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SAS/STAT® 9.2 User's Guide

The KRIGE2D Procedure

(Book Excerpt)

SAS® Documentation

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Chapter 46

The KRIGE2D Procedure

Contents

Overview: KRIGE2D Procedure

The KRIGE2D procedure performs ordinary kriging in two dimensions. PROC KRIGE2D can handle anisotropic and nested semivariogram models. Four semivariogram models are supported: the Gaussian, exponential, spherical, and power models. A single nugget effect is also supported.

You can specify the locations of kriging predictions in a GRID statement, or they can be read from a SAS data set. The grid specification is most suitable for a regular grid; the data set specification can handle any irregular pattern of points.

Local kriging is supported through the specification of a radius around a grid point or the specification of the number of nearest neighbors to use in the kriging system. When you perform local kriging, a separate kriging system is solved at each grid point by using a neighborhood of the data point established by the radius or number specification.

The KRIGE2D procedure writes the kriging predictions and associated standard errors for each grid to an output data set. When you perform local kriging, PROC KRIGE2D writes the neighborhood information for each grid point to an additional, optional data set. The KRIGE2D procedure does not produce any displayed output.

The KRIGE2D procedure now uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." For more information about the graphics available in PROC KRIGE2D, see the section "ODS Graphics" on page 2967.

Introduction to Spatial Prediction

Many activities in science and technology involve measurements of one or more quantities at given spatial locations, with the goal of predicting the measured quantities at unsampled locations. Application areas include reservoir prediction in mining and petroleum exploration, as well as modeling in a broad spectrum of fields (for example, environmental health, environmental pollution, natural resources and energy, hydrology, risk analysis). Often, the unsampled locations are on a regular grid, and the predictions are used to produce surface plots or contour maps.

The preceding tasks fall within the scope of *spatial prediction*, which, in general, is any prediction method that incorporates spatial dependence. The study of these tasks involves naturally occurring uncertainties that cannot be ignored. Stochastic analysis frameworks and methods are used to account for these uncertainties. Hence, the terms *stochastic spatial prediction* and *stochastic modeling* are also used to characterize this type of analysis.

A popular method of spatial prediction is *ordinary kriging*, which produces both predicted values and associated standard errors. Ordinary kriging requires the complete specification (the form and parameter values) of the spatial dependence characterizing the spatial process. For this purpose, models for the spatial dependence are expressed in terms of the distance between any two locations in the spatial domain of interest. These models take the form of a covariance or semivariance function.

Spatial prediction, then, involves two steps. First, you model the covariance or semivariance of the spatial process. These measures are typically not known in advance. This step involves computing an empirical estimate, as well as determining both the mathematical form and the values of any parameters for a theoretical form of the dependence model. Second, you use this dependence model to solve the kriging system at a specified set of spatial points, resulting in predicted values and associated standard errors.

The KRIGE2D procedure performs the second of these steps by using ordinary kriging of two-dimensional data.

This introduction concludes with a note on terminology. You might commonly encounter the terms *estimation* and *prediction* used interchangeably by experts in different fields; this could be a source of confusion. A precise statistical vernacular uses the term *estimation* to refer to inferences about the value of fixed but unknown parameters, whereas *prediction* concerns inferences about the value of random variables—see, for example, Cressie (1993, p. 106). In light of these definitions, kriging methods are clearly predictive techniques, since they are concerned with making inferences about the value of a spatial random field at observed or unobserved locations. The SAS/STAT suite of procedures for spatial analysis and prediction (VARIOGRAM, KRIGE2D, and SIM2D) follows the statistical vernacular in the use of the terms *estimation* and *prediction*.

Getting Started: KRIGE2D Procedure

Spatial Prediction Using Kriging, Contour Plots

After an appropriate semivariogram model is chosen, there are a number of choices involved in producing the kriging surface. In order to illustrate these choices, you use the theoretical semivariogram model that was selected for the coal seam thickness data in "Example 95.1: Theoretical Semivariogram Model Fitting" on page 7562 in the VARIOGRAM procedure. This model is Gaussian,

$$\gamma_z(h) = c_0\left[1 - \exp\left(-\frac{h^2}{a_0^2}\right)\right]$$

with a scale of $c_0 = 7.2881$ (that is, the model sill) and a range of $a_0 = 30.6239$, based on the weighted least squares fitting results in the PROC VARIOGRAM example.

