_b = number of bivariate thin-plate spline smoothers

 $p = p_r + p_s + p_l + p_b$

 $p_n = p_s + p_l + p_b$

m = maximum number of iterations for the backfitting algorithm

In addition to the space to store the data (8np bytes), the minimum working space (in bytes) needed for fitting a model using PROC GAM is

$$(16+8p_r)(n+2p_r)+(160+48p+16p_s+8p_b+8p_l)n+8p+32p_b+32p_s+8m+8n+(4n+4)p_s+4.$$

For fitting bivariate thin-plate smoothing spline variables, an extra $80 + 120n + 8n^2 + 8p_b$ bytes of memory are needed. For fitting loess variables, an extra $48n + 16p_l$ bytes of memory are needed. If model inference or confidence limits are requested, additional memory is required.

It is difficult to provide accurate estimates of the time required to fit a GAM model. Both the backfitting algorithm and the local scoring algorithm are iterative techniques whose convergence rates depend on the particular data being analyzed. Furthermore, the time required depends on the types of smoothers that you specify, as well as on the inferential information you request.

You can estimate the time required for problems with a larger number of observations by observing the time required for smaller problems and then using the following growth rules (obtained using by simulations) that show that the time required grows proportionally with the following:

- n^3 when at least one bivariate thin-plate spline is used
- $n^{3/2}$ when only loess smoothers are used
- *n* when only univariate smoothing splines are used

For additive models (models with Gaussian response distribution) with a fixed number of observations, the time required is roughly proportional to $p_n^{3/2}$. For generalized additive models (models with non-Gaussian distributions), the computation time grows more rapidly as p_n increases. This is harder to quantify as it depends on the distribution family and the number of iterations required for the local scoring algorithm to converge.

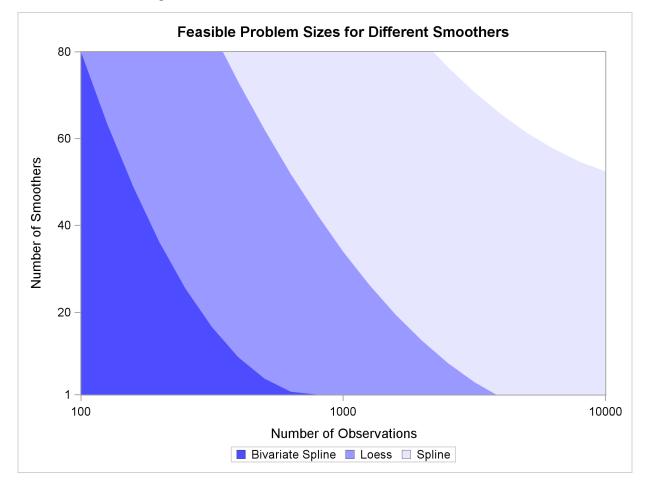


Figure 41.4 Feasible Problem Sizes for Different Smoothers

Figure 41.4 shows a rough estimation of feasible sizes for the smoothers that you can use, as a function of the number of observations and number of smoothing components. This figure depicts the regions where you can expect a single fit of an additive model to finish within a few minutes on a typical Pentium 4 system.

Note that the times reflected in Figure 41.4 are based on fitting additive models (no local scoring iterations) when no analysis of deviance or confidence limits are computed. The time required for fitting generalized additive models grows proportionally with the number of the local scoring iterations. Furthermore, analysis of deviance (if you do not request the fast approximations with the ANODEV option) requires fitting multiple GAM models as each smoothing component is omitted sequentially, and so the time estimates need to be multiplied by the number of smoothing components when analysis of deviance is performed. Finally computation of confidence limits for each individual smoother increases the time required, especially when loess smoothers are utilized.

For univariate spline smoothers, subject to the aforementioned caveats, problems that correspond to all shaded regions in Figure 41.4 can be completed within a few minutes. For univariate loess smoothers, the two darkest regions are feasible. For bivariate spline smoothers, problems that correspond to only the darkest shading can be completed in the order of a few minutes. The problems that correspond to the upper right unshaded region might be possible, but they require long computation times.

ODS Table Names

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

| ODS Table Name | Description | Statement | Option |
|--------------------|--|-----------|---------------|
| ANODEV | Analysis of deviance table for smoothing variables | PROC | Default |
| ClassSummary | Summary of classification variables | PROC | Default |
| ConvergenceStatus | Convergence status of the local scoring algorithm | PROC | Default |
| InputSummary | Input data summary | PROC | Default |
| IterHistory | Iteration history table | MODEL | ITPRINT |
| IterSummary | Iteration summary | PROC | Default |
| FitSummary | Fit parameters and fit summary | PROC | Default |
| ParameterEstimates | Parameter estimation for regression variables | PROC | Default |
| ResponseProfile | Frequency counts for binary models | MODEL | DIST=BINOMIAL |

Table 41.5 ODS Tables Produced by PROC GAM

By referring to the names of such tables, you can use the ODS OUTPUT statement to place one or more of these tables in output data sets.

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 GRAPH-ICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 609 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 608 in Chapter 21, "Statistical Graphics Using ODS."

When ODS Graphics is enabled, the GAM procedure by default produces plots of the partial predictions for each nonparametric predictor in the model. Use the PLOTS option in the PROC GAM statement to control aspects of these plots.

ODS Graph Names

PROC GAM assigns a name to each graph it creates by using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 41.6.

Table 41.6 Graphs Produced by PROC GAM

| ODS Graph Name | Plot Description | PLOTS= Option |
|------------------------|--------------------------------------|--------------------|
| SmoothingComponentPlot | Panel of multiple partial prediction | COMPONENTS |
| | curves | |
| SmoothingComponentPlot | Unpacked partial prediction curves | COMPONENTS(UNPACK) |

By default, partial prediction plots for each component are displayed in panels containing at most six plots. If you specify more than six smoothing components, multiple panels are used. Use the PLOTS(UNPACK) option in the PROC GAM statement to display these plots individually.

Examples: GAM Procedure

Example 41.1: Generalized Additive Model with Binary Data

This example illustrates the capabilities of the GAM procedure and compares it to the GENMOD procedure. From this example, you can see that PROC GAM is very useful in visualizing the data and detecting the nonlinearity among the variables.

