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SAS/STAT® 15.1 User's Guide

The RSREG Procedure

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Chapter 105
The RSREG Procedure

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Overview: RSREG Procedure

The RSREG procedure uses the method of least squares to fit quadratic response surface regression models. Response surface models are a kind of general linear model in which attention focuses on characteristics of the fit response function and in particular, where optimum estimated response values occur.

In addition to fitting a quadratic function, you can use the RSREG procedure to do the following:

- test for lack of fit
- test for the significance of individual factors
- analyze the canonical structure of the estimated response surface
- compute the ridge of optimum response
- predict new values of the response

The RSREG procedure uses ODS Graphics to display the response surfaces, residuals, fit diagnostics, and ridges of optimum response. For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS."

Comparison to Other SAS Software

Other SAS/STAT procedures can be used to fit the response surface, but the RSREG procedure is more specialized. PROC RSREG uses a much more compact model syntax than other procedures; for example, the following statements model a three-factor response surface in the REG, GLM, and RSREG procedures:

```
proc reg;
   model y=x1 x1*x1
           x2 x1*x2 x2*x2
           x3 x1*x3 x2*x3 x3*x3;
run;

proc glm;
   model y=x1|x2|x3@2 x1*x1 x2*x2 x3*x3;
run;

proc rsreg;
   model y=x1 x2 x3;
run;
```

Additionally, PROC RSREG includes specialized methodology for analyzing the fitted response surface, such as canonical analysis and optimum response ridges.

Terminology

Variables are referred to according to the following conventions:

factor variables	independent variables used to construct the quadratic response surface. To estimate the necessary parameters, each variable must have at least three distinct values in the data. Independent variables must be numeric.
response variables	the dependent variables to which the quadratic response surfaces are fit. Dependent variables must be numeric.
covariates	additional independent variables for use in the regression but not in the formation of the quadratic response surface. Covariates must be numeric.
WEIGHT variable	a variable for weighting the observations in the regression. The WEIGHT variable must be numeric.
ID variables	variables not previously described that are transferred to an output data set containing statistics for each observation in the input data set. This data set is created by using the OUT= option in the PROC RSREG statement. ID variables can be either character or numeric.
BY variables	variables for grouping observations. Separate analyses are obtained for each BY group. BY variables can be either character or numeric.

Getting Started: RSREG Procedure

A Response Surface with a Simple Optimum

This example uses the three-factor quadratic model discussed in John (1971). Settings of the temperature, gas–liquid ratio, and packing height are controlled factors in the production of a certain chemical; Schneider and Stockett (1963) performed an experiment in order to determine the values of these three factors that minimize the unpleasant odor of the chemical. The following statements input the SAS data set smell; the variable Odor is the response, while the variables T, R, and H are the independent factors.

```
title 'Response Surface with a Simple Optimum';
data smell;
   input Odor T R H @@;
   label
      T = "Temperature"
      R = "Gas-Liquid Ratio"
      H = "Packing Height";
   datalines;
 66 40 .3 4     39 120 .3 4     43 40 .7 4     49 120 .7  4
 58 40 .5 2     17 120 .5 2     -5 40 .5 6    -40 120 .5  6
 65 80 .3 2      7  80 .7 2     43 80 .3 6    -22  80 .7  6
-31 80 .5 4    -35  80 .5 4    -26 80 .5 4
;
```

The following statements invoke PROC RSREG on the data set smell. Figure 105.1 through Figure 105.3 display the results of the analysis, including a lack-of-fit test requested with the LACKFIT option.

```
proc rsreg data=smell;
   model Odor = T R H / lackfit;
run;
```

Figure 105.1 displays the coding coefficients for the transformation of the independent variables to lie between –1 and 1, simple statistics for the response variable, hypothesis tests for linear, quadratic, and crossproduct terms, and the lack-of-fit test. The hypothesis tests can be used to gain a rough idea of importance of the effects; here the crossproduct terms are not significant. However, the lack of fit for the model is significant, so more complicated modeling or further experimentation with additional variables should be performed before firm conclusions are made concerning the underlying process.

Figure 105.1 Summary Statistics and Analysis of Variance

Response Surface with a Simple Optimum

The RSREG Procedure

Coding Coefficients for the Independent Variables		
Factor	Subtracted off	Divided by
T	80.000000	40.000000
R	0.500000	0.200000
H	4.000000	2.000000

Response Surface for Variable Odor	
Response Mean	15.200000
Root MSE	22.478508
R-Square	0.8820
Coefficient of Variation	147.8849

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Linear	3	7143.250000	0.3337	4.71	0.0641
Quadratic	3	11445	0.5346	7.55	0.0264
Crossproduct	3	293.500000	0.0137	0.19	0.8965
Total Model	9	18882	0.8820	4.15	0.0657

Residual	DF	Sum of Squares	Mean Square	F Value	Pr > F
Lack of Fit	3	2485.750000	828.583333	40.75	0.0240
Pure Error	2	40.666667	20.333333		
Total Error	5	2526.416667	505.283333		

Parameter estimates and the factor ANOVA are shown in Figure 105.2. Looking at the parameter estimates, you can see that the crossproduct terms are not significantly different from zero, as noted previously. The Estimate column contains estimates based on the raw data, and the Parameter Estimate from Coded Data column contains estimates based on the coded data. The factor ANOVA table displays tests for all four parameters corresponding to each factor—the parameters corresponding to the linear effect, the quadratic

effect, and the effects of the crossproducts with each of the other two factors. The only factor with a significant overall effect is R, indicating that the level of noise left unexplained by the model is still too high to estimate the effects of T and H accurately. This might be due to the lack of fit.

Figure 105.2 Parameter Estimates and Hypothesis Tests

Parameter	DF	Estimate	Standard Error	t Value	Pr > |t|	Parameter Estimate from Coded Data
Intercept	1	568.958333	134.609816	4.23	0.0083	-30.666667
T	1	-4.102083	1.489024	-2.75	0.0401	-12.125000
R	1	-1345.833333	335.220685	-4.01	0.0102	-17.000000
H	1	-22.166667	29.780489	-0.74	0.4902	-21.375000
T*T	1	0.020052	0.007311	2.74	0.0407	32.083333
R*T	1	1.031250	1.404907	0.73	0.4959	8.250000
R*R	1	1195.833333	292.454665	4.09	0.0095	47.833333
H*T	1	0.018750	0.140491	0.13	0.8990	1.500000
H*R	1	-4.375000	28.098135	-0.16	0.8824	-1.750000
H*H	1	1.520833	2.924547	0.52	0.6252	6.083333

Factor	DF	Sum of Squares	Mean Square	F Value	Pr > F	Label
T	4	5258.016026	1314.504006	2.60	0.1613	Temperature
R	4	11045	2761.150641	5.46	0.0454	Gas-Liquid Ratio
H	4	3813.016026	953.254006	1.89	0.2510	Packing Height

Figure 105.3 displays the canonical analysis and eigenvectors. The canonical analysis indicates that the directions of principal orientation for the predicted response surface are along the axes associated with the three factors, confirming the small interaction effect in the regression ANOVA (Figure 105.1). The largest eigenvalue (48.8588) corresponds to the eigenvector (0.238091, 0.971116, -0.015690), the largest component of which (0.971116) is associated with R; similarly, the second-largest eigenvalue (31.1035) is associated with T. The third eigenvalue (6.0377), associated with H, is quite a bit smaller than the other two, indicating that the response surface is relatively insensitive to changes in this factor. The coded form of the canonical analysis indicates that the estimated response surface is at a minimum when T and R are both near the middle of their respective ranges (that is, the coded critical values for T and R are both near 0) and H is relatively high; in uncoded terms, the model predicts that the unpleasant odor is minimized when T = 84.876502, R = 0.539915, and H = 7.541050.

Figure 105.3 Canonical Analysis and Eigenvectors

	Critical Value		
Factor	Coded	Uncoded	Label
T	0.121913	84.876502	Temperature
R	0.199575	0.539915	Gas-Liquid Ratio
H	1.770525	7.541050	Packing Height
Predicted value at stationary point: -52.024631			