The first choice is whether to use local or global kriging. Local kriging uses only data points in the neighborhood of a grid point, and you choose this type of analysis by specifying a data search radius around the grid point. Global kriging uses all data points.

The most important consideration in this decision is the spatial covariance structure. Global kriging is appropriate when the correlation range ϵ is approximately equal to the length of the spatial domain. The correlation range ϵ is the distance r_ϵ (also known as *effective* or *practical* range, too) at which the covariance is 5% of its value at zero. That is,

$$C_Z(r_\epsilon) = 0.05C_z(0)$$

For a Gaussian model, r_ϵ is $\sqrt{3}a_0 \approx 52{,}000$ feet. The data points are scattered uniformly throughout a 100×100 (10^6 ft^2) area. Hence, the linear dimension of the data is nearly double the r_ϵ range. This indicates that local kriging rather than global kriging is appropriate because data that are farther away than r_ϵ essentially add to the computational burden without significant contribution to the prediction. The following DATA step is used to input the thickness data set:

```
data thick;
   input East North Thick @@;
   label Thick='Coal Seam Thickness';
   datalines;
    0.7  59.6  34.1   2.1  82.7  42.2   4.7  75.1  39.5
    4.8  52.8  34.3   5.9  67.1  37.0   6.0  35.7  35.9
    6.4  33.7  36.4   7.0  46.7  34.6   8.2  40.1  35.4
   13.3   0.6  44.7  13.3  68.2  37.8  13.4  31.3  37.8
   17.8   6.9  43.9  20.1  66.3  37.7  22.7  87.6  42.8
   23.0  93.9  43.6  24.3  73.0  39.3  24.8  15.1  42.3
   24.8  26.3  39.7  26.4  58.0  36.9  26.9  65.0  37.8
   27.7  83.3  41.8  27.9  90.8  43.3  29.1  47.9  36.7
   29.5  89.4  43.0  30.1   6.1  43.6  30.8  12.1  42.8
   32.7  40.2  37.5  34.8   8.1  43.3  35.3  32.0  38.8
   37.0  70.3  39.2  38.2  77.9  40.7  38.9  23.3  40.5
   39.4  82.5  41.4  43.0   4.7  43.3  43.7   7.6  43.1
   46.4  84.1  41.5  46.7  10.6  42.6  49.9  22.1  40.7
   51.0  88.8  42.0  52.8  68.9  39.3  52.9  32.7  39.2
   55.5  92.9  42.2  56.0   1.6  42.7  60.6  75.2  40.1
   62.1  26.6  40.1  63.0  12.7  41.8  69.0  75.6  40.1
   70.5  83.7  40.9  70.9  11.0  41.7  71.5  29.5  39.8
   78.1  45.5  38.7  78.2   9.1  41.7  78.4  20.0  40.8
   80.5  55.9  38.7  81.1  51.0  38.6  83.8   7.9  41.6
   84.5  11.0  41.5  85.2  67.3  39.4  85.5  73.0  39.8
   86.7  70.4  39.6  87.2  55.7  38.8  88.1   0.0  41.6
   88.4  12.1  41.3  88.4  99.6  41.2  88.8  82.9  40.5
   88.9   6.2  41.5  90.6   7.0  41.5  90.7  49.6  38.9
   91.5  55.4  39.0  92.9  46.8  39.1  93.4  70.9  39.7
   55.8  50.5  38.1  96.2  84.3  40.3  98.2  58.2  39.5
   ;
```

Local kriging is performed by using only data points within a specified radius of each grid point. In this example, a radius of 60,000 feet is used. Other choices involved in local kriging are the minimum and maximum number of data points in each neighborhood (around a grid point). The minimum number is left at the default value of 20; the maximum number defaults to all observations in the data set within the specified radius.

The last step in contouring the data is to define the prediction grid point (node) locations. The prediction grid is typically rectangular, and you decide on the grid points population and spacing based on your available data as well as your application needs. A convenient area that encompasses all the data points is a square of side length 100,000 feet. In the present analysis, a distance of 2,500 feet between nodes in the prediction grid is selected to obtain a smooth contour plot. Based on this choice, you will obtain predictions on a square grid with 41 nodes on each side, which yields a total of 1681 grid points.