The data used in this example are based on a study by Bell et al. (1994). Bell and his associates studied the result of multiple-level thoracic and lumbar laminectomy, a corrective spinal surgery commonly performed on children. The data in the study consist of retrospective measurements on 83 patients. The specific outcome of interest is the presence (1) or absence (0) of kyphosis, defined as a forward flexion of the spine of at least 40 degrees from vertical. The available predictor variables are age in months at time of the operation (Age), the starting of vertebrae levels involved in the operation (StartVert), and the number of levels involved (NumVert). The goal of this analysis is to identify risk factors for kyphosis. PROC GENMOD can be used to investigate the relationship among kyphosis and the predictors. The following statements create the data kyphosis and fit a logistic model specifying linear effects for the three predictors:

```
title 'Comparing PROC GAM with PROC GENMOD';
data kyphosis;
  input Age StartVert NumVert Kyphosis @@;
  datalines;
71 5 3 0
              158 14 3 0
                           128 5
                                   4 1
2
   1 5 0
              1
                  15 4 0
                           1
                               16
                                  2 0
              37 16 3 0
61 17 2 0
                           113 16
                                  2 0
              82 14 5 1
59
   12 6
        1
                           148 16
18 2 5 0
              1
                  12 4 0
                           243 8
                                   8 0
168 18 3 0
              1
                  16 3 0
                           78 15 6 0
              80 16 5 0
175 13 5 0
                           27 9
                                   4 0
22 16 2 0
              105 5 6 1
                           96
                              12
                                  3 1
131 3 2 0
              15 2 7 1
                           9
                               13 5 0
                           100 14 3 0
12 2 14 1
              8
                  6 3 0
   16 3
        0
              151 16 2 0
                           31 16
                                  3 0
                           112 16 3 0
125 11 2 0
              130 13 5 0
140 11 5 0
              93 16 3 0
                               9
                                  3 0
```

```
91 12 5 1
52 6 5 1
                20 9 6 0
73 1 5 1
                35 13 3 0
                               143 3
                                        9 0
61 1 4 0 97 16 3 0
136 15 4 0 131 13 5 0
177 14 2 0 68 10 5 0
                               139 10 3 1
                               121 3
                               9 17 2 0
139 6 10 1
              2 17 2 0 140 15 4 0
72 15 5 0 2 13 3 0
                               120 8 5 1
51 9 7 0 102 13 3 0
                               130 1
                                        4 1
114 8 7 1 81 1 4 0
                               118 16 3 0
118 16 4 0 17 10 4 0
                               195 17 2 0
159 13 4 0 18 11 4 0 15 16 5 0
158 15 4 0 127 12 4 0 87 16 4 0
206 10 4 0 11 15 3 0 178 15 4 0
157 13 3 1 26 13 7 0 120 13 2 0
42 6 7 1 36 13 4 0
proc genmod data=kyphosis descending;
   model Kyphosis = Age StartVert NumVert/link=logit dist=binomial;
```

The GENMOD analysis of the independent variable effects is shown in Output 41.1.1. Based on these results, the only significant factor is StartVert with a log odds ratio of -0.1972. The variable NumVert has a p-value of 0.0904 with a log odds ratio of 0.3031.

Output 41.1.1 GENMOD Analysis: Partial Output

Comparing PROC GAM with PROC GENMOD

The GENMOD Procedure

| Analysis Of Maximum Likelihood Parameter Estimates | | | | | | | |
|--|--|---------|--------|---------|---------|------|--------|
| Parameter | Wald 95% Standard Confidence Wald rameter DF Estimate Error Limits Chi-Square Pr > ChiSq | | | | | | |
| Intercept | 1 | -1.2497 | | -3.6848 | 1.1853 | 1.01 | 0.3145 |
| Age | 1 | 0.0061 | 0.0055 | -0.0048 | 0.0170 | 1.21 | 0.2713 |
| StartVert | 1 | -0.1972 | 0.0657 | -0.3260 | -0.0684 | 9.01 | 0.0027 |
| NumVert | 1 | 0.3031 | 0.1790 | -0.0477 | 0.6540 | 2.87 | 0.0904 |
| Scale | 0 | 1.0000 | 0.0000 | 1.0000 | 1.0000 | | |

Note: The scale parameter was held fixed.

The GENMOD procedure assumes a strict linear relationship between the predictors and the response function, which is the logit (log odds) in this model. The following SAS statements use PROC GAM to investigate a less restrictive model, with moderately flexible spline terms for each of the predictors:

The MODEL statement requests an additive model with a univariate smoothing spline for each term. The response variable option EVENT= chooses Kyphosis=1 (presence) as the event so that the probability of

presence of kyphosis is modeled. The option DIST=BINOMIAL with binary responses specifies a logistic model. Each term is fit by using a univariate smoothing spline with three degrees of freedom. Of these three degrees of freedom, one is taken up by the linear portion of the fit and two are left for the nonlinear spline portion. Although this might seem to be an unduly modest amount of flexibility, it is better to be conservative with a data set this small.

Output 41.1.2 and Output 41.1.3 list the output from PROC GAM.

Output 41.1.2 Summary Statistics

Comparing PROC GAM with PROC GENMOD

The GAM Procedure **Dependent Variable: Kyphosis** Smoothing Model Component(s): spline(Age) spline(StartVert) spline(NumVert)

| Summary of Input Data Set | | | |
|---------------------------------------|----------|--|--|
| Number of Observations | 83 | | |
| Number of Missing Observations | 0 | | |
| Distribution | Binomial | | |
| Link Function | Logit | | |

| Response Profile | | | | |
|------------------|----------|-----------|--|--|
| Ordered Total | | | | |
| Value | Kyphosis | Frequency | | |
| 1 | 0 | 65 | | |
| 2 | 1 | 18 | | |

Note: PROC GAM is modeling the probability that Kyphosis=1. One way to change this to model the probability that Kyphosis=0 is to specify the response variable option EVENT='0'.

| Iteration Summary and Fit Statistics | | | | |
|--|--------------|--|--|--|
| Number of local scoring iterations | 9 | | | |
| Local scoring convergence criterion | 2.6635661E-9 | | | |
| Final Number of Backfitting Iterations | 1 | | | |
| Final Backfitting Criterion | 5.2326593E-9 | | | |
| The Deviance of the Final Estimate | 46.610922438 | | | |

Output 41.1.3 Model Fit Statistics

| Regression Model Analysis Parameter Estimates | | | | | | | |
|--|--------------------|---------|-------|--------|--|--|--|
| | Parameter Standard | | | | | | |
| Parameter Estimate Error t Value Pr > | | | | | | | |
| Intercept | -2.01533 | 1.45620 | -1.38 | 0.1706 | | | |
| Linear(Age) | 0.01213 | 0.00794 | 1.53 | 0.1308 | | | |
| Linear(StartVert) | -0.18615 | 0.07628 | -2.44 | 0.0171 | | | |
| Linear(NumVert) 0.38347 0.19102 2.01 0.0484 | | | | | | | |

Output 41.1.3 continued

Smoothing Model Analysis Fit Summary for Smoothing Components Num

| | Smoothing | | | Unique |
|-------------------|-----------|----------|------------|--------|
| Component | Parameter | DF | GCV | Obs |
| Spline(Age) | 0.999996 | 2.000000 | 328.512831 | 66 |
| Spline(StartVert) | 0.999551 | 2.000000 | 317.646685 | 16 |
| Spline(NumVert) | 0.921758 | 2.000000 | 20.144056 | 10 |