Figure 105.3 *continued*

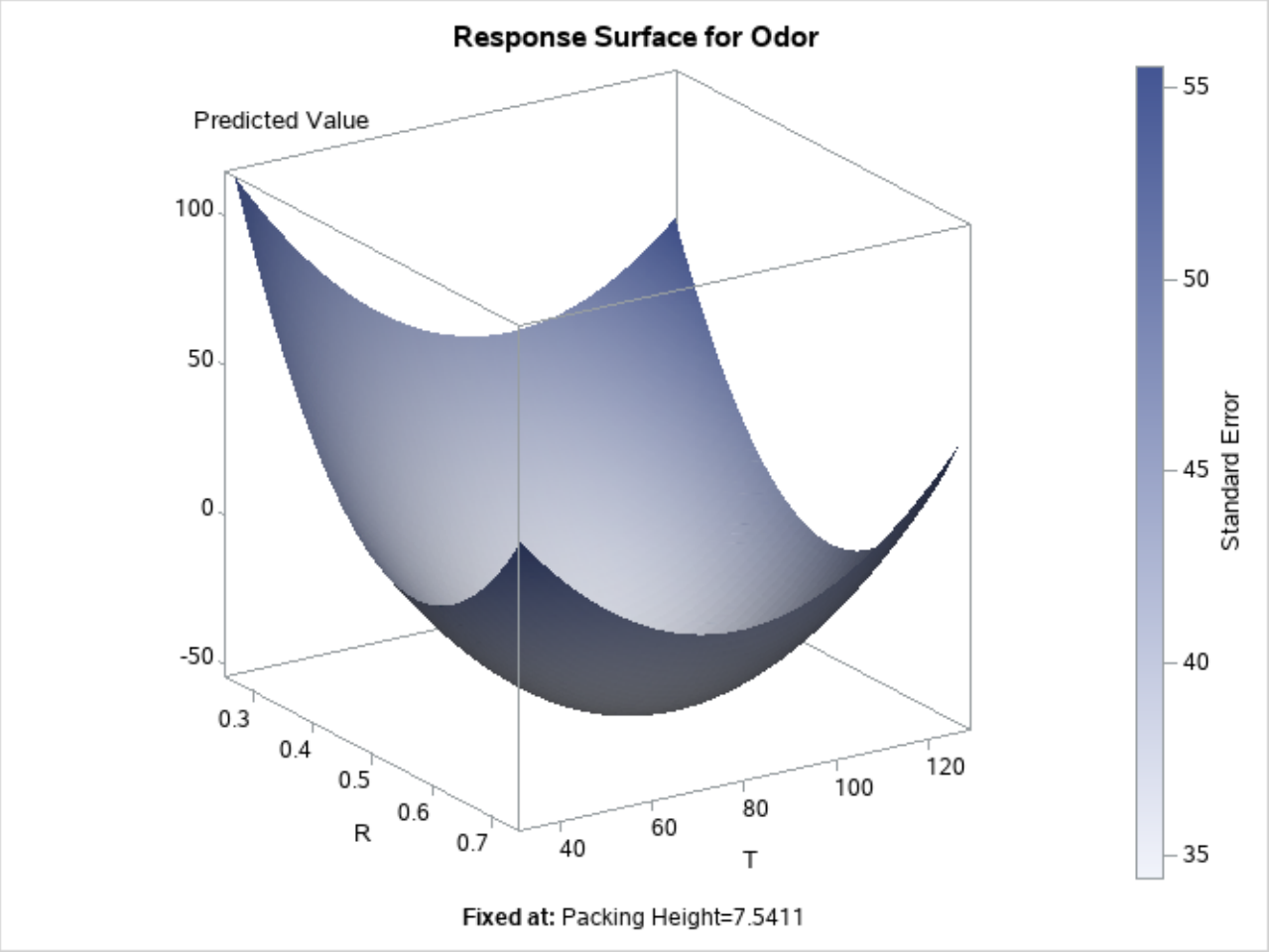
	Eigenvectors		
Eigenvalues	**T**	**R**	**H**
48.858807	0.238091	0.971116	-0.015690
31.103461	0.970696	-0.237384	0.037399
6.037732	-0.032594	0.024135	0.999177
Stationary point is a minimum.			

To plot the response surface with respect to two of the factor variables, fix H, the least significant factor variable, at its estimated optimum value. The following statements use ODS Graphics to display the surface:

```
ods graphics on;
proc rsreg data=smell
           plots(unpack)=surface(3d at(H=7.541050));
   model Odor = T R H;
   ods select 'T * R = Pred';
run;
ods graphics off;
```

Note that the ODS SELECT statement is specified to select the plot of interest.

Figure 105.4 The Response Surface at the Optimum H



Alternatively, the following statements produce an output data set containing the surface information, which you can then use for plotting surfaces or searching for optima. The first DATA step fixes H, the least significant factor variable, at its estimated optimum value (7.541), and generates a grid of points for T and R. To ensure that the grid data do not affect parameter estimates, the response variable (Odor) is set to missing. (See the section "Missing Values" on page 8767.) The second DATA step concatenates these grid points to the original data. Then PROC RSREG computes predictions for the combined data. The last DATA step subsets the predicted values over just the grid points, which excludes the predictions at the original data.

```
data grid;
   do;
      Odor =  .  ;
      H    = 7.541;
      do T = 20 to 140 by 5;
         do R = .1 to .9 by .05;
            output;
         end;
      end;
   end;
run;
data grid;
   set smell grid;
run;

proc rsreg data=grid out=predict noprint;
   model Odor = T R H / predict;
run;

data grid;
   set predict;
   if H = 7.541;
run;
```

Syntax: RSREG Procedure

The following statements are available in the RSREG procedure.

PROC RSREG < *options* > **;**
MODEL *responses* **=** *independents* < / *options* > **;**
RIDGE < *options* > **;**
WEIGHT *variable* **;**
ID *variables* **;**
BY *variables* **;**

The PROC RSREG and MODEL statements are required.

The BY, ID, MODEL, RIDGE, and WEIGHT statements are described after the PROC RSREG statement, and they can appear in any order.

PROC RSREG Statement

PROC RSREG < *options* > **;**

The PROC RSREG statement invokes the RSREG procedure. Table 105.1 summarizes the *options* available in the PROC RSREG statement.

Table 105.1 PROC RSREG Statement Options

Option	Description
DATA=	Names the input SAS data set
NOPRINT	Suppresses the normal display of results
OUT=	Creates the output SAS data set
PLOTS	Controls the plots produced through ODS Graphics

The following list describes these *options*.

DATA=*SAS-data-set*
specifies the input SAS data set that contains the data to be analyzed. By default, PROC RSREG uses the most recently created SAS data set.

NOPRINT
suppresses the normal display of results when only the output data set is required.

For more information, see the description of the NOPRINT option in the MODEL and RIDGE statements.

Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, "Using the Output Delivery System," for more information.

OUT=*SAS-data-set*
creates an output SAS data set that contains statistics for each observation in the input data set. In particular, this data set contains the BY variables, the ID variables, the WEIGHT variable, the variables in the MODEL statement, and the output options requested in the MODEL statement. You must specify output statistic options in the MODEL statement; otherwise, the output data set is created but contains no observations. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For more details, see the section "OUT=SAS-data-set" on page 8772.

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

PLOTS<(*global-plot-option***)>=(***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 from around the *plot-request*. For example:

```
plots = all
plots = (diagnostics ridge surface(unpack))
plots(unpack) = surface(overlaypairs)
```