You can visualize the outcome of your analysis by using the PLOTS= option in the PROC KRIGE2D statement. PROC KRIGE2D will produce by default one plot that displays the kriging prediction and its corresponding standard error at each output grid point. The locations of the Thick observations are displayed too, as outlines in the default plot. You can also ask for a plot of the thick data set observations and their values by specifying the OBSERV option in the PLOTS option.

The kriging analysis with the KRIGE2D procedure requires that you provide the prediction parameters in the PREDICT statement. You use the VAR= option to specify that you will be using the Thick variable in the kriging system, and the RADIUS= option to specify the radius of the local kriging regression. In this scenario you want to consider for your predictions all the neighboring data within a radius of 60,000 feet from each prediction location. You can specify more than one PREDICT statements; for example, you can do this when you want predictions for different variables in your DATA= data set.

The coordinates of your variable are specified in the COORDINATES statement. The MODEL statement contains the parameters that describe your data spatial correlation. Namely, the FORM= option specifies the model type, based on its mathematical form. The SCALE= and RANGE= options specify the model sill and range, respectively. You can specify more than one MODEL statement for the same PREDICT statement in order to obtain predictions based on different correlation models.

When you use the RADIUS= option to perform local kriging, as in the present example, it is suggested that the radius parameter is at least as large as your model range, so that you do not exclude data points that can contribute to your prediction.

Eventually, you specify the region of predictions with the GRID statement. The following SAS statements compute the kriged surface by using the preceding options and grid choice:

```
title 'Coal Seam Thickness Kriging';
ods graphics on;

proc krige2d data=thick;
   coordinates xc=East yc=North;
   predict var=Thick radius=60;
   model scale=7.2881 range=30.6239 form=gauss;
   grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;
```

The table in Figure 46.1 shows the number of observations read and used in the kriging prediction. This table provides you with useful information in case you have missing values in the input data.

Figure 46.1 Number of Observations for the thick Data Set

```
                    Coal Seam Thickness Kriging

                       The KRIGE2D Procedure
                     Dependent Variable: Thick

                 Number of Observations Read          75
                 Number of Observations Used          75
```

Figure 46.2 shows some general information about the kriging analysis. This includes the count of the output grid points. You have specified the RADIUS= option; therefore you also see that local kriging is requested. Because this is a local analysis, the table also displays the parameters related to the neighborhood search around the grid points.

Figure 46.2 Kriging Analysis Information

```
                        Kriging Information

              Prediction Grid Points                    1681
              Type of Analysis                         Local
              Neighborhood Search Radius                  60
              Minimum Neighbors                           20
              Maximum Neighbors            All Within Radius
```