Smoothing Model Analysis Analysis of Deviance

| | Sum of | | | | |
|-------------------|---------|-----------|------------|------------|--|
| Source | DF | Squares | Chi-Square | Pr > ChiSq | |
| Spline(Age) | 2.00000 | 10.494369 | 10.4944 | 0.0053 | |
| Spline(StartVert) | 2.00000 | 5.494968 | 5.4950 | 0.0641 | |
| Spline(NumVert) | 2.00000 | 2.184518 | 2.1845 | 0.3355 | |

The critical part of the GAM results is the "Analysis of Deviance" table, shown in Output 41.1.3. For each smoothing effect in the model, this table gives a χ^2 test comparing the deviance between the full model and the model without the nonparametric component of this variable. The analysis of deviance results indicate that the nonparametric effect of Age is highly significant, the nonparametric effect of StartVert is nearly significant, and the nonparametric effect of NumVert is insignificant at the 5% level.

PROC GAM can also perform approximate analysis of deviance for smoothing effects by using the AN-ODEV=NOREFIT option, as in the following statements:

```
title 'PROC GAM with Approximate Analysis of Deviance';
proc gam data=kyphosis;
                                                  ,df=3)
   model Kyphosis (event='1') = spline(Age
                                 spline(StartVert, df=3)
                                 spline (NumVert , df=3) /
                                     dist=binomial anodev=norefit;
run;
```

Output 41.1.4 Approximate Analysis of Deviance Table

PROC GAM with Approximate Analysis of Deviance

The GAM Procedure **Dependent Variable: Kyphosis** Smoothing Model Component(s): spline(Age) spline(StartVert) spline(NumVert)

| Smoothing Model Analysis Approximate Analysis of Deviance | | | | | |
|--|---------|------------|------------|--|--|
| Source | DF | Chi-Square | Pr > ChiSq | | |
| Spline(Age) | 2.00000 | 7.0888 | 0.0289 | | |
| Spline(StartVert) | 2.00000 | 5.0431 | 0.0803 | | |
| Spline(NumVert) | 2.00000 | 2.2471 | 0.3251 | | |

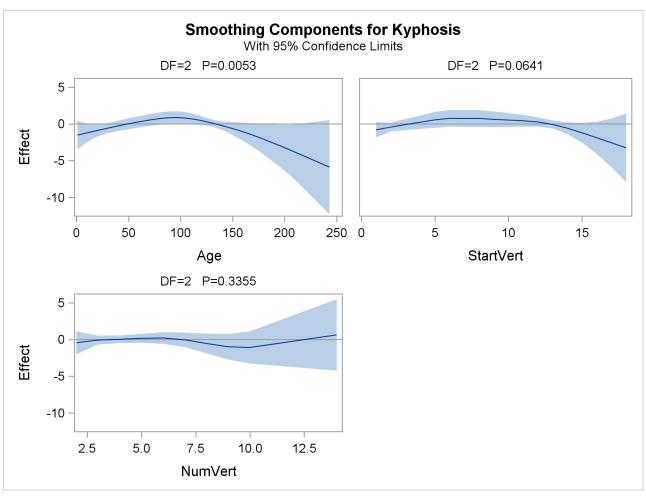
The "Approximate Analysis of Deviance" table shown in Output 41.1.4 yields similar conclusions to those of the "Analysis of Deviance" table (Output 41.1.3). In addition to fitting the model using all the specified

smoothing effects, the default ANODEV=REFIT option requires fitting p additional subset models to p smoothing effects. Each submodel is fit by omitting one smoothing term from the model. By contrast, the ANODEV=NOREFIT option keeps the nonparametric terms fixed and requires a weighted least squares fit for only the parametric part of the model. Hence, GAM with the ANODEV=NOREFIT option is computationally inexpensive and is useful for obtaining approximate analysis of deviance results for models with many smoothing effects. This option assumes that the remaining nonparametric terms do not change much with the deletion of one nonparametric component. It should be used with caution when a model contains highly correlated predictors.

Plots of the partial predictions for each predictor can be used to investigate why PROC GAM and PROC GENMOD produce different results. The following statements use ODS Graphics to produce plots of the individual smoothing components. The CLM suboption in the PLOTS=COMPONENTS option adds a curvewise Bayesian confidence band to each smoothing component, while the COMMONAXES suboption forces all three smoothing component plots to share the same vertical axis limits, allowing a visual judgment of the relative nonparametric effect sizes.

```
ods graphics on;
proc gam data=kyphosis plots=components(clm commonaxes);
                                                  , df=3)
   model Kyphosis (event='1') = spline(Age
                                 spline(StartVert, df=3)
                                 spline(NumVert , df=3) / dist=binomial;
run;
ods graphics off;
```

For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." For specific information about the graphics available in the GAM procedure, see the section "ODS Graphics" on page 2834. The smoothing component plots are displayed in Output 41.1.5.



Output 41.1.5 Partial Prediction for Each Predictor

The plots show that the partial predictions corresponding to both Age and StartVert have a quadratic pattern, while NumVert has a more complicated but ultimately nonsignificant pattern.

An important difference between the first analysis of these data with PROC GENMOD and the subsequent analysis with PROC GAM is that PROC GAM indicates that Age has a significant but nonlinear association with kyphosis. The difference is due to the fact that the generalized linear model includes only the linear effect of Age whereas the generalized additive model allows a more complex relationship, which the plots indicate is nearly quadratic. Having used the GAM procedure to discover an appropriate form of the dependence of Kyphosis on each of the three independent variables, you can use the GENMOD procedure to fit and assess the corresponding parametric model. The following statements fit a generalized linear model with quadratic terms for all three variables. The parameter estimates are shown in Output 41.1.6.

Output 41.1.6 Logistic Model with Quadratic Terms

Comparing PROC GAM with PROC GENMOD

The GENMOD Procedure

| Analysis Of Maximum Likelihood Parameter Estimates | | | | | | | |
|--|----|----------|-------------------|-----------------------|---------|--------------------|------------|
| Parameter | DF | Estimate | Standard Error | Wald Confid Lim | lence | Wald Chi-Square | Pr > ChiSq |
| Intercept | 1 | -5.8134 | 2.5618 | -10.8345 | -0.7923 | 5.15 | 0.0233 |
| Age | 1 | 0.0819 | 0.0345 | 0.0143 | 0.1496 | 5.63 | 0.0176 |
| Age*Age | 1 | -0.0004 | 0.0002 | -0.0008 | -0.0000 | 4.32 | 0.0376 |
| StartVert | 1 | 0.4394 | 0.3234 | -0.1944 | 1.0733 | 1.85 | 0.1742 |
| StartVert*StartVert | 1 | -0.0396 | 0.0202 | -0.0791 | -0.0001 | 3.86 | 0.0495 |
| NumVert | 1 | 0.3798 | 0.5988 | -0.7939 | 1.5535 | 0.40 | 0.5259 |
| NumVert*NumVert | 1 | 0.0020 | 0.0420 | -0.0803 | 0.0843 | 0.00 | 0.9621 |
| Scale | 0 | 1.0000 | 0.0000 | 1.0000 | 1.0000 | | |

Note: The scale parameter was held fixed.