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

```
ods graphics on;
proc rsreg plots=all;
   model y=x;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 623 in Chapter 21, "Statistical Graphics Using ODS."

By default, no graphs are created; you must specify the PLOTS= option to make graphs. See Figure 105.4, Output 105.1.5, Output 105.2.3, and Output 105.2.4 for examples of the ODS graphical displays.

The following *global-plot-option* is available.

UNPACKPANELS | UNPACK
suppresses paneling. By default, multiple plots can appear in some output *panels*. Specify the UNPACK option to display each plot separately.

The following *plot-requests* are available.

ALL
produces all appropriate plots. You can specify other options with ALL; for example, to display all plots and unpack the SURFACE contours you can specify `plots=(all surface(unpack))`.

DIAGNOSTICS < (LABEL | UNPACK) >
displays a panel of summary fit diagnostic plots. The plots produced and their usage are discussed in Table 105.2.

Table 105.2 Diagnostic Plots

Diagnostic Plot	Usage
Cook's *D* statistic versus observation number	Evaluate influence of an observation on the entire parameter estimate vector
Dependent variable values versus predicted values	Evaluate adequacy of fit and detect influential observations
Externally studentized residuals (RStudent) versus leverage	Detect outliers and influential (high-leverage) observations
Externally studentized residuals versus predicted values	Evaluate adequacy of fit and detect outliers
Histogram of residuals	Confirm normality of error terms
Normal quantile plot of residuals	Confirm normality and homogeneity of error terms, and detect outliers
Residuals versus predicted values	Evaluate adequacy of fit and detect outliers
Residual-fit (RF) spread plot	side-by-side quantile plots of the centered fit and the residuals show "how much variation in the data is explained by the fit and how much remains in the residuals" (Cleveland 1993)

Observations satisfying RStudent > 2 or RStudent < –2 are called *outliers*, and observations with leverage > $2p/n$ are called *influential*, where n is the number of observations used in fitting the model and p is the number of parameters used in the model (Rawlings, Pantula, and Dickey 1998). Specifying the LABEL option labels the influential and outlying observations—the label is the first ID variable if the ID statement is specified; otherwise, it is the observation number. Note in the Cook's D plot that only observations with D exceeding $4/n$ are labeled; these are also called influential observations. The UNPACK option displays each diagnostic plot separately. See Output 105.2.3 for an example of the diagnostics panel.

FIT < (GRIDSIZE=*number*) >
plots the predicted values against a single predictor when you have only one factor or only one covariate in the model. The GRIDSIZE= option specifies the number of points at which the fitted values are computed; by default, GRIDSIZE=200.

NONE
suppresses all plots.

RESIDUALS < (UNPACK | SMOOTH) >
displays plots of residuals against each factor and covariate. The UNPACK option displays each residual plot separately. The SMOOTH option overlays a loess smooth on each residual plot; see Chapter 75, "The LOESS Procedure," for more information. See Output 105.2.4 for an example of this plot.

RIDGE < (UNPACK) >
displays the maximum and/or minimum ridge plots. This option is available only when a MAXIMUM or MINIMUM option is specified in the RIDGE statement. The UNPACK option displays the estimated response and factor level ridge plots separately. See Output 105.1.5 for an example of this plot.

SURFACE < (*surface-options*) >
displays the response surface for each response variable and each pair of factors with all other factors and covariates fixed at their means. By default a panel of contour plots is produced; see Output 105.1.5 for an example of this plot. The following *surface-options* can be specified:

3D
displays three-dimensional surface plots instead of contour plots. See Figure 105.4 for an example of this plot.

AT < *keyword* >< (*variable=value-list* | *keyword* < ...*variable=value-list* | *keyword* >) >
specifies fixed values for factors and covariates. You can specify one or more numbers in the *value-list* or one of the following *keywords*:

MIN	sets the variable to its minimum value.
MEAN	sets the variable to its mean value.
MIDRANGE	sets the variable to the middle value: $\frac{\max + \min}{2}$.
MAX	sets the variable to its maximum value.

Specifying a *keyword* immediately after AT sets the default value of all variables; for example, **AT MIN** sets all variables not displayed on an axis to their minimum values. By default, continuous variables are set to their means (**AT MEAN**) when they are not used on an axis. For example, if your model contains variables X1, X2, and X3, then specifying

AT(X1=7 9) produces a contour plot of X2 versus X3 fixing X1 = 7 and then another contour plot with X1 = 9, along with contour plots of X1 versus X2 fixing X3 at its mean, and X1 versus X3 fixing X2 at its mean.

EXTEND=*value*
extends the surface *value*-times the range of each factor in each direction, which enables you to see more of the fitted surface. For example, if factor A has range [0, 10], then specifying **EXTEND=0.1** will compute and display the surface for A in [-1, 11]. You can specify *value* ≥ 0; by default, *value* = 0.1.

FILL=PRED | SE | NONE
produces a filled contour plot for either the predicted values or the standard errors. FILL=SE is the default. If the 3D option is also specified, then the contour plot is projected onto the surface.

GRIDSIZE=*n*
creates an $n \times n$ grid of points at which the estimated values for the surface and standard errors are computed, for $n \geq 1$. By default, $n = 50$.

LINE< =PRED | SE | NONE >
produces a contour line plot for either the predicted values or the standard errors. LINE=PRED is the default. If the 3D option is also specified, then specifying LINE displays a grid on the surface, and the other LINE= specifications are ignored.

NODESIGN
suppresses the display of the design points on the contour surface plots and the overlaid contour-line plots.

OVERLAYPAIRS
produces overlaid contour line plots for all pairs of response variables in addition to the contour surface plots. See Figure 105.6 for an example of this plot.

ROTATE=*angle*
rotates the 3-D surface plots *angle* degrees, $-180 < angle < 180$. By default, *angle* = 57.

TILT=*angle*
tilts the 3-D surface plots *angle* degrees, $-180 < angle < 180$. By default, *angle* = 20.

UNPACKPANELS | UNPACK
suppresses paneling, and displays each surface plot separately.

BY Statement

BY *variables* **;**

You can specify a BY statement in PROC RSREG 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 in the RSREG 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*.

ID Statement

ID *variables* **;**

The ID statement names variables that are to be transferred to the data set created by the OUT= option in the PROC RSREG statement.

MODEL Statement

MODEL *responses* **=** *independents* < / *options* > **;**

In the MODEL statement, you specify the response (dependent) variables followed by an equal sign and then the independent variables, some of which can be covariates.

Table 105.3 summarizes the *options* available in the MODEL statement. The output statistics specify which statistics are output to the OUT= data set. If none of the output statistics are specified, the data set is created but contains no observations. The keywords for the output statistics become values of the special variable _TYPE_ in the output data set.

Table 105.3 MODEL Statement Options

Option	Description
BYOUT	Uses only the first BY group to estimate the model
COVAR=	Declares variables to be simple linear regressors
LACKFIT	Performs a lack-of-fit test
NOCODE	Performs the canonical and ridge analyses using original values
PRESS	Displays the predicted residual sum of squares (PRESS) statistic
Suppress Displayed Output	
NOANOVA	Suppresses the analysis of variance and parameter estimates
NOOPTIMAL	Suppresses the canonical analysis
NOPRINT	Suppresses both the analysis of variance and the canonical analysis

Table 105.3 *continued*

Option	Description
Output Statistics	
ACTUAL	Includes observed response values
PREDICT	Includes values predicted by the model
RESIDUAL	Includes the residuals
L95	Includes the lower bound of a 95% confidence interval for an individual predicted value
U95	Includes the upper bound of a 95% confidence interval for an individual predicted value
L95M	Includes the lower bound of a 95% confidence interval for the expected value of the dependent variable
U95M	Includes the upper bound of a 95% confidence interval for the expected value of the dependent variable
D	Includes Cook's *D* influence statistic

The following list describes these *options* in alphabetical order.

ACTUAL
specifies that the observed response values from the input data set be written to the output data set.

BYOUT
uses only the first BY group to estimate the model. Subsequent BY groups have scoring statistics computed in the output data set only. The BYOUT option is used only when a BY statement is specified.

COVAR=*n*
declares that the first *n* variables on the right side of the model are simple linear regressors (covariates) and not factors in the quadratic response surface. By default, PROC RSREG forms quadratic and crossproduct effects for all regressor variables in the MODEL statement.

See the section "Handling Covariates" on page 8770 for more details and Example 105.2 for an example that uses covariates.

D
specifies that Cook's *D* influence statistic be written to the output data set.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

LACKFIT
performs a lack-of-fit test.

See Draper and Smith (1981) for a discussion of lack-of-fit tests.

L95
specifies that the lower bound of a 95% confidence interval for an individual predicted value be written to the output data set. The variance used in calculating this bound is a function of both the mean square error and the variance of the parameter estimates.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

L95M
specifies that the lower bound of a 95% confidence interval for the expected value of the dependent variable be written to the output data set. The variance used in calculating this bound is a function of the variance of the parameter estimates.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

NOANOVA
NOAOV
suppresses the display of the analysis of variance and parameter estimates from the model fit.

NOCODE
performs the canonical and ridge analyses with the parameter estimates derived from fitting the response to the original values of the factor variables, rather than their coded values (see the section "Coding the Factor Variables" on page 8767 for more details). Use this option if the data are already stored in a coded form.

NOOPTIMAL
NOOPT
suppresses the display of the canonical analysis for the quadratic response surface.

NOPRINT
suppresses the display of both the analysis of variance and the canonical analysis.

PREDICT
specifies that the values predicted by the model be written to the output data set.

PRESS
computes and displays the predicted residual sum of squares (PRESS) statistic for each dependent variable in the model. The PRESS statistic is added to the summary information at the beginning of the analysis of variance, so if the NOANOVA or NOPRINT option is specified, then the PRESS option has no effect.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

RESIDUAL
specifies that the residuals, calculated as ACTUAL – PREDICTED, be written to the output data set.

U95
specifies that the upper bound of a 95% confidence interval for an individual predicted value be written to the output data set. The variance used in calculating this bound is a function of both the mean square error and the variance of the parameter estimates.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

U95M
specifies that the upper bound of a 95% confidence interval for the expected value of the dependent variable be written to the output data set. The variance used in calculating this bound is a function of the variance of the parameter estimates.

See Chapter 4, "Introduction to Regression Procedures," for details and formulas.

RIDGE Statement

RIDGE < *options* > **;**

A RIDGE statement computes the ridge of optimum response. The ridge starts at a given point $\mathbf{x}_0$, and the point on the ridge at radius r from $\mathbf{x}_0$ is the collection of factor settings that optimizes the predicted response at this radius. You can think of the ridge as climbing or falling as fast as possible on the surface of predicted response. Thus, the ridge analysis can be used as a tool to help interpret an existing response surface or to indicate the direction in which further experimentation should be performed.

The default starting point, $\mathbf{x}_0$, has each coordinate equal to the point midway between the highest and lowest values of the factor in the design. The default radii at which the ridge is computed are 0, 0.1, . . ., 0.9, 1. If the ridge analysis is based on the response surface fit to coded values for the factor variables (see the section "Coding the Factor Variables" on page 8767 for details), then this results in a ridge that starts at the point with a coded zero value for each coordinate and extends toward, but not beyond, the edge of the range of experimentation. Alternatively, both the center point of the ridge and the radii at which it is to be computed can be specified.

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

CENTER=*uncoded-factor-values*
gives the coordinates of the point $\mathbf{x}_0$ from which to begin the ridge. The coordinates should be given in the original (uncoded) factor variable values and should be separated by commas. There must be as many coordinates specified as there are factors in the model, and the order of the coordinates must be the same as that used in the MODEL statement. This starting point should be well inside the range of experimentation. The default sets each coordinate equal to the value midway between the highest and lowest values for the associated factor.

MAXIMUM
MAX
computes the ridge of maximum response. Both the MIN and MAX options can be specified; at least one must be specified.

MINIMUM
MIN
computes the ridge of minimum response. Both the MIN and MAX options can be specified; at least one must be specified.

NOPRINT
suppresses the display of the ridge analysis when only an output data set is required.

OUTR=*SAS-data-set*
creates an output SAS data set containing the computed optimum ridge.

For details, see the section "OUTR=SAS-data-set" on page 8772.

RADIUS=*coded-radii*
gives the distances from the ridge starting point at which to compute the optima. The values in the list represent distances between coded points. The list can take any of the following forms or can be composed of mixtures of them:

$m_1, m_2, \ldots, m_n$	specifies several values.
m TO n	specifies a sequence where m equals the starting value, n equals the ending value, and the increment equals 1.
m TO n BY i	specifies a sequence where m equals the starting value, n equals the ending value, and i equals the increment.

Mixtures of the preceding forms should be separated by commas. The default list runs from 0 to 1 by increments of 0.1. The following are examples of valid lists.