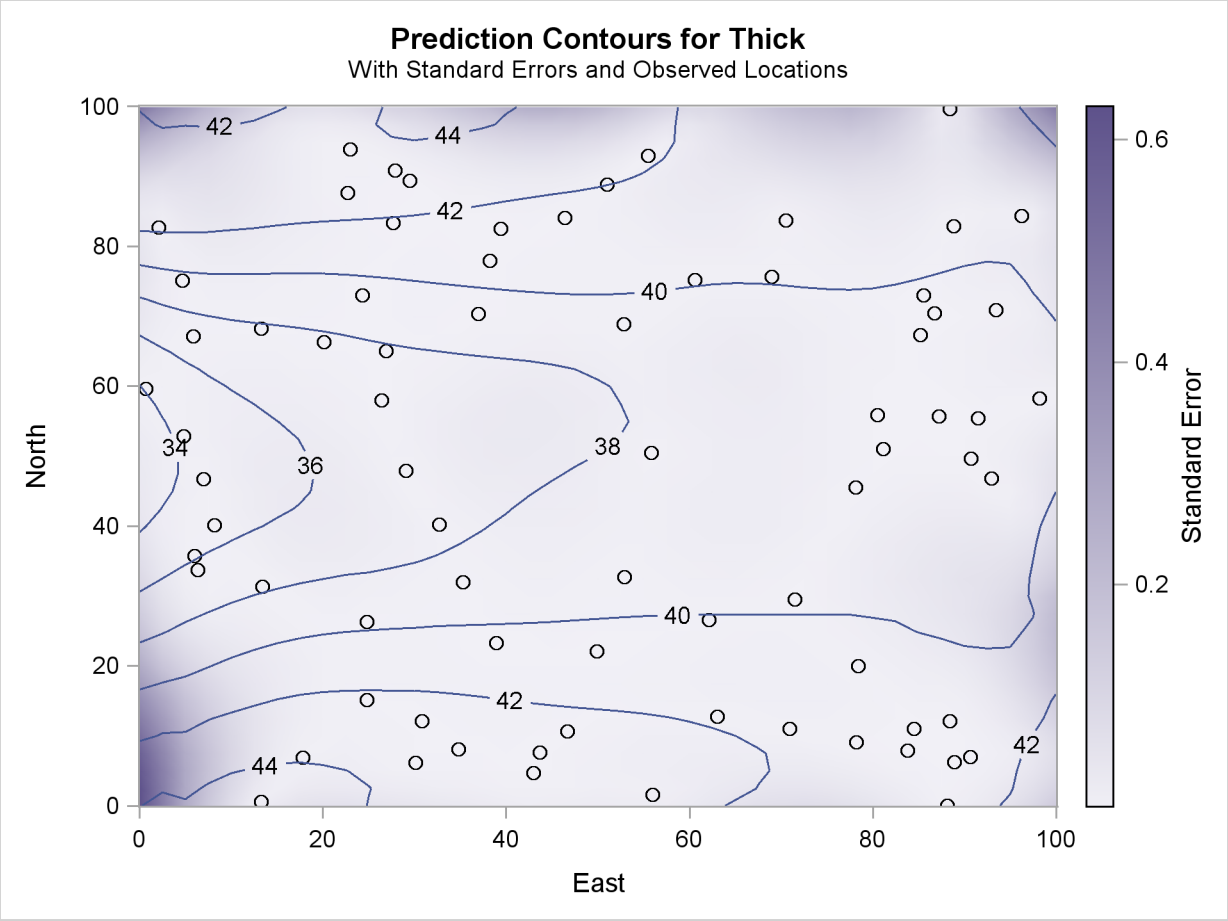
The covariance model parameters, including the effective range of the Gaussian model you specified, are shown in Figure 46.3.

Figure 46.3 Kriging Covariance Model Information

```
                    Coal Seam Thickness Kriging

                       The KRIGE2D Procedure
                     Dependent Variable: Thick
                Prediction: Pred1, Model: Model1

                    Covariance Model Information

                    Type                Gaussian
                    Sill                  7.2881
                    Range                30.6239
                    Effective Range    53.042151
                    Nugget Effect              0
```

Figure 46.4 shows a map of the kriging prediction contours based on the Thick observations in the specified spatial domain. The prediction error is displayed as a surface in the background.

Figure 46.4 Contour Plot of Kriged Coal Seam Thickness



Note the locations of the observed data in Figure 46.4. The figure suggests that the Thick sampling locations are not ideally spread around the prediction area; however, there are no extended areas lacking measurements.

Based on the spatial distribution of the Thick data and the range r_ϵ of your covariance model, you can roughly see that for each prediction location there are at least several neighboring data points that will contribute to the prediction value. Except perhaps for the nodes close to the boundaries of the prediction grid, you can then expect the prediction errors to be reasonably low compared to the predicted Thick values.

The kriging outcome in Figure 46.4 indicates that the standard errors are smaller in the neighborhoods where data are available. The size of these neighborhoods depends on the range of the specified covariance model that characterizes the spatial continuity of the domain, and the prediction radius, if one is specified as in this example. The standard errors tend to increase toward the borders of the prediction area, beyond which no observations are available.

Syntax: KRIGE2D Procedure

The following statements are available in PROC KRIGE2D:

PROC KRIGE2D *options* ;
BY *variables* ;
COORDINATES | **COORD** *coordinate-variables* ;
GRID *grid-options* ;
PREDICT | **PRED** | **P** *predict-options* ;
MODEL *model-options* ;

The PREDICT and MODEL statements are hierarchical; the PREDICT statement is followed by a MODEL statement. If more than one MODEL statement is given, only the last one is used for the analysis. The MODEL statement following a PREDICT statement uses the variable and neighborhood specifications in that PREDICT statement.

You must specify at least one PREDICT statement and one MODEL statement. You must supply a single COORDINATES statement to identify the x and y coordinate variables in the input data set. You must also specify a single GRID statement to include the grid information.