The p-value for the χ^2 test is 0.0376 for dropping the quadratic term of Age, 0.0495 for dropping the quadratic term of StartVert, and 0.9621 for dropping this quadratic term of NumVert. The results for the quadratic GENMOD model are consistent with the GAM results.

Example 41.2: Poisson Regression Analysis of Component Reliability

In this example, the number of maintenance repairs on a complex system are modeled as realizations of Poisson random variables. The system under investigation has a large number of components, which occasionally break down and are replaced or repaired. During a four-year period, the system was observed to be in a state of steady operation, meaning that the rate of operation remained approximately constant. A monthly maintenance record is available for that period, which tracks the number of components removed for maintenance each month. The data are listed in the following statements, which create a SAS data set:

```
title 'Analysis of Component Reliability';
data equip;
   input year month removals @@;
  datalines;
1987
       1 2 1987
                   2
                     4 1987
                               3
                                 3
         3 1987
                   5
                     3 1987
                                 8
1987
                               6
         2 1987
                     6 1987
1987
      7
                   8
                                  3
                             12 10
1987 10
         9 1987
                 11
                     4 1987
1988
      1
         4 1988
                  2
                     6 1988
                              3
                                  4
1988
         4 1988
                   5
                     3 1988
                                 5
       4
                               6
1988
      7
         3 1988
                  8
                     4 1988
                              9
                                  5
1988 10 3 1988 11
                     6 1988
                              12
                                 3
1989
      1 2 1989
                  2
                     6 1989
                                 1
         5 1989
                   5
                     5 1989
                               6
                                  4
1989
1989
      7
         2 1989
                  8
                     2 1989
                                 2
                               9
1989 10 5 1989 11 1 1989
                             12 10
      1 3 1990
                 2 8 1990
```

```
1990  4 7 1990  5 3 1990  6 2
1990  7 4 1990  8 3 1990  9 0
1990  10 6 1990  11 6 1990  12 6
:
```

For planning purposes, it is of interest to understand the long- and short-term trends in the maintenance needs of the system. Over the long term, it is suspected that the quality of new components and repair work improves over time, so the number of component removals would tend to decrease from year to year. It is not known whether the robustness of the system is affected by seasonal variations in the operating environment, but this possibility is also of interest.

Because the maintenance record is in the form of counts, the number of removals are modeled as realizations of Poisson random variables. Denote by λ_{ij} the unobserved component removal rate for year i and month j. Since the data were recorded at regular intervals (from a system operating at a constant rate), each λ_{ij} is assumed to be a function of year and month only.

A preliminary two-way analysis is performed by using PROC GENMOD to make broad inferences on repair trends. A log-link is specified for the model

$$\log \lambda_{ij} = \mu + \alpha_i^Y + \alpha_i^M$$

where μ is a grand mean, α_i^Y is the effect of the *i*th year, and α_j^M is the effect of the *j*th month.

In the following statements, the CLASS statement declares the variables year and month as categorical. Type III sum of squares are requested to test whether there is an overall effect of year and/or month.

```
title2 'Two-way model';
proc genmod data=equip;
  class year month;
  model removals=year month / dist=Poisson link=log type3;
run;
```

Output 41.2.1 displays the listed Type III statistics for the fitted model. With the test for year effects yielding a p-value of 0.4527, there is no evidence of a long-term trend in maintenance rates. Apparently, the quality of new or repaired components did not change between 1987 and 1990. However, the test for monthly trends does yield a small p-value of 0.0321, indicating that seasonal trends are significant at the $\alpha = 0.05$ level.

Output 41.2.1 PROC GENMOD Listing for Type III Analysis

Analysis of Component Reliability Two-way model

The GENMOD Procedure

| LR Statistics For Type 3 Analysis | | | | |
|-----------------------------------|----|------------|------------|--|
| Source | DF | Chi-Square | Pr > ChiSq | |
| year | 3 | 2.63 | 0.4527 | |
| month | 11 | 21.12 | 0.0321 | |

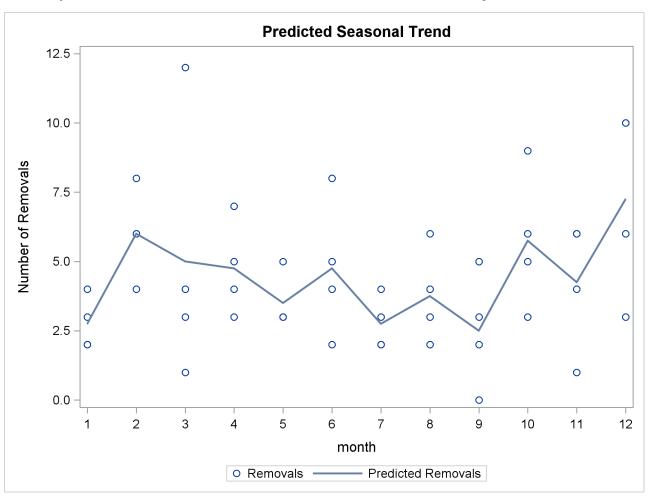
If year is dropped from the model, the focus of the analysis is now on identifying the form of the underlying seasonal trend, which is a task that PROC GAM is especially suited for. PROC GAM will be used to fit both a reduced categorical model, with year eliminated, and a nonparametric spline model. Although PROC

GENMOD also has the capability to fit categorical models, as demonstrated earlier, PROC GAM will be used here to fit both models for a better comparison.

The following PROC GAM statements specify the reduced categorical model and write predicted values to a data set. For this part of the analysis, a CLASS statement is again used to specify that month is a categorical variable. In the follow-up, the seasonal effect will be treated as a nonparametric function of month.

```
title2 'One-way model';
proc gam data=equip;
  class month;
  model removals=param(month) / dist=Poisson;
  output out=est p;
run;
```

The following statements use the SGPLOT procedure to generate a plot of the estimated seasonal trend. The plot is displayed in Output 41.2.2.



Output 41.2.2 Predicted Seasonal Trend from a Parametric Model Fit Using a CLASS Statement

The predicted repair rates shown in Output 41.2.2 form a jagged seasonal pattern. Ignoring the month-to-month fluctuations, which are difficult to explain and can be artifacts of random noise, the general removal rate trend is high in winter and low in summer.