```
radius=0 to 5 by .5;
radius=0, .2, .25, .3, .5 to 1.0 by .1;
```

WEIGHT Statement

WEIGHT *variable* **;**

When a WEIGHT statement is specified, a weighted residual sum of squares

$$\sum_i w_i (y_i - \hat{y}_i)^2$$

is minimized, where w_i is the value of the variable specified in the WEIGHT statement, y_i is the observed value of the response variable, and $\hat{y}_i$ is the predicted value of the response variable.

The observation is used in the analysis only if the value of the WEIGHT statement variable is greater than zero. The WEIGHT statement has no effect on degrees of freedom or number of observations. If the weights for the observations are proportional to the reciprocals of the error variances, then the weighted least squares estimates are best linear unbiased estimators (BLUE).

Details: RSREG Procedure

Introduction to Response Surface Experiments

Many industrial experiments are conducted to discover which values of given factor variables optimize a response. If each factor is measured at three or more values, a quadratic response surface can be estimated by least squares regression. The predicted optimal value can be found from the estimated surface if the surface is shaped like a simple hill or valley. If the estimated surface is more complicated, or if the predicted optimum is far from the region of experimentation, then the shape of the surface can be analyzed to indicate the directions in which new experiments should be performed.

Suppose that a response variable y is measured at combinations of values of two factor variables, x_1 and x_2. The quadratic response surface model for this variable is written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + \epsilon$$

The steps in the analysis for such data are as follows:

1. model fitting and analysis of variance, including lack-of-fit testing, to estimate parameters
2. canonical analysis to investigate the shape of the predicted response surface
3. ridge analysis to search for the region of optimum response

Model Fitting and Analysis of Variance

The first task in analyzing the response surface is to estimate the parameters of the model by least squares regression and to obtain information about the fit in the form of an analysis of variance. The estimated surface is typically curved: a *hill* with the peak occurring at the unique estimated point of maximum response, a *valley,* or a *saddle surface* with no unique minimum or maximum. Use the results of this phase of the analysis to answer the following questions:

- What is the contribution of each type of effect—linear, quadratic, and crossproduct—to the statistical fit? The ANOVA table with sources labeled "Regression" addresses this question.
- What part of the residual error is due to lack of fit? Does the quadratic response model adequately represent the true response surface? If you specify the LACKFIT option in the MODEL statement, then the ANOVA table with sources labeled "Residual" addresses this question. See the section "Lack-of-Fit Test" on page 8765 for details.
- What is the contribution of each factor variable to the statistical fit? Can the response be predicted accurately if the variable is removed? The ANOVA table with sources labeled "Factor" addresses this question.
- What are the predicted responses for a grid of factor values? (See the section "Plotting the Surface" on page 8767 and the section "Searching for Multiple Response Conditions" on page 8768.)

Lack-of-Fit Test

The lack-of-fit test compares the variation around the model with *pure* variation within replicated observations. This measures the adequacy of the quadratic response surface model. In particular, if there are n_i replicated observations $Y_{i1}, \ldots, Y_{in_i}$ of the response all at the same values $\mathbf{x}_i$ of the factors, then you can predict the true response at $\mathbf{x}_i$ either by using the predicted value $\hat{Y}_i$ based on the model or by using the mean $\bar{Y}_i$ of the replicated values. The lack-of-fit test decomposes the residual error into a component due to the variation of the replications around their mean value (the *pure* error) and a component due to the variation of the mean values around the model prediction (the *bias* error):

$$\sum_i \sum_{j=1}^{n_i} \left(Y_{ij} - \hat{Y}_i\right)^2 = \sum_i \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_i\right)^2 + \sum_i n_i \left(\bar{Y}_i - \hat{Y}_i\right)^2$$

If the model is adequate, then both components estimate the nominal level of error; however, if the bias component of error is much larger than the pure error, then this constitutes evidence that there is significant lack of fit.

If some observations in your design are replicated, you can test for lack of fit by specifying the LACKFIT option in the MODEL statement. Note that, since all other tests use total error rather than pure error, you

might want to hand-calculate the tests with respect to pure error if the lack of fit is significant. On the other hand, significant lack of fit indicates that the quadratic model is inadequate, so if this is a problem you can also try to refine the model, possibly by using PROC GLM for general polynomial modeling; see Chapter 50, "The GLM Procedure," for more information. Example 105.1 illustrates the use of the LACKFIT option.

Canonical Analysis

The second task in analyzing the response surface is to examine the overall shape of the curve and determine whether the estimated stationary point is a maximum, a minimum, or a saddle point. The canonical analysis can be used to answer the following questions:

- Is the surface shaped like a hill, a valley, or a saddle, or is it flat?
- If there is a unique optimum combination of factor values, where is it?
- To which factor or factors are the predicted responses most sensitive?

The eigenvalues and eigenvectors in the matrix of second-order parameters characterize the shape of the response surface. The eigenvectors point in the directions of principal orientation for the surface, and the signs and magnitudes of the associated eigenvalues give the shape of the surface in these directions. Positive eigenvalues indicate directions of upward curvature, and negative eigenvalues indicate directions of downward curvature. The larger an eigenvalue is in absolute value, the more pronounced is the curvature of the response surface in the associated direction. Often, all the coefficients of an eigenvector except for one are relatively small, indicating that the vector points roughly along the axis associated with the factor corresponding to the single large coefficient. In this case, the canonical analysis can be used to determine the relative sensitivity of the predicted response surface to variations in that factor. (See the section "Getting Started: RSREG Procedure" on page 8751 for an example.)

Ridge Analysis

If the estimated surface is found to have a simple optimum well within the range of experimentation, the analysis performed by the preceding two steps might be sufficient. In more complicated situations, further search for the region of optimum response is required. The method of ridge analysis computes the estimated ridge of optimum response for increasing radii from the center of the original design. The ridge analysis answers the following question:

- If there is not a unique optimum of the response surface within the range of experimentation, in which direction should further searching be done in order to locate the optimum?

You can use the RIDGE statement to compute the ridge of maximum or minimum response.

Coding the Factor Variables

For the results of the canonical and ridge analyses to be interpretable, the values of different factor variables should be comparable. This is because the canonical and ridge analyses of the response surface are not invariant with respect to differences in scale and location of the factor variables. The analysis of variance is not affected by these changes. Although the actual predicted surface does not change, its parameterization does. The usual solution to this problem is to code each factor variable so that its minimum in the experiment is –1 and its maximum is 1 and to carry through the analysis with the coded values instead of the original ones. This practice has the added benefit of making 1 a reasonable boundary radius for the ridge analysis since 1 represents approximately the edge of the experimental region. By default, PROC RSREG computes the linear transformation to perform this coding as the data are initially read in, and the canonical and ridge analyses are performed on the model fit to the coded data. The actual form of the coding operation for each value of a variable is

$$\textit{coded value} = (\textit{original value} - M)/S$$

where M is the average of the highest and lowest values for the variable in the design and S is half their difference.

Missing Values

If an observation has missing data for any of the variables used by the procedure, then that observation is not used in the estimation process. If one or more response variables are missing, but no factor or covariate variables are missing, then predicted values and confidence limits are computed for the output data set, but the residual and Cook's D statistic are missing.

Plotting the Surface

Specifying the PLOTS=SURFACE option in the PROC RSREG statement displays contour plots for all pairs of factors in the model (see Example 105.1), while specifying the PLOTS=SURFACE(3D) option displays a three-dimensional surface as shown in Figure 105.4.

You can also generate predicted values for a grid of points with the PREDICT option (see the section "Getting Started: RSREG Procedure" on page 8751 for an example) and then use these values to create a contour plot or a three-dimensional plot of the response surface over a two-dimensional grid. Any two factor variables can be chosen to form the grid for the plot. Several plots can be generated by using different pairs of factor variables.

Searching for Multiple Response Conditions

Suppose you have the following data with two factors and three responses, and you want to find the factor setting that produces responses in a certain region:

```
data a;
   input x1 x2 y1 y2 y3;
   datalines;
-1      -1         1.8 1.940  3.6398
-1       1         2.6 1.843  4.9123
 1      -1         5.4 1.063  6.0128
 1       1         0.7 1.639  2.3629
 0       0         8.5 0.134  9.0910
 0       0         3.0 0.545  3.7349
 0       0         9.8 0.453 10.4412
 0       0         4.1 1.117  5.0042
 0       0         4.8 1.690  6.6245
 0       0         5.9 1.165  6.9420
 0       0         7.3 1.013  8.7442
 0       0         9.3 1.179 10.2762
 1.4142  0         3.9 0.945  5.0245
-1.4142  0         1.7 0.333  2.4041
 0       1.4142    3.0 1.869  5.2695
 0      -1.4142    5.7 0.099  5.4346
;
```

You want to find the values of x1 and x2 that maximize y1 subject to y2<2 and y3<y2+y1. The exact answer is not easy to obtain analytically, but you can obtain a practically feasible solution by checking conditions across a grid of values in the range of interest. First, append a grid of factor values to the observed data, with missing values for the responses:

```
data b;
   set a end=eof;
   output;
   if eof then do;
      y1=.;
      y2=.;
      y3=.;
      do x1=-2 to 2 by .1;
         do x2=-2 to 2 by .1;
            output;
         end;
      end;
   end;
run;
```

Next, use PROC RSREG to fit a response surface model to the data and to compute predicted values for both the observed data and the grid, putting the predicted values in a data set c:

```
proc rsreg data=b out=c;
   model y1 y2 y3=x1 x2 / predict;
run;
```

Finally, find the subset of predicted values that satisfy the constraints, sort by the unconstrained variable, and display the top five predictions:

```
data d;
   set c;
   if y2<2;
   if y3<y2+y1;

proc sort data=d;
   by descending y1;
run;