The following table outlines the options available in PROC KRIGE2D classified by function.

Table 46.1 Options Available in the KRIGE2D Procedure

Task	Statement	Option
Data Set Options		
Specify input data set	PROC KRIGE2D	DATA=
Specify grid data set	GRID	GDATA=
Specify model data set	MODEL	MDATA=
Write kriging predictions and standard errors	PROC KRIGE2D	OUTEST=
Write neighborhood information for each grid point	PROC KRIGE2D	OUTNBHD=
Specify plot display and options	PROC KRIGE2D	PLOTS=
Declaring the Role of Variables		
Specify variables to define analysis subgroups	BY	
Specify the variables to be predicted (kriged)	PREDICT	VAR=
Specify the x and y coordinate variables in the DATA= data set	COORDINATES	XC= YC=
Specify the x and y coordinate variables in the GDATA= data set	GRID	XC= YC=
Controlling Kriging Neighborhoods		
Specify the radius of a neighborhood for all grid points	PREDICT	RADIUS=
Specify the number of neighbors for all grid points	PREDICT	NUMPOINTS=
Specify the maximum of neighbors for all grid points	PREDICT	MAXPOINTS=
Specify the minimum of neighbors for all grid points	PREDICT	MINPOINTS=
Specify action when maximum not met	PREDICT	NODECREMENT

Table 46.1 *continued*

Task	Statement	Option
Specify action when minimum not met	PREDICT	NOINCREMENT
Controlling the Semivariogram Model		
Specify a nugget effect	MODEL	NUGGET=
Specify a type with a functional form	MODEL	FORM=
Specify a range parameter	MODEL	RANGE=
Specify a scale parameter	MODEL	SCALE=
Specify an angle for an anisotropic model	MODEL	ANGLE=
Specify a minor-major axis ratio for an anisotropic model	MODEL	RATIO=

PROC KRIGE2D Statement

PROC KRIGE2D *options* **;**

You can specify the following options in the PROC KRIGE2D statement.

DATA=*SAS-data-set*
specifies a SAS data set containing the x and y coordinate variables and the VAR= variables in the PREDICT statement.

NOPRINT
suppresses the normal display of results. The NOPRINT option is useful when you want only to create one or more output data sets with the procedure. Note that this option temporarily disables the Output Delivery System (ODS); see the section "ODS Graphics" on page 2967 for more information.

OUTEST=*SAS-data-set*

OUTE=*SAS-data-set*
specifies a SAS data set in which to store the kriging predictions, standard errors, and grid location. For details, see the section "OUTEST=*SAS-data-set*" on page 2965.

OUTNBHD=*SAS-data-set*

OUTN=*SAS-data-set*
specifies a SAS data set in which to store the neighborhood information for each grid point. Information is written to this data set only if one or more PREDICT statements have options specifying local kriging. For details, see the section "OUTNBHD=*SAS-data-set*" on page 2965.

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 around the plot request. Here are some examples:

```
plots=none
plots=observ
plots=(observ(outl) prediction)
plots=(prediction(fill=pred line=se obs=grad) prediction(fill=se))
```

You must enable ODS Graphics before requesting plots, for example, like this:

```
ods graphics on;

proc krige2d data=thick;
   coordinates xc=East yc=North;
   predict var=thick r=60;
   model scale=7.2881 range=30.6239 form=gauss;
   grid x=0 to 100 by 10 y=0 to 100 by 10;
run;

ods graphics off;
```

For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." If you have enabled ODS Graphics but do not specify the PLOTS= option or have specified PLOTS=ALL, then PROC KRIGE2D produces a default plot for each MODEL statement of every PREDICT statement that you specify. The default PROC KRIGE2D plot displays a contour plot of the kriging prediction and the gradient of the kriging prediction standard error at every location of the prediction grid, as well as empty circles that indicate the observation locations. See Figure 46.4 for an example of the default KRIGE2D plot.

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

ONLY
suppresses the default plot. Only plots specifically requested are displayed.

The following individual *plot-requests* and plot *options* are available:

ALL
produces all appropriate plots. You can specify other options with ALL. For example, to request the default plot and an additional plot of the predictions, specify PLOTS=(ALL PREDICTION).

EQUATE
specifies that all appropriate plots be produced in a way that the axes coordinates have equal size units.