One advantage of nonparametric regression is its ability to highlight general trends in the data, such as those described earlier, and to attribute local fluctuations to unexplained random noise. The nonparametric regression model used by PROC GAM specifies that the underlying removal rates λ_i are of the form

$$\log \lambda_j = \beta_0 + \beta_1 Month_j + s(Month_j)$$

where β_1 is a linear coefficient and s() is a nonparametric regression function. β_1 and s() define the linear and nonparametric parts, respectively, of the seasonal trend.

The following statements request that PROC GAM fit a cubic spline model to the monthly repair data. The output listing is displayed in Output 41.2.3 and Output 41.2.4.

```
title 'Analysis of Component Reliability';
title2 'Spline model';
proc gam data=equip;
   model removals=spline(month) / dist=Poisson method=gcv;
run;
```

The METHOD=GCV option is used to determine an appropriate level of smoothing.

Output 41.2.3 PROC GAM Listing for Cubic Spline Regression Using the METHOD=GCV Option

Analysis of Component Reliability Spline model

The GAM Procedure Dependent Variable: removals **Smoothing Model Component(s): spline(month)**

| Summary of Input Data Set | | | |
|----------------------------------|---------|--|--|
| Number of Observations | 48 | | |
| Number of Missing Observations 0 | | | |
| Distribution | Poisson | | |
| Link Function | Log | | |

Output 41.2.4 Model Fit Statistics

| Regression Model Analysis Parameter Estimates | | | | |
|---|-------------------------|---------|-----------------|--|
| Parameter | Parameter : Estimate | | t Value Pr > t | |
| Intercept | 1.34594 | 0.14509 | 9.28 <.0001 | |
| Linear(month) | 0.02274 | 0.01893 | 1.20 0.2362 | |

Smoothing Model Analysis Fit Summary for Smoothing Components

| Component | Smoothing Parameter | DF | GCV | Num Unique Obs |
|---------------|------------------------|----------|----------|----------------------|
| Spline(month) | 0.901512 | 1.879980 | 0.115848 | 12 |

Smoothing Model Analysis Analysis of Deviance

| Source | DF | Sum of Squares | Chi-Square | Pr > ChiSq |
|---------------|---------|-------------------|------------|------------|
| Spline(month) | 1.87998 | 8.877764 | 8.8778 | 0.0103 |

Notice in the listing in Output 41.2.4 that the DF value chosen for the nonlinear portion of the spline by minimizing GCV is about 1.88, which is smaller than the default value of 3. This indicates that the spline model of the seasonal trend is relatively simple. As indicated by the "Analysis of Deviance" table, it is a significant feature of the data. The table lists a p-value of 0.0103 for the hypothesis of no seasonal trend. Note also that the "Parameter Estimates" table lists a p-value of 0.2362 for the hypothesis of no linear factor in the seasonal trend indicating no significant linear trend.

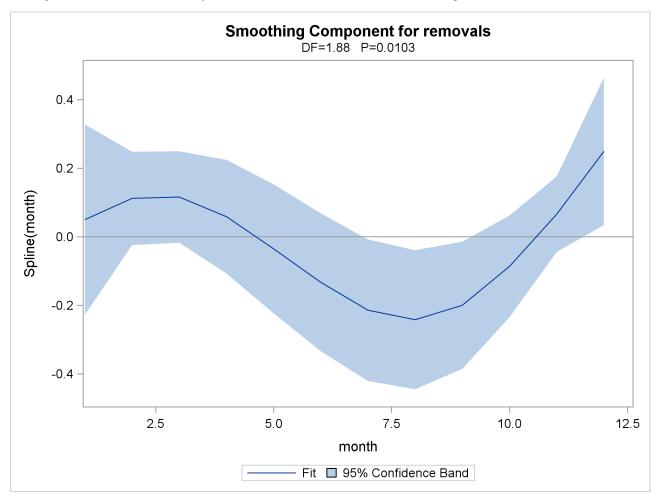
The following statements use ODS Graphics to plot the smoothing component for the effect of Month on predicted repair rates. The CLM suboption for the PLOTS=COMPONENTS option adds a 95% confidence band to the fit.

```
ods graphics on;
proc gam data=equip plots=components(clm);
   model removals=spline(month) / dist=Poisson method=gcv;
run;
ods graphics off;
```

For general information about ODS graphics, see Chapter 21, "Statistical Graphics Using ODS." For specific information about the graphics available in the GAM procedure, see the section "ODS Graphics" on page 2834. The smoothing component plot is displayed in Output 41.2.5.

In Output 41.2.5, it is apparent that the pattern of repair rates follows the general pattern observed in Output 41.2.2. However, the plot in Output 41.2.5 is much cleaner because the month-to-month fluctuations are smoothed out to reveal the broader seasonal trend.

Output 41.2.5 Estimated Nonparametric Factor of Seasonal Trend, Along with 95% Confidence Bounds



In Output 41.2.1 the small p-value (p = 0.0321) for the hypothesis of no seasonal trend indicates that the data exhibit significant seasonal structure. Output 41.2.5 is a graphical illustration of the seasonality of the number of removals.

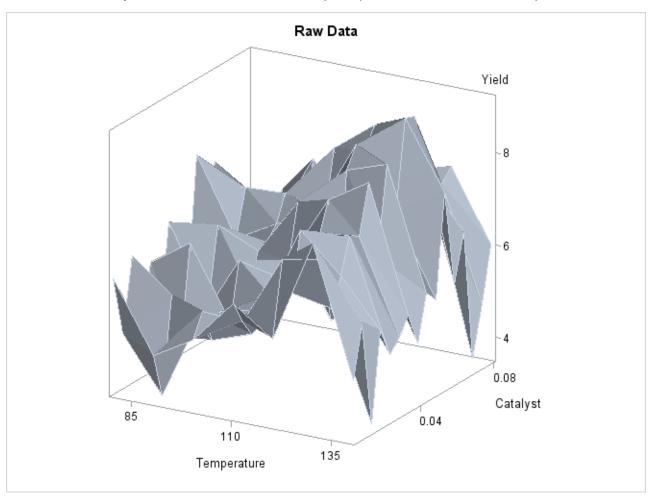
In an analysis of simulated data from a hypothetical chemistry experiment, additive nonparametric regression performed by PROC GAM is compared to the unrestricted multidimensional procedure of PROC LOESS.