data d; set d;
   if (_n_ <= 5);
proc print;
run;
```

The results are displayed in Figure 105.5. They indicate that optimal values of the factors are around 0.3 for x1 and around –0.5 for x2.

Figure 105.5 Top Five Predictions

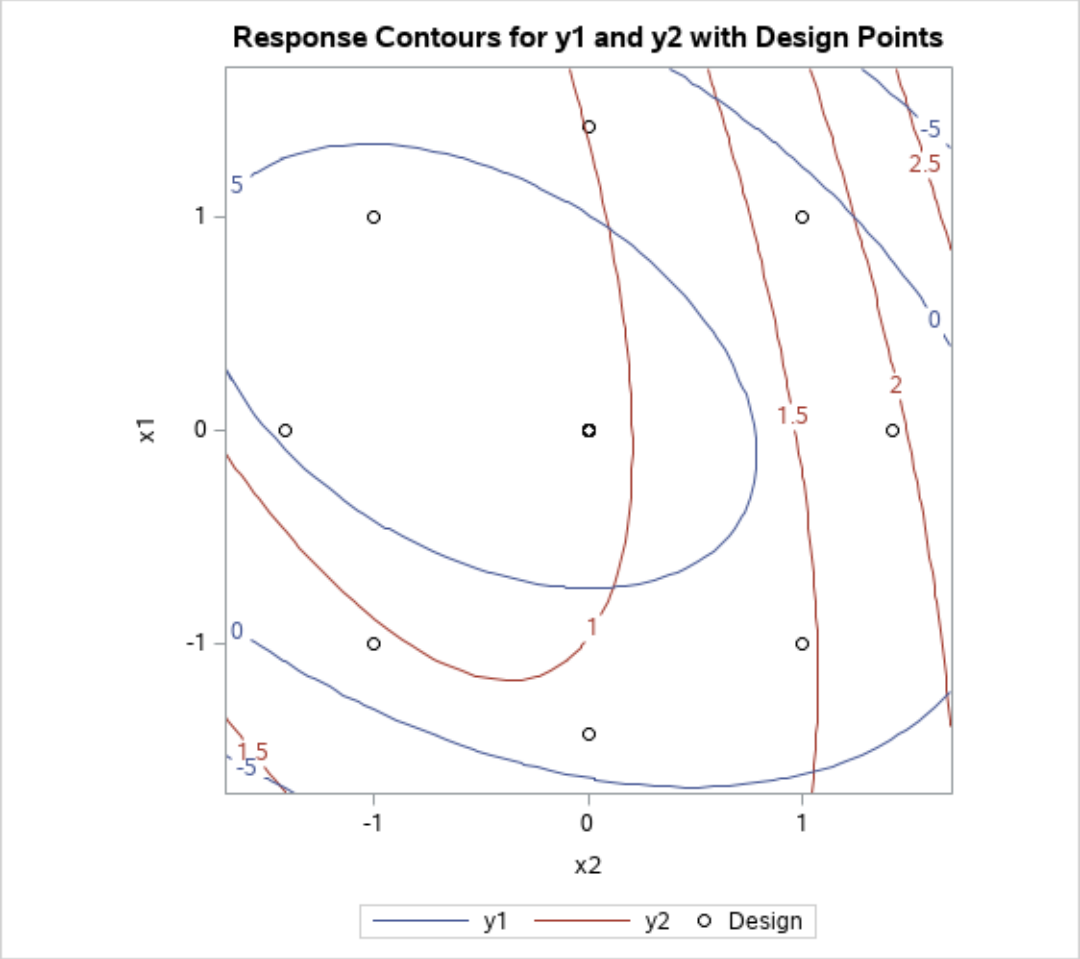
Obs	x1	x2	_TYPE_	y1	y2	y3
1	0.3	-0.5	PREDICT	6.92570	0.75784	7.60471
2	0.3	-0.6	PREDICT	6.91424	0.74174	7.54194
3	0.3	-0.4	PREDICT	6.91003	0.77870	7.64341
4	0.4	-0.6	PREDICT	6.90769	0.73357	7.51836
5	0.4	-0.5	PREDICT	6.90540	0.75135	7.56883

If you are also interested in simultaneously optimizing y1 and y2, you can specify the following statements to make a visual comparison of the two response surfaces by overlaying their contour plots:

```
ods graphics on;
proc rsreg data=a plots=surface(overlaypairs);
   model y1 y2=x1 x2;
run;
ods graphics off;
```

Figure 105.6 shows that you have to make some compromises in any attempt to maximize both y1 and y2; however, you might be able to maximize y1 while minimizing y2.

Figure 105.6 Overlaid Line Contours of Predicted Responses



Handling Covariates

Covariate regressors are added to a response surface model because they are believed to account for a sizable yet relatively uninteresting portion of the variation in the data. What the experimenter is really interested in is the response corrected for the effect of the covariates. A common example is the block effect in a block design. In the canonical and ridge analyses of a response surface, which estimate responses at hypothetical levels of the factor variables, the actual value of the predicted response is computed by using the average values of the covariates. The estimated response values do optimize the estimated surface of the response corrected for covariates, but true prediction of the response requires actual values for the covariates. You can use the COVAR= option in the MODEL statement to include covariates in the response surface model. Example 105.2 illustrates the use of this option.

Computational Method

Canonical Analysis

For each response variable, the model can be written in the form

$$y_i = \mathbf{x}_i' \mathbf{A} \mathbf{x}_i + \mathbf{b}' \mathbf{x}_i + \mathbf{c}' \mathbf{z}_i + \epsilon_i$$

where

y_i is the ith observation of the response variable.

$\mathbf{x}_i$ $= (x_{i1}, x_{i2}, \ldots, x_{ik})'$ are the k factor variables for the ith observation.

$\mathbf{z}_i$ $= (z_{i1}, z_{i2}, \ldots, z_{iL})'$ are the L covariates, including the intercept term.

$\mathbf{A}$ is the $k \times k$ symmetrized matrix of quadratic parameters, with diagonal elements equal to the coefficients of the pure quadratic terms in the model and off-diagonal elements equal to half the coefficient of the corresponding crossproduct.

$\mathbf{b}$ is the $k \times 1$ vector of linear parameters.

$\mathbf{c}$ is the $L \times 1$ vector of covariate parameters, one of which is the intercept.

ϵ_i is the error associated with the ith observation. Tests performed by PROC RSREG assume that errors are independently and normally distributed with mean zero and variance σ^2.

The parameters in $\mathbf{A}$, $\mathbf{b}$, and $\mathbf{c}$ are estimated by least squares. To optimize $\mathbf{y}$ with respect to $\mathbf{x}$, take partial derivatives, set them to zero, and solve:

$$\frac{\partial y}{\partial \mathbf{x}} = 2\mathbf{x}'\mathbf{A} + \mathbf{b}' = \mathbf{0} \quad \Longrightarrow \quad \mathbf{x} = -\frac{1}{2}\mathbf{A}^{-1}\mathbf{b}$$

You can determine if the solution is a maximum or minimum by looking at the eigenvalues of $\mathbf{A}$:

If the eigenvalues...	then the solution is...
are all negative	a maximum
are all positive	a minimum
have mixed signs	a saddle point
contain zeros	in a flat area

Ridge Analysis

If the largest eigenvalue is positive, its eigenvector gives the direction of steepest ascent from the stationary point; if the largest eigenvalue is negative, its eigenvector gives the direction of steepest descent. The eigenvectors corresponding to small or zero eigenvalues point in directions of relative flatness.

The point on the optimum response ridge at a given radius R from the ridge origin is found by optimizing

$$(\mathbf{x}_0 + \mathbf{d})'\mathbf{A}(\mathbf{x}_0 + \mathbf{d}) + \mathbf{b}'(\mathbf{x}_0 + \mathbf{d})$$

over $\mathbf{d}$ satisfying $\mathbf{d}'\mathbf{d} = R^2$, where $\mathbf{x}_0$ is the $k \times 1$ vector containing the ridge origin and $\mathbf{A}$ and $\mathbf{b}$ are as previously discussed. By the method of Lagrange multipliers, the optimal $\mathbf{d}$ has the form

$$\mathbf{d} = -(\mathbf{A} - \mu\mathbf{I})^{-1}(\mathbf{A}\mathbf{x}_0 + 0.5\mathbf{b})$$

where $\mathbf{I}$ is the $k \times k$ identity matrix and μ is chosen so that $\mathbf{d}'\mathbf{d} = R^2$. There can be several values of μ that satisfy this constraint; the correct one depends on which sort of response ridge is of interest. If you are searching for the ridge of maximum response, then the appropriate μ is the unique one that satisfies the constraint and is greater than all the eigenvalues of $\mathbf{A}$. Similarly, the appropriate μ for the ridge of minimum response satisfies the constraint and is less than all the eigenvalues of $\mathbf{A}$. (See Myers and Montgomery (1995) for details.)

Output Data Sets

OUT=SAS-data-set

An output data set containing statistics requested with options in the MODEL statement for each observation in the input data set is created whenever the OUT= option is specified in the PROC RSREG statement. The data set contains the following variables:

- the BY variables
- the ID variables
- the WEIGHT variable
- the independent variables in the MODEL statement
- the variable _TYPE_, which identifies the observation type in the output data set. _TYPE_ is a character variable with a length of eight, and it takes on the values 'ACTUAL', 'PREDICT', 'RESIDUAL', 'U95M', 'L95M', 'U95', 'L95', and 'D', corresponding to the options specified.
- the response variables containing special output values identified by the _TYPE_ variable

All confidence limits use the two-tailed Student's t value.

OUTR=SAS-data-set

An output data set containing the optimum response ridge is created when the OUTR= option is specified in the RIDGE statement. The data set contains the following variables:

- the current values of the BY variables
- a character variable _DEPVAR_ containing the name of the dependent variable
- a character variable _TYPE_ identifying the type of ridge being computed, MINIMUM or MAXIMUM. If both MAXIMUM and MINIMUM are specified, the data set contains observations for the minimum ridge followed by observations for the maximum ridge.
- a numeric variable _RADIUS_ giving the distance from the ridge starting point
- the values of the model factors at the estimated optimum point at distance _RADIUS_ from the ridge starting point

- a numeric variable _PRED_, which is the estimated expected value of the dependent variable at the optimum
- a numeric variable _STDERR_, which is the standard error of the estimated expected value

Displayed Output

All estimates and hypothesis tests assume that the model is correctly specified and the errors are distributed according to classical statistical assumptions.

The output displayed by PROC RSREG includes the following.

Estimation and Analysis of Variance

- The actual form of the coding operation for each value of a variable is

$$coded\ value = \frac{1}{S}(original\ value - M)$$

  where M is the average of the highest and lowest values for the variable in the design and S is half their difference. The Subtracted off column contains the M values for this formula for each factor variable, and S is found in the Divided by column.

- The summary table for the response variable contains the following information.
  - "Response Mean" is the mean of the response variable in the sample. When a WEIGHT statement is specified, the mean $\bar{y}$ is calculated by