NONE
suppresses all plots.

OBSERVATIONS < (*observations-plot-options*) >
OBSERV < (*observations-plot-options*) >
OBS < (*observations-plot-options*) >
produces the observed data plot. Only one observations plot will be created if you specify the OBSERVATIONS option more than once within a PLOTS option.

The OBSERVATIONS option has the following suboptions:

GRADIENT
specifies that observations be displayed as circles colored by the observed measurement.

OUTLINE
specifies that observations be displayed as circles with a border but with a completely transparent fill.

OUTLINEGRADIENT
is the same as OBSERVATIONS(GRADIENT) except that a border is shown around each observation.

SHOWMISSING
specifies that observations with missing values be displayed in addition to the observations with nonmissing values. By default, missing values locations are not shown on the plot. If you specify multiple instances of the OBSERVATIONS option, and you specify the SHOWMISSING suboption in any of those, then the resulting observations plot will display the observations with missing values.

For the GRADIENT, OUTLINE, and OUTLINEGRADIENT suboptions: The OUTLINEGRADIENT is the default suboption if you do not specify any of those three. If you specify multiple instances of the OBSERVATIONS option or multiple suboptions for OBSERVATIONS, then the resulting observations plot will honor the last specified GRADIENT, OUTLINE, or OUTLINEGRADIENT suboption.

PREDICTION < (*prediction-plot-options*) >
PRED < (*prediction-plot-options*) >
specifies that the kriging prediction plot be produced. You can specify the PREDICTION option multiple times in the same PLOTS option to request instances of plots with the following *prediction-plot-options*:

FILL=NONE | PRED | SE
produces a surface plot for either the predicted values or the standard errors. FILL=SE is the default; however, if you do not specify the FILL suboption the behavior depends on the LINE suboption as follows: If you specify LINE=NONE or do not specify the LINE suboption at all, then the FILL suboption will be set to its default value. If LINE=PRED or LINE=SE, then the FILL suboption will be set to the same value as the LINE suboption.

LINE=NONE | PRED | SE
produces a contour line plot for either the predicted values or the standard errors. LINE=PRED is the default; however, if you do not specify the LINE suboption the behavior depends on the FILL suboption as follows: If you specify FILL=NONE or do not specify the FILL suboption at all, then the LINE suboption will be set to its default value. If FILL=PRED or FILL=SE, then the LINE suboption will be set to the same value as the FILL suboption.

OBS=*obs-options*
produces an overlaid scatter plot of the observations in addition to the specified contour plots. The following *obs-options* are available:

GRAD
specifies that observations be displayed as circles colored by the observed measurement. The same color gradient is used to display the prediction surface and the observations. Observations where the prediction is close to the observed values have similar colors—the greater the contrast between the color of an observation and the surface, the larger the prediction standard error is at that point.

LINEGRAD
is the same as OBS=GRAD except that a border is shown around each observation. This option is useful to identify the location of observations where the standard errors are small, because at these points the color of the observations and the color of the surface are indistinguishable.

NONE
specifies that no observations be displayed.

OUTL
specifies that observations be displayed as circles with a border but with a completely transparent fill.

OBS=NONE is the default; however, the default plot in PROC KRIGE2D displays the observations locations as outlines.

If you specify multiple instances of the FILL, LINE, or OBS suboptions in the same PREDICTION option, then the resulting predictions plot will honor the last value specified for any of the suboptions.

Any combination where you specify FILL=NONE and LINE=NONE is not available.

The PREDICTION option requires that predictions be requested at more than one location on a rectangular grid. The plot is not available when you use the GRIDDATA= data set option in the GRID statement, because the GRIDDATA= option allows you to specify any coordinates for the prediction locations.

SINGULARMSG=*number*
SMSG=*number*
controls the number of warning messages displayed for a singular matrix. When local kriging is performed, a separate kriging system is solved for each grid point. Anytime a singular matrix is encountered, a warning message is displayed up to a total of SINGULARMSG=*n* times. The default is SINGULARMSG=10.

BY Statement

BY *variables* **;**

You can specify a BY statement with PROC KRIGE2D to obtain separate analyses on observations in groups 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. The *variables* are one or more variables in the input data set.

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 BY statement options NOTSORTED or DESCENDING in the BY statement for the KRIGE2D 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 the BY statement, see *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the *Base SAS Procedures Guide*.