In each repetition of the experiment, a catalyst is added to a chemical solution, thereby inducing synthesis of a new material. The data are measurements of the temperature of the solution, the amount of catalyst added, and the yield of the chemical reaction. The following statements read and plots the raw data.

```
data ExperimentA;
   format Temperature f4.0 Catalyst f6.3 Yield f8.3;
   input Temperature Catalyst Yield @@;
  datalines;
80 0.005 6.039 80 0.010 4.719 80 0.015 6.301
80 0.020 4.558 80 0.025 5.917 80 0.030 4.365
80 0.035 6.540 80 0.040 5.063 80 0.045 4.668
80 0.050 7.641 80 0.055 6.736 80 0.060 7.255
80 0.065 5.515 80 0.070 5.260 80 0.075 4.813
80 0.080 4.465 90 0.005 4.540 90 0.010 3.553
90 0.015 5.611 90 0.020 4.586 90 0.025 6.503
90 0.030 4.671 90 0.035 4.919 90 0.040 6.536
90 0.045 4.799 90 0.050 6.002 90 0.055 6.988
90 0.060 6.206 90 0.065 5.193 90 0.070 5.783
90 0.075 6.482 90 0.080 5.222 100 0.005 5.042
100 0.010 5.551 100 0.015 4.804 100 0.020 5.313
100 0.025 4.957 100 0.030 6.177 100 0.035 5.433
100 0.040 6.139 100 0.045 6.217 100 0.050 6.498
100 0.055 7.037 100 0.060 5.589 100 0.065 5.593
100 0.070 7.438 100 0.075 4.794 100 0.080 3.692
110 0.005 6.005 110 0.010 5.493 110 0.015 5.107
110 0.020 5.511 110 0.025 5.692 110 0.030 5.969
110 0.035 6.244 110 0.040 7.364 110 0.045 6.412
110 0.050 6.928 110 0.055 6.814 110 0.060 8.071
110 0.065 6.038 110 0.070 6.295 110 0.075 4.308
110 0.080 7.020 120 0.005 5.409 120 0.010 7.009
120 0.015 6.160 120 0.020 7.408 120 0.025 7.123
120 0.030 7.009 120 0.035 7.708 120 0.040 5.278
120 0.045 8.111 120 0.050 8.547 120 0.055 8.279
120 0.060 8.736 120 0.065 6.988 120 0.070 6.283
120 0.075 7.367 120 0.080 6.579 130 0.005 7.629
130 0.010 7.171 130 0.015 5.997 130 0.020 6.587
130 0.025 7.335 130 0.030 7.209 130 0.035 8.259
130 0.040 6.530 130 0.045 8.400 130 0.050 7.218
130 0.055 9.167 130 0.060 9.082 130 0.065 7.680
130 0.070 7.139 130 0.075 7.275 130 0.080 7.544
140 0.005 4.860 140 0.010 5.932 140 0.015 3.685
140 0.020 5.581 140 0.025 4.935 140 0.030 5.197
140 0.035 5.559 140 0.040 4.836 140 0.045 5.795
140 0.050 5.524 140 0.055 7.736 140 0.060 5.628
140 0.065 6.644 140 0.070 3.785 140 0.075 4.853
140 0.080 6.006
```

```
proc sort data=ExperimentA;
   by Temperature Catalyst;
run;
proc template;
   define statgraph surface;
      dynamic _X _Y _Z _T;
      begingraph;
         entrytitle _T;
         layout overlay3d/
            xaxisopts=(linearopts=(tickvaluesequence=
                        (start=85 end=135 increment=25)))
            yaxisopts=(linearopts=(tickvaluesequence=
                        (start=0 end=0.08 increment=0.04)))
            rotate=30 cube=false;
         surfaceplotparm x=_X y=_Y z=_Z;
         endlayout;
      endgraph;
   end;
run;
proc sgrender data=ExperimentA template=surface;
   dynamic _X='Temperature' _Y='Catalyst' _Z='Yield' _T='Raw Data';
run;
```

The plot is displayed in Output 41.3.1. A surface fitted to the plot of Output 41.3.1 by PROC LOESS will be of a very general (and flexible) type, since the procedure requires only weak assumptions about the structure of the dependencies among the data. PROC GAM, on the other hand, makes stronger structural assumptions by restricting the fitted surface to an additive form. These differences will be demonstrated in this example.



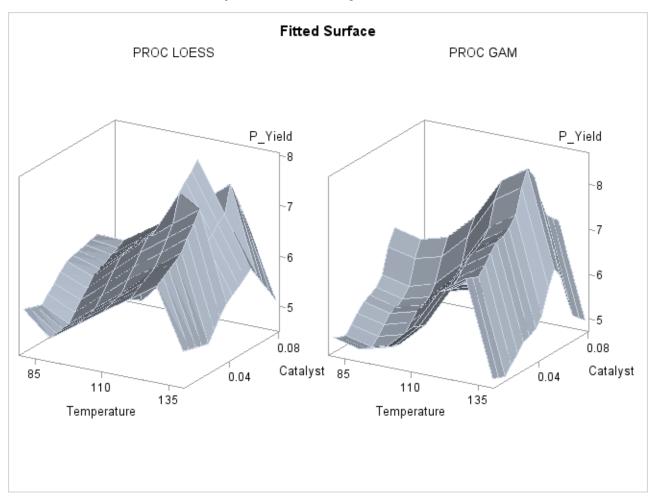
Output 41.3.1 Surface Plot of Yield by Temperature and Amount of Catalyst

The following statements request that both PROC LOESS and PROC GAM fit surfaces to the data:

In both cases the smoothing parameter was chosen as the value that minimizes GCV. This is performed automatically by PROC LOESS and PROC GAM.

The following statements generate plots of the predicted yields, which are displayed in Output 41.3.2:

```
proc template;
   define statgraph surface1;
      begingraph;
         entrytitle "Fitted Surface";
         layout lattice/columns=2;
            layout
            overlay3d/xaxisopts=(linearopts=(tickvaluesequence=
                                 (start=85 end=135 increment=25)))
                     yaxisopts=(linearopts=(tickvaluesequence=
                                 (start=0 end=0.08 increment=0.04)))
                     zaxisopts=(label="P_Yield")
                     rotate=30 cube=0;
               entry "PROC LOESS"/location=outside valign=top
                                   textattrs=graphlabeltext;
               surfaceplotparm x=Temperature y=Catalyst z=p_Yield;
            endlayout;
            layout
            overlay3d/xaxisopts=(linearopts=(tickvaluesequence=
                                 (start=85 end=135 increment=25)))
                     yaxisopts=(linearopts=(tickvaluesequence=
                                 (start=0 end=0.08 increment=0.04)))
                     rotate=30 cube=0
                     zaxisopts=(label="P_Yield")
                     rotate=30 cube=0;
               entry "PROC GAM"/location=outside valign=top
                                textattrs=graphlabeltext;
               surfaceplotparm x=Temperature y=Catalyst z=Gam_p_Yield;
            endlayout;
         endlayout;
      endgraph;
   end;
run;
proc sgrender data=PredGAM template=surface1;
run;
```