$$\bar{y} = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

  - "Root MSE" estimates the standard deviation of the response variable and is calculated as the square root of the "Total Error" mean square.
  - The "R-Square" value is R^2, or the coefficient of determination. R^2 measures the proportion of the variation in the response that is attributed to the model rather than to random error.
  - The "Coefficient of Variation" is 100 times the ratio of the "Root MSE" to the "Response Mean."
- A table analyzing the significance of the terms of the regression is displayed. Terms are brought into the regression in four steps: (1) the "Intercept" and any covariates in the model, (2) "Linear" terms like X1 and X2, (3) pure "Quadratic" terms like X1*X1 or X2*X2, and (4) "Crossproduct" terms like X1*X2. The table displays the following information:
  - the degrees of freedom in the DF column, which should be the same as the number of corresponding parameters unless one or more of the parameters are not estimable
  - Type I Sum of Squares, also called the sequential sums of squares, which measures the reduction in the error sum of squares as sets of terms (Linear, Quadratic, and so forth) are added to the model

  - R-Square, which measures the portion of total R^2 contributed as each set of terms (Linear, Quadratic, and so forth) is added to the model
  - F Value, which tests the null hypothesis that all parameters in the term are zero by using the Total Error mean square as the denominator. This is a test of a Type I hypothesis, containing the usual F test numerator, conditional on the effects of subsequent variables not being in the model.
  - Pr > F, which is the significance value or probability of obtaining at least as great an F ratio given that the null hypothesis is true.

- The Sum of Squares column partitions the "Total Error" into "Lack of Fit" and "Pure Error." When "Lack of Fit" is significant, there is variation around the model other than random error (such as cubic effects of the factor variables).
  - The "Total Error" Mean Square estimates σ^2, the variance.
  - F Value tests the null hypothesis that the variation is adequately described by random error.

- A table containing the parameter estimates from the model is displayed.
  - The Estimate column contains the parameter estimates based on the *uncoded* values of the factor variables. If an effect is a linear combination of previous effects, the parameter for the effect is not estimable. When this happens, the degrees of freedom are zero, the parameter estimate is set to zero, and estimates and tests on other parameters are conditional on this parameter being zero.
  - The Standard Error column contains the estimated standard deviations of the parameter estimates based on *uncoded* data.
  - The t Value column contains t values of a test of the null hypothesis that the true parameter is zero when the *uncoded* values of the factor variables are used.
  - The Pr > |T| column gives the significance value or probability of a greater absolute t ratio given that the true parameter is zero.
  - The Parameter Estimate from Coded Data column contains the parameter estimates based on the *coded* values of the factor variables. These are the estimates used in the subsequent canonical and ridge analyses.

- The sum of squares are partitioned by the factors in the model, and an analysis table is displayed. The test on a factor is a joint test on all the parameters involving that factor. For example, the test for the factor X1 tests the null hypothesis that the true parameters for X1, X1*X1, and X1*X2 are all zero.

Canonical Analysis

- The Critical Value columns contain the values of the factor variables that correspond to the stationary point of the fitted response surface. The critical values can be at a minimum, maximum, or saddle point.

- The eigenvalues and eigenvectors are from the matrix of quadratic parameter estimates based on the coded data. They characterize the shape of the response surface.

Ridge Analysis

- The Coded Radius column contains the distance from the coded version of the associated point to the coded version of the origin of the ridge. The origin is given by the point at radius zero.
- The Estimated Response column contains the estimated value of the response variable at the associated point. The standard error of this estimate is also given. This quantity is useful for assessing the relative credibility of the prediction at a given radius. Typically, this standard error increases rapidly as the ridge moves up to and beyond the design perimeter, reflecting the inherent difficulty of making predictions beyond the range of experimentation.
- The Uncoded Factor Values columns contain the values of the uncoded factor variables that give the optimum response at this radius from the ridge origin.

ODS Table Names

PROC RSREG 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 Table 105.4. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

Table 105.4 ODS Tables Produced by PROC RSREG

ODS Table Name	Description	Statement
Coding	Coding coefficients for the independent variables	default
ErrorANOVA	Error analysis of variance	default
FactorANOVA	Factor analysis of variance	default
FitStatistics	Overall statistics for fit	default
ModelANOVA	Model analysis of variance	default
ParameterEstimates	Estimated linear parameters	default
Ridge	Ridge analysis for optimum response	RIDGE
Spectral	Spectral analysis	default
StationaryPoint	Stationary point of response surface	default

ODS Graphics

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

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 623 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 622 in Chapter 21, "Statistical Graphics Using ODS."

PROC RSREG assigns a name to each graph it creates using ODS. The names are listed in Table 105.5. You can use these names to reference the graphs when using ODS. You must also specify the PLOTS= option and any other options indicated in Table 105.5.

Table 105.5 Graphs Produced by PROC RSREG

ODS Graph Name	Plot Description	PLOTS= Option
FitPlot	Fit plot for 1 predictor	FIT
DiagnosticsPanel	Panel of fit diagnostics	DIAGNOSTICS
CooksDPlot	Cook's *D* plot	DIAGNOSTICS(UNPACK)
ObservedByPredicted	Observed by predicted	DIAGNOSTICS(UNPACK)
QQPlot	Residual Q-Q plot	DIAGNOSTICS(UNPACK)
ResidualByPredicted	Residual by predicted values	DIAGNOSTICS(UNPACK)
ResidualHistogram	Residual histogram	DIAGNOSTICS(UNPACK)
RFPlot	RF plot	DIAGNOSTICS(UNPACK)
RStudentByPredicted	Studentized residuals by predicted	DIAGNOSTICS(UNPACK)
RStudentByLeverage	RStudent by hat diagonals	DIAGNOSTICS(UNPACK)
ResidualPlots	Panel of residuals by predictors	RESIDUALS
	Residuals by predictors	RESIDUALS(UNPACK)
RidgePlots	Panel of ridge plot and factors	RIDGE (with RIDGE MAX or MIN)
	Ridge plot	RIDGE(UNPACK) (with RIDGE MAX or MIN)
	Ridge factors	RIDGE(UNPACK) (with RIDGE MAX or MIN)
Contour	Panel of contour plots	SURFACE
	Contour plots	SURFACE(UNPACK)
Surface	Panel of 3-D surface plots	SURFACE(3D)
	3-D surface plots	SURFACE(3D UNPACK)
ContourOverlay	Panel of overlaid line-contour plots	SURFACE(OVERLAYPAIRS)
	Overlaid line-contour plots	SURFACE(OVERLAYPAIRS UNPACK)

Examples: RSREG Procedure

Example 105.1: A Saddle Surface Response Using Ridge Analysis

Myers (1976) analyzes an experiment reported by Frankel (1961) aimed at maximizing the yield of mercaptobenzothiazole (MBT) by varying processing time and temperature. Myers (1976) uses a two-factor model in which the estimated surface does not have a unique optimum. A ridge analysis is used to determine the region in which the optimum lies. The objective is to find the settings of time and temperature in the processing of a chemical that maximize the yield. The following statements produce Output 105.1.1 through Output 105.1.5:

```
data d;
   input Time Temp MBT;
   label Time = "Reaction Time (Hours)"
         Temp = "Temperature (Degrees Centigrade)"
         MBT  = "Percent Yield Mercaptobenzothiazole";
   datalines;
 4.0   250   83.8
20.0   250   81.7
12.0   250   82.4
12.0   250   82.9
12.0   220   84.7
12.0   280   57.9
12.0   250   81.2
 6.3   229   81.3
 6.3   271   83.1
17.7   229   85.3
17.7   271   72.7
 4.0   250   82.0
;

ods graphics on;
proc rsreg data=d plots=(ridge surface);
   model MBT=Time Temp / lackfit;
   ridge max;
run;
ods graphics off;
```

Output 105.1.1 displays the coding coefficients for the transformation of the independent variables to lie between –1 and 1 and some simple statistics for the response variable.

Output 105.1.1 Coding and Response Variable Information

The RSREG Procedure

Coding Coefficients for the Independent Variables		
Factor	Subtracted off	Divided by
Time	12.000000	8.000000
Temp	250.000000	30.000000

Output 105.1.1 *continued*

Response Surface for Variable MBT: Percent Yield Mercaptobenzothiazole	
Response Mean	79.916667
Root MSE	4.615964
R-Square	0.8003
Coefficient of Variation	5.7760

Output 105.1.2 shows that the lack of fit for the model is highly significant. Since the quadratic model does not fit the data very well, firm statements about the underlying process should not be based only on the current analysis. Note from the analysis of variance for the model that the test for the time factor is not significant. If further experimentation is undertaken, it might be best to fix Time at a moderate to high value and to concentrate on the effect of temperature. In the actual experiment discussed here, extra runs were made that confirmed the results of the following analysis.

Output 105.1.2 Analyses of Variance

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Linear	2	313.585803	0.4899	7.36	0.0243
Quadratic	2	146.768144	0.2293	3.44	0.1009
Crossproduct	1	51.840000	0.0810	2.43	0.1698
Total Model	5	512.193947	0.8003	4.81	0.0410

Residual	DF	Sum of Squares	Mean Square	F Value	Pr > F
Lack of Fit	3	124.696053	41.565351	39.63	0.0065
Pure Error	3	3.146667	1.048889		
Total Error	6	127.842720	21.307120		

Parameter	DF	Estimate	Standard Error	t Value	Pr > |t|	Parameter Estimate from Coded Data
Intercept	1	-545.867976	277.145373	-1.97	0.0964	82.173110
Time	1	6.872863	5.004928	1.37	0.2188	-1.014287
Temp	1	4.989743	2.165839	2.30	0.0608	-8.676768
Time*Time	1	0.021631	0.056784	0.38	0.7164	1.384394
Temp*Time	1	-0.030075	0.019281	-1.56	0.1698	-7.218045
Temp*Temp	1	-0.009836	0.004304	-2.29	0.0623	-8.852519

Factor	DF	Sum of Squares	Mean Square	F Value	Pr > F	Label
Time	3	61.290957	20.430319	0.96	0.4704	Reaction Time (Hours)
Temp	3	461.250925	153.750308	7.22	0.0205	Temperature (Degrees Centigrade)

The canonical analysis (Output 105.1.3) indicates that the predicted response surface is shaped like a saddle. The eigenvalue of 2.5 shows that the valley orientation of the saddle is less curved than the hill orientation, with an eigenvalue of –9.99. The coefficients of the associated eigenvectors show that the valley is more aligned with Time and the hill with Temp. Because the canonical analysis resulted in a saddle point, the estimated surface does not have a unique optimum.

Output 105.1.3 Canonical Analysis

	Critical Value		
Factor	**Coded**	**Uncoded**	**Label**
Time	-0.441758	8.465935	Reaction Time (Hours)
Temp	-0.309976	240.700718	Temperature (Degrees Centigrade)
Predicted value at stationary point: 83.741940			

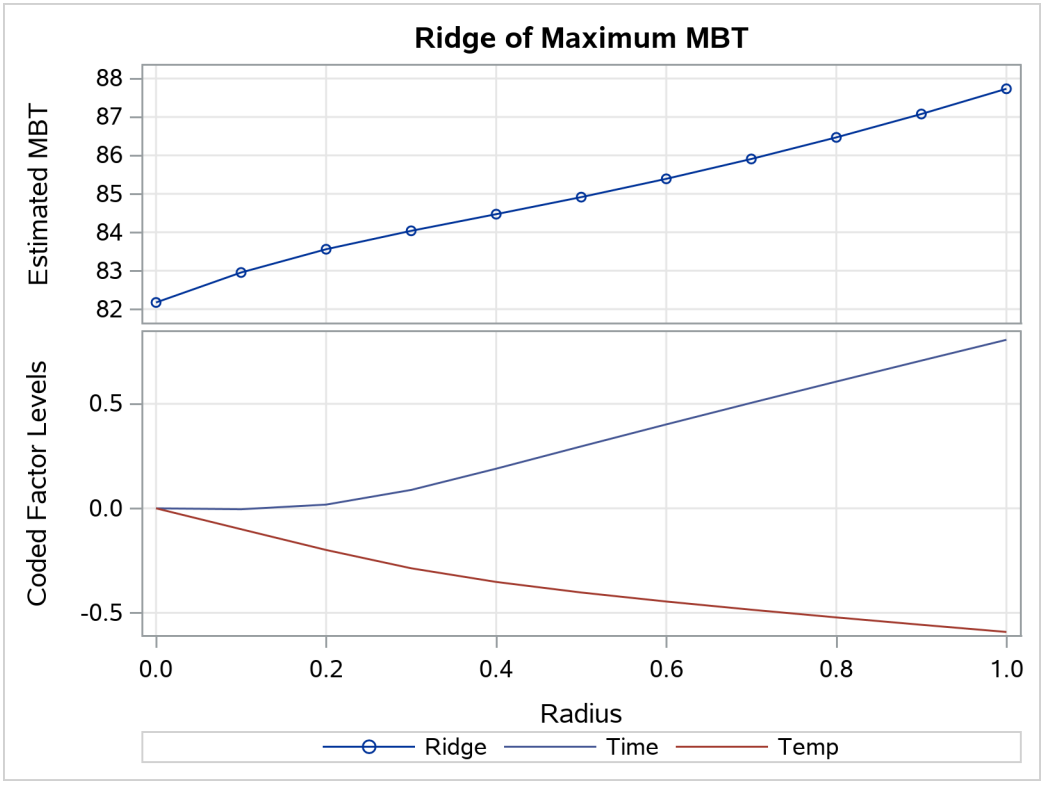
	Eigenvectors	
Eigenvalues	**Time**	**Temp**
2.528816	0.953223	-0.302267
-9.996940	0.302267	0.953223
Stationary point is a saddle point.		

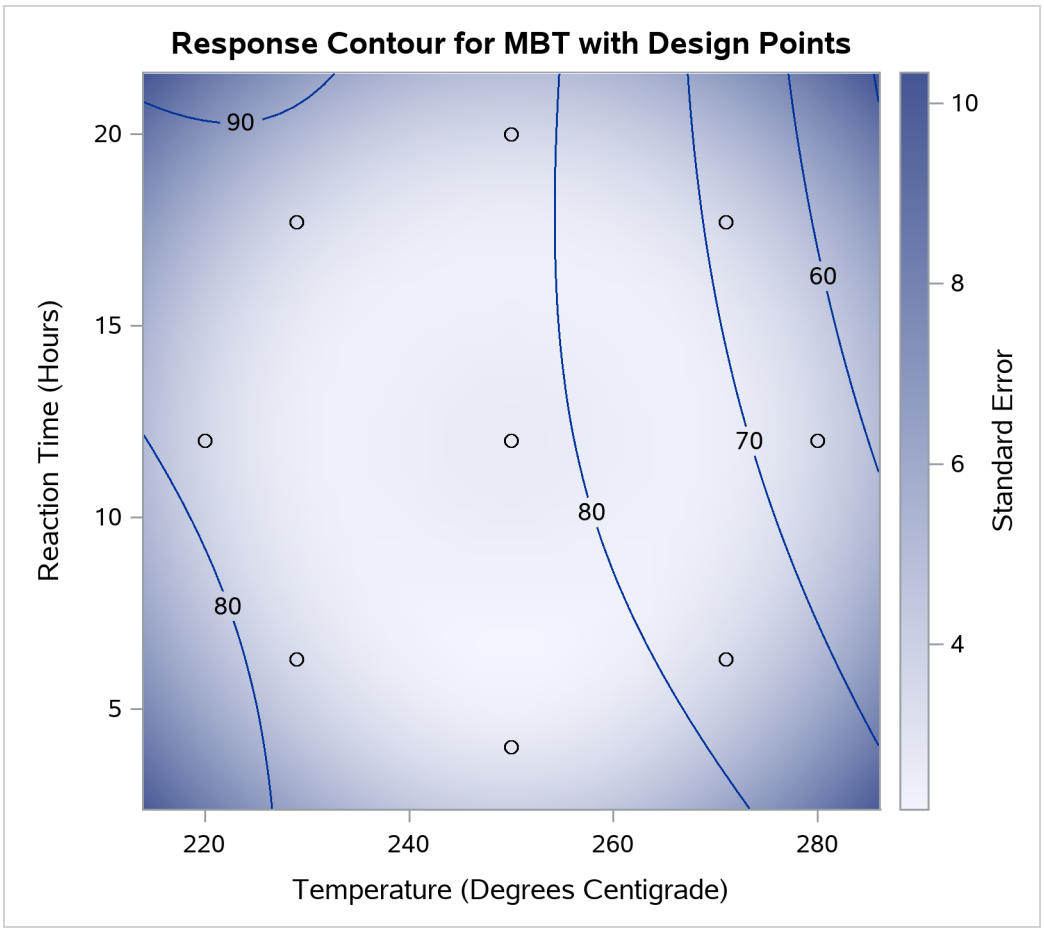
However, the ridge analysis in Output 105.1.4 and the ridge plot in Output 105.1.5 indicate that maximum yields result from relatively high reaction times and low temperatures. A contour plot of the predicted response surface, shown in Output 105.1.5, confirms this conclusion.

Output 105.1.4 Ridge Analysis

Estimated Ridge of Maximum Response for Variable MBT: Percent Yield Mercaptobenzothiazole				
			Uncoded Factor Values	
Coded Radius	**Estimated Response**	**Standard Error**	**Time**	**Temp**
0.0	82.173110	2.665023	12.000000	250.000000
0.1	82.952909	2.648671	11.964493	247.002956
0.2	83.558260	2.602270	12.142790	244.023941
0.3	84.037098	2.533296	12.704153	241.396084
0.4	84.470454	2.457836	13.517555	239.435227
0.5	84.914099	2.404616	14.370977	237.919138
0.6	85.390012	2.410981	15.212247	236.624811
0.7	85.906767	2.516619	16.037822	235.449230
0.8	86.468277	2.752355	16.850813	234.344204
0.9	87.076587	3.130961	17.654321	233.284652
1.0	87.732874	3.648568	18.450682	232.256238

Output 105.1.5 Ridge and Contour Plot of Predicted Response Surface





Example 105.2: Response Surface Analysis with Covariates

One way of viewing covariates is as extra sources of variation in the dependent variable that can mask the variation due to primary factors. This example demonstrates the use of the COVAR= option in PROC RSREG to fit a response surface model to the dependent variables corrected for the covariates.

You have a chemical process with a yield that you hypothesize to be dependent on three factors: reaction time, reaction temperature, and reaction pressure. You perform an experiment to measure this dependence. You are willing to include up to 20 runs in your experiment, but you can perform no more than 8 runs on the same day, so the design for the experiment is composed of three blocks. Additionally, you know that the grade of raw material for the reaction has a significant impact on the yield. You have no control over this, but you keep track of it. The following statements create a SAS data set containing the results of the experiment:

```
data Experiment;
   input Day Grade Time Temp Pressure Yield;
   datalines;
1 67      -1     -1     -1         32.98
1 68      -1      1      1         47.04
1 70       1     -1      1         67.11
1 66       1      1     -1         26.94
1 74       0      0      0        103.22
1 68       0      0      0         42.94
2 75      -1     -1      1        122.93
2 69      -1      1     -1         62.97
2 70       1     -1     -1         72.96
2 71       1      1      1         94.93
2 72       0      0      0         93.11
2 74       0      0      0        112.97
3 69       1.633  0      0         78.88
3 67      -1.633  0      0         52.53
3 68       0      1.633  0         68.96
3 71       0     -1.633  0         92.56
3 70       0      0      1.633     88.99
3 72       0      0     -1.633    102.50
3 70       0      0      0         82.84
3 72       0      0      0        103.12
;
```

Your first analysis neglects to take the covariates into account. The following statements use PROC RSREG to fit a response surface to the observed yield, but note that Day and Grade are omitted:

```
proc rsreg data=Experiment;
   model Yield = Time Temp Pressure;
run;
```

The ANOVA results shown in Output 105.2.1 indicate that *no* process variable effects are significantly larger than the background noise.

Output 105.2.1 Analysis of Variance Ignoring Covariates

The RSREG Procedure

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Linear	3	1880.842426	0.1353	0.67	0.5915
Quadratic	3	2370.438681	0.1706	0.84	0.5023
Crossproduct	3	241.873250	0.0174	0.09	0.9663
Total Model	9	4493.154356	0.3233	0.53	0.8226

Residual	DF	Sum of Squares	Mean Square
Total Error	10	9405.129724	940.512972

However, when the yields are adjusted for covariate effects of day and grade of raw material, very strong process variable effects are revealed. The following statements produce the ANOVA results in Output 105.2.2. Note that in order to include the effects of the classification factor Day as covariates, you need to create dummy variables indicating each day separately.