COORDINATES Statement

COORDINATES | COORD *coordinate-variables* **;**

The following two options specify the names of the variables in the DATA= data set containing the values of the x and y coordinates of the data.

Only one COORDINATES statement is allowed, and it is applied to all PREDICT statements. In other words, it is assumed that all the VAR= variables in all PREDICT statements have the same x and y coordinates.

This is not a limitation. Since each VAR= variable is processed separately, observations for which the current VAR= variable is missing are excluded. With the next VAR= variable, the entire data are read again, this time excluding missing values in this next variable. Hence, a single run of PROC KRIGE2D can be used for variables measured at different locations without overlap.

XCOORD= *(variable-name)*

XC= *(variable-name)*

specifies the name of the variable containing the x coordinate of the data locations in the DATA= data set.

YCOORD= *(variable-name)*

YC= *(variable-name)*

specifies the name of the variable containing the y coordinate of the data locations in the DATA= data set.

GRID Statement

GRID *grid-options* **;**

You can use the following options to specify the grid of spatial locations for the kriging predictions. The grid specification is applied to all PREDICT and MODEL statements.

There are two basic methods for specifying the grid. You can specify the x and y coordinates explicitly, or they can be read from a SAS data set. The options for the explicit specification of grid locations are as follows:

X=*number*

X=$x_1, \ldots, x_m$

X=x_1 *to* x_m

X=x_1 *to* x_m *by* δx

specifies the x coordinate of the grid locations.

Y=*number*

Y=$y_1, \ldots, y_m$

Y=y_1 *to* y_m

Y=y_1 *to* y_m *by* δy

specifies the y coordinate of the grid locations.

For example, the following two GRID statements are equivalent.

```
grid x=1,2,3,4,5  y=0,2,4,6,8,10;
grid x=1 to 5 y=0 to 10 by 2;
```

To specify grid locations from a SAS data set, you must provide the name of the data set and the variables containing the values of the x and y coordinates.

GRIDDATA=*SAS-data-set*

GDATA=*SAS-data-set*

specifies a SAS data set containing the x and y grid coordinates.

XCOORD= *(variable-name)*

XC= *(variable-name)*

specifies the name of the variable containing the x coordinate of the grid locations in the GRIDDATA= data set.

YCOORD= *(variable-name)*

YC= *(variable-name)*

specifies the name of the variable containing the y coordinate of the grid locations in the GRIDDATA= data set.

PREDICT Statement

PREDICT | PRED | P *predict-options* **;**

You can specify the following options in a PREDICT statement.

MAXPOINTS=*number*

MAXP=*number*

MAX=*number*

specifies the maximum number of data points in a neighborhood. You specify this option in conjunction with the RADIUS= option. When the number of data points in the neighborhood formed at a given grid point by the RADIUS= option is greater than the MAXPOINTS= value, the RADIUS= value is decreased just enough to honor the MAXPOINTS= value unless you specify the NODECREMENT option. The default is to include all data points within the specified RADIUS= value. Neighborhoods with very large numbers of data points might lead to unnecessarily slow execution times and potential lack of memory issues, depending on the problem setup and your computational resources. In that case, you could use the MAXPOINTS= option to set a cap for your neighborhood size. For details about numerical considerations see the section "Computational Resources" on page 2964. Unless the RADIUS= option is also specified, when the MAXPOINTS= and NUMPOINTS= options are specified in the same PREDICT statement the MAXPOINTS= option is ignored.

MINPOINTS=*number*

MINP=*number*

MIN=*number*

specifies the minimum number of data points in a neighborhood. You specify this option in conjunction with the RADIUS= option. When the number of data points in the neighborhood formed at a given grid point by the RADIUS= option is less than the MINPOINTS= value, the RADIUS= value is increased just enough to honor the MINPOINTS= value unless you specify the NOINCREMENT option. The default is MINPOINTS=20. When enough data are available, you might improve prediction if you increase this value. When the MINPOINTS= and NUMPOINTS= options are specified in the same PREDICT statement the MINPOINTS= option is set to the value of NUMPOINTS=.