Output 41.3.2 Fitted Regression Surfaces

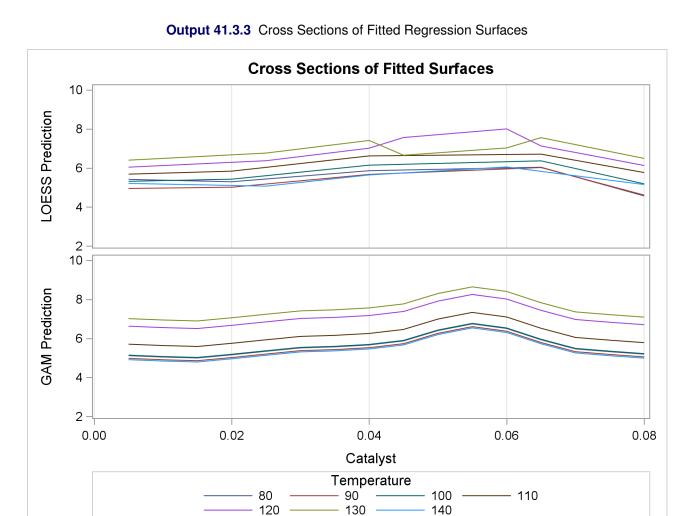
Though both PROC LOESS and PROC GAM use the statistical technique loess, it is apparent from Output 41.3.2 that the manner in which it is applied is very different. By smoothing out the data in local neighborhoods, PROC LOESS essentially fits a surface to the data in pieces, one neighborhood at a time. The local regions are treated independently, so separate areas of the fitted surface are only weakly related. PROC GAM imposes additive structure, requiring that cross sections of the fitted surface always have the same shape and thereby relating regions that have a common value of the same individual regressor variable. Under that restriction, the loess technique need not be applied to the entire multidimensional scatter plot, but only to one-dimensional cross sections of the data.

The advantage of using additive model fitting is that its statistical power is directed toward univariate smoothing, and so it is able to discern the finer details of any underlying structure in the data. Regression data can be very sparse when viewed in the context of multidimensional space, even when every individual set of regressor values densely covers its range. This is the familiar curse of dimensionality. Sparse data greatly restrict the effectiveness of nonparametric procedures, but additive model fitting, when appropriate, is one way to overcome this limitation.

To examine these properties, you can use ODS Graphics to generate plots of cross sections of the unrestricted (PROC LOESS) and additive (PROC GAM) fitted surfaces for the variable Catalyst, as shown in the following statements:

```
proc template;
   define statgraph projection;
      begingraph;
         entrytitle "Cross Sections of Fitted Surfaces";
         layout lattice/rows=2 columndatarange=unionall
                       columngutter=10;
            columnAxes;
               columnAxis / display=all griddisplay=auto_on;
            endColumnAxes;
            layout overlay/
               xaxisopts=(display=none)
               yaxisopts=(label="LOESS Prediction"
               linearopts=(viewmin=2 viewmax=10));
               seriesplot x=Catalyst y=p_Yield /
                  group=temperature
                  name="Temperature";
            endlayout;
            layout overlay/
               xaxisopts=(display=none)
               yaxisopts=(label="GAM Prediction"
               linearopts=(viewmin=2 viewmax=10));
               seriesplot x=Catalyst y=Gam_p_Yield /
                  group=temperature
                  name="Temperature";
            endlayout;
            columnheaders;
               discreteLegend "Temperature" / title = "Temperature";
            endcolumnheaders;
         endlayout;
      endgraph;
   end;
run;
proc sgrender data=PredGAM template=projection;
```

The plots are displayed in Output 41.3.3.

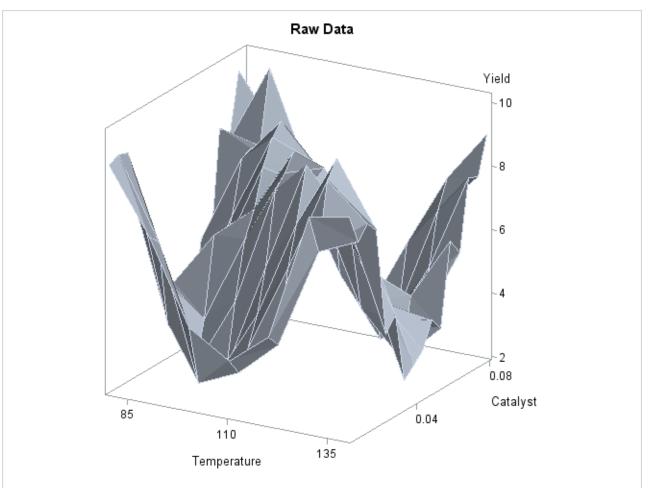


Notice that the cross sections in the top panel (PROC LOESS) of Output 41.3.3 have varying shapes, while every cross section in the bottom panel (PROC GAM) is the same curve shifted vertically. This illustrates precisely the kind of structural differences that distinguish additive models. A second important comparison to make between Output 41.3.2 and Output 41.3.3 is the level of detail in the fitted regression surfaces. Cross sections of the PROC LOESS surface are rather flat, but those of the additive surface have a clear shape. In particular, the ridge near Catalyst=0.055 is only vaguely evident in the PROC LOESS surface, but it is plainly revealed by the additive procedure.

For an example of a situation where unrestricted multidimensional fitting is preferred over additive regression, consider the following simulated data from a similar experiment. The following statements create another SAS data set and plot.

```
data ExperimentB;
   format Temperature f4.0 Catalyst f6.3 Yield f8.3;
  input Temperature Catalyst Yield @@;
   datalines;
80 0.005 9.115 80 0.010 9.275 80 0.015
   0.020 7.065 80 0.025 6.054 80 0.030
80
                                           4.899
   0.035 4.504 80 0.040 4.238 80 0.045
                                           3.232
80 0.050 3.135 80 0.055 5.100 80 0.060
                                          4.802
80 0.065 8.218 80 0.070 7.679 80 0.075
                                           9.669
80 0.080 9.071 90 0.005 7.085 90 0.010
                                           6.814
90 0.015 4.009 90 0.020 4.199 90 0.025
                                           3.377
90 0.030 2.141 90 0.035 3.500 90 0.040
                                          5.967
90 0.045 5.268 90 0.050 6.238 90 0.055 7.847
90 0.060 7.992 90 0.065 7.904 90 0.070 10.184
90 0.075 7.914 90 0.080
                          6.842 100 0.005
                                           4.497
100 0.010 2.565 100 0.015 2.637 100 0.020
                                           2.436
100 0.025 2.525 100 0.030 4.474 100 0.035
                                          6.238
100 0.040 7.029 100 0.045 8.183 100 0.050
                                           8.939
100 0.055 9.283 100 0.060 8.246 100 0.065
                                          6.927
100 0.070 7.062 100 0.075 5.615 100 0.080
110 0.005 3.706 110 0.010 3.154 110 0.015
                                           3.726
110 0.020 4.634 110 0.025 5.970 110 0.030
                                           8.219
110 0.035 8.590 110 0.040 9.097 110 0.045
                                          7.887
110 0.050 8.480 110 0.055 6.818 110 0.060
                                          7.666
110 0.065 4.375 110 0.070 3.994 110 0.075 3.630
110 0.080 2.685 120 0.005 4.697 120 0.010
                                           4.268
120 0.015 6.507 120 0.020 7.747 120 0.025
                                          9.412
120 0.030 8.761 120 0.035 8.997 120 0.040
                                          7.538
120 0.045 7.003 120 0.050 6.010 120 0.055
                                           3.886
120 0.060 4.897 120 0.065 2.562 120 0.070
                                           2.714
120 0.075 3.141 120 0.080 5.081 130 0.005
                                          8.729
130 0.010 7.460 130 0.015 9.549 130 0.020 10.049
130 0.025 8.131 130 0.030 7.553 130 0.035
                                           6.191
130 0.040 6.272 130 0.045 4.649 130 0.050
                                          3.884
                                          3.272
130 0.055 2.522 130 0.060 4.366 130 0.065
130 0.070 4.906 130 0.075 6.538 130 0.080
                                           7.380
140 0.005 8.991 140 0.010
                          8.029 140 0.015
                                           8.417
140 0.020 8.049 140 0.025 4.608 140 0.030
                                          5.025
140 0.035 2.795 140 0.040 3.123 140 0.045
                                          3.407
140 0.050 4.183 140 0.055 3.750 140 0.060
                                           6.316
140 0.065 5.799 140 0.070 7.992 140 0.075
140 0.080 8.985
proc sort data=ExperimentB;
  by Temperature Catalyst;
run;
proc sgrender data=ExperimentB template=surface;
   dynamic _X='Temperature' _Y='Catalyst' _Z='Yield' _T='Raw Data';
```