```
data Experiment;
   set Experiment;
   d1 = (Day = 1);
   d2 = (Day = 2);
   d3 = (Day = 3);

ods graphics on;
proc rsreg data=Experiment plots=all;
   model Yield = d1-d3 Grade Time Temp Pressure / covar=4;
run;
ods graphics off;
```

The results show very strong effects due to both the covariates and the process variables.

Output 105.2.2 Analysis of Variance Including Covariates

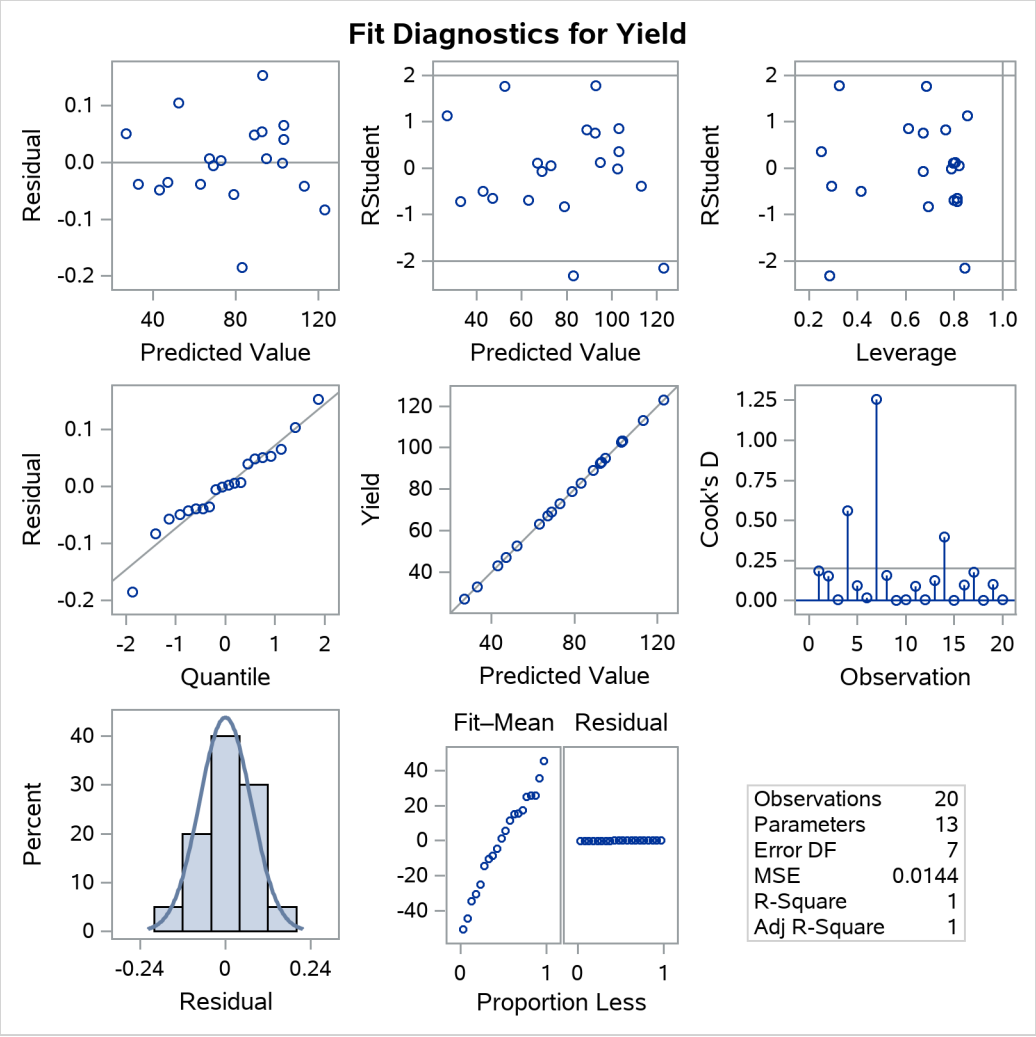
The RSREG Procedure

Regression	DF	Type I Sum of Squares	R-Square	F Value	Pr > F
Covariates	3	13695	0.9854	316957	<.0001
Linear	3	156.524497	0.0113	3622.53	<.0001
Quadratic	3	22.989775	0.0017	532.06	<.0001
Crossproduct	3	23.403614	0.0017	541.64	<.0001
Total Model	12	13898	1.0000	80413.2	<.0001

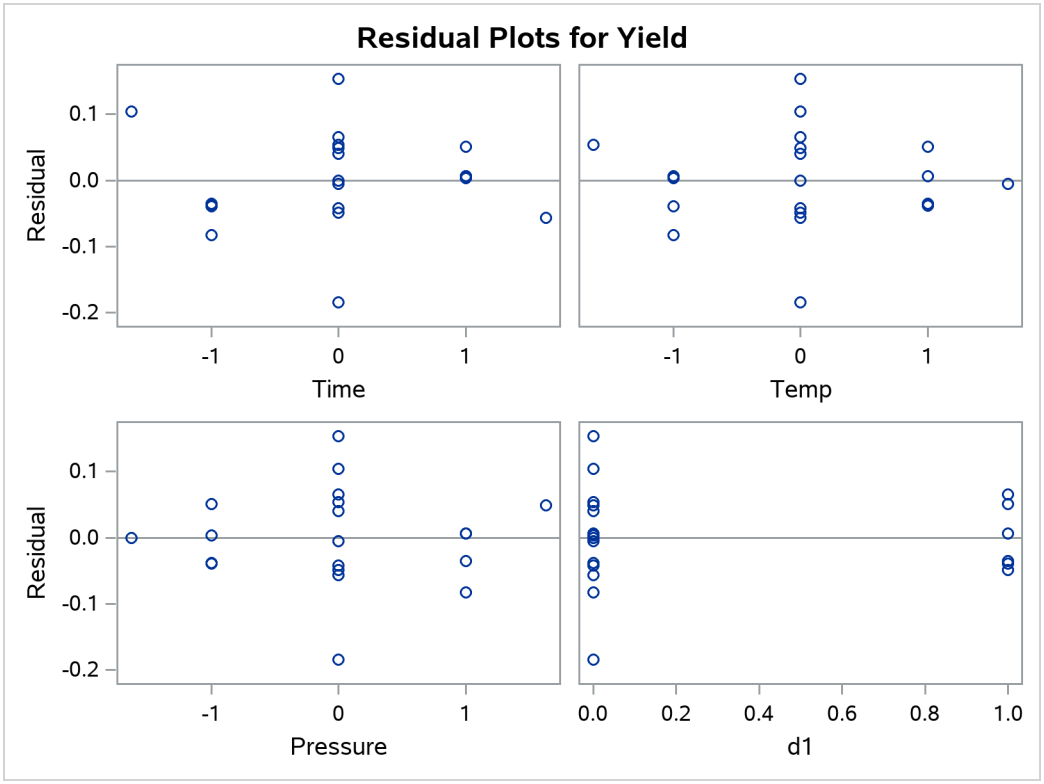
Residual	DF	Sum of Squares	Mean Square
Total Error	7	0.100820	0.014403

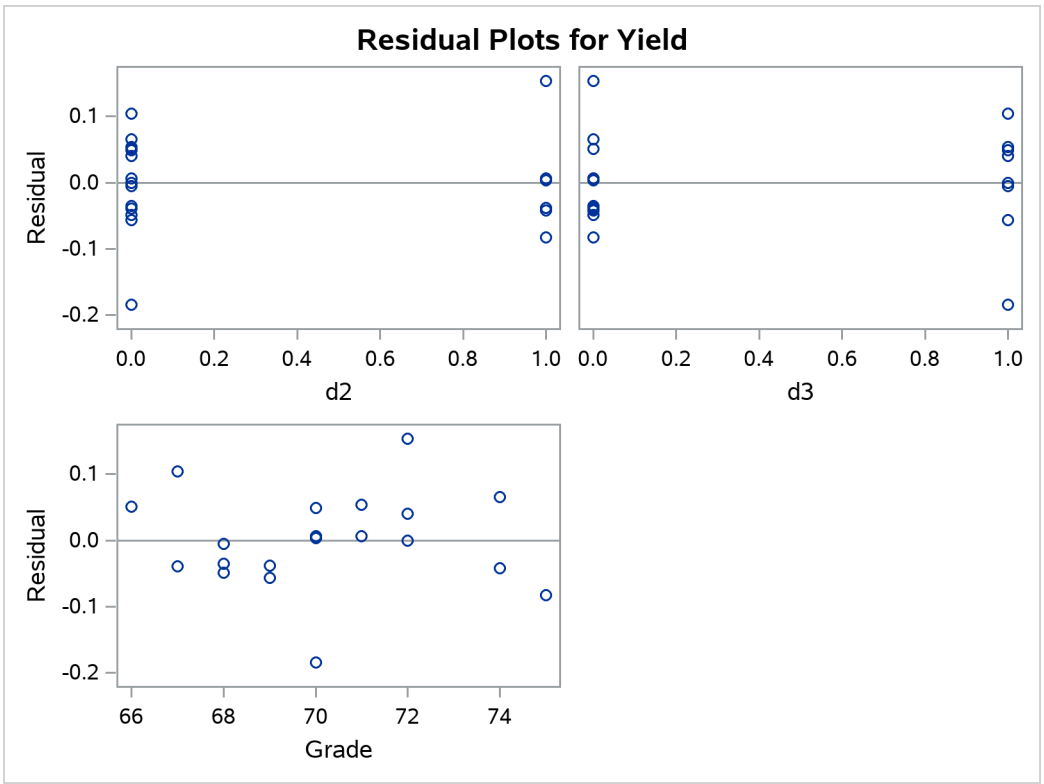
The number of observations in the data set might be too small for the diagnostic plots in Output 105.2.3 to dependably identify problems; however, some outliers are indicated. The residual plots in Output 105.2.4 do not display any obvious structure.

Output 105.2.3 Fit Diagnostics



Output 105.2.4 Residual Plots





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