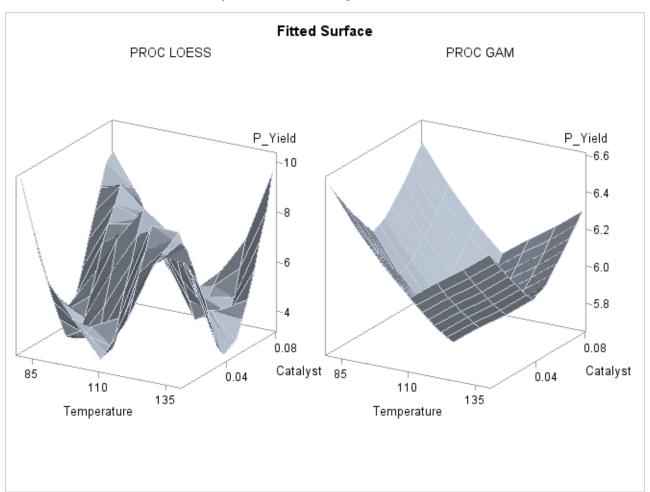
A plot of the raw data is displayed in Output 41.3.4.



Output 41.3.4 Raw Data from Experiment B

Though the surface displayed in Output 41.3.4 is quite jagged, a distinct feature of the plot is a large ridge that runs diagonally across its surface. One would expect that the ridge would appear in the fitted regression surface of an appropriate nonparametric procedure. Nevertheless, between PROC LOESS and PROC GAM, only PROC LOESS is able to capture this significant feature.

The SAS program for fitting the new data is essentially the same as that for the data set from the first experiment and produces output data set PredGAMb for this experiment. As in Output 41.3.2, multivariate and additive fitted surfaces for these data are displayed in Output 41.3.5.



Output 41.3.5 Fitted Regression Surfaces

It is clear from Output 41.3.5 that the results of PROC LOESS and PROC GAM are completely different. While the plot in the left panel resembles the raw data plot in Output 41.3.4, the plot in the right panel is essentially featureless.

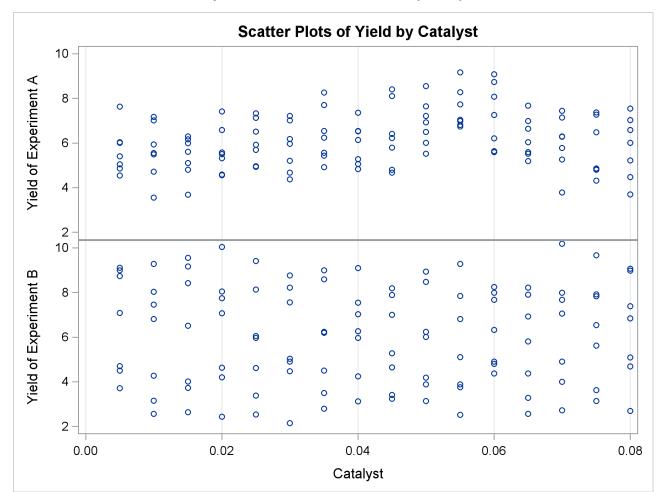
To understand what is happening, compare the scatter plots of Yield by Catalyst for the two data sets in this example. These are generated by the following statements and displayed in Output 41.3.6.

```
data PredGAM;
    set PredGAM;
    rename Yield=Yield_a;
run;

data PredGAMb;
    set PredGAMb;
    set PredGAM(keep=Yield_a);
run;
```

```
proc template;
   define statgraph scatter2;
      dynamic _X _Y1 _Y2;
      begingraph;
         entrytitle "Scatter Plots of Yield by Catalyst";
         layout lattice/rows=2 columndatarange=unionall
                         rowdatarange=unionall
                         columngutter=15;
            columnAxes;
               columnAxis / display=all griddisplay=auto_on;
            endColumnAxes;
            layout overlay/
               xaxisopts=(display=none)
               yaxisopts=(label="Yield of Experiment A"
               linearopts=(viewmin=2 viewmax=10));
               scatterplot x=_X y=_Y1;
            endlayout;
            layout overlay/
               xaxisopts=(display=none)
               yaxisopts=(label="Yield of Experiment B"
               linearopts=(viewmin=2 viewmax=10));
               scatterplot x=_X y=_Y2;
            endlayout;
         endlayout;
      endgraph;
   end:
run;
proc sgrender data=PredGAMb template=scatter2;
   dynamic _X='Catalyst' _Y1='Yield_a' _Y2='Yield';
run;
ods graphics off;
```

The top panel of Output 41.3.6 hints at the same kind of structure exhibited in the fitted cross sections of Output 41.3.3. In PROC GAM, the additive model component corresponding to Catalyst is fit to a similar scatter plot, with the partial residuals computed in the backfitting algorithm, so it is able to capture the trend seen here. In contrast, when the second data set is viewed from the perspective of Output 41.3.6, the diagonal ridge apparent in Output 41.3.4 is washed out, and no clear structure shows up in the scatter plot. As a result, the additive model fit produced by PROC GAM is relatively featureless.



Output 41.3.6 Scatter Plots of Yield by Catalyst

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