NODECREMENT | NODECR

requests that the RADIUS= value not be decremented when the MAXPOINTS= value is exceeded at a grid point. This option is relevant only when you specify both a RADIUS= value and a MAXPOINTS= value. In this case, when the number of points in the neighborhood constructed from the RADIUS= specification is greater than the MAXPOINTS= value, the RADIUS= value is decremented enough to honor the MAXPOINTS= value, and the kriging system is solved for this grid point. If you specify the NODECREMENT option, no decrementing is done, prediction is skipped at this grid point, and a message is written to the log.

NOINCREMENT | NOINCR

requests that the RADIUS= value not be incremented when the MINPOINTS= value is not met at a grid point. This option is relevant only when you specify both a RADIUS= value and

a MINPOINTS= number. In this case, when the number of points in the neighborhood constructed from the RADIUS= specification is less than the MINPOINTS= value, the RADIUS= value is incremented enough to honor the MINPOINTS= value, and the kriging system is solved for this grid point. If you specify the NOINCREMENT option, no incrementing is done, prediction is skipped at this grid point, and a message is written to the log.

NUMPOINTS=*number*
NPOINTS=*number*
NPTS=*number*
NP=*number*

specifies the exact size of a neighborhood. This option is incompatible with all other PREDICT statement options that control the neighborhood; it must appear by itself. In particular, if you specify both NUMPOINTS= and the RADIUS= option in the same PREDICT statement, then RADIUS= is honored, instead. In this event the value of the MINPOINTS= option is set to NUMPOINTS=, and the value of the MAXPOINTS= option is set to default, regardless whether these options have been specified or not. If you specify any of the MINPOINTS= or MAXPOINTS= option without the RADIUS= option in the same PREDICT statement as NUMPOINTS=, then the NUMPOINTS= option will be honored.

RADIUS=*number*
R=*number*

specifies the radius to use in a local kriging regression. When you specify this option, a separate kriging system is solved at each grid point by finding the neighborhood of this grid point consisting of all data points within the distance specified by the RADIUS= value. Note that if you specify the RADIUS= value to include data points situated beyond the extent of your problem's spatial correlation, this could result in unnecessary computational burden in your analysis. For additional control on the neighborhood see the MAXPOINTS= and MINPOINTS= options. When you specify the RADIUS= and NUMPOINTS= options in the same PREDICT statement, then RADIUS= is honored.

VAR= *variable-name*

specifies the single numeric variable used in the kriging system.

MODEL Statement

MODEL *model-options* **;**

You can use the following options to specify a semivariogram or covariance model. The specified model is used in the kriging system defined by the most previous PREDICT statement.

There are two ways to specify a semivariogram or covariance model. In the first method, you specify the required parameters SCALE, RANGE, and FORM, and possibly the optional parameters NUGGET, ANGLE, and RATIO, explicitly in the MODEL statement. In the second method, you specify an MDATA= data set. This data set contains variables corresponding to the required SCALE, RANGE, and FORM parameters, and optionally variables for the NUGGET, ANGLE, and RATIO parameters. The two methods are exclusive; either you specify all parameters explicitly, or they all are read from the MDATA= data set.

ANGLE=*angle*

ANGLE=*(angle*$_1$*,...,angle*$_k$*)*

specifies the angle of the major axis for anisotropic models, measured in degrees clockwise from the N-S axis. In the case of a nested semivariogram model, you can specify an angle for each nesting. The default is ANGLE=0.

FORM=SPHERICAL | EXPONENTIAL | GAUSSIAN | POWER

FORM=SPH | EXP | GAUSS | POW

specifies the functional form (type) of the semivariogram model. All the supported models are two-parameter models (SCALE= and RANGE=). A FORM= value is required; in the case of a nested semivariogram model, you must specify a form for each nesting.

See the section "Theoretical Semivariogram Models" on page 2945 for details on how the FORM= forms are determined.

MDATA=*SAS-data-set*

specifies the input data set that contains parameter values for the covariance or semivariogram model. The MDATA= data set must contain variables named SCALE, RANGE, and FORM=, and it can optionally contain variables NUGGET, ANGLE, and RATIO.

The FORM variable must be a character variable, assuming only the values allowed in the explicit FORM= syntax described previously. The RANGE and SCALE variables must be numeric. The optional variables ANGLE, RATIO, and NUGGET must also be numeric if present.

The number of observations present in the MDATA= data set corresponds to the level of nesting of the semivariogram model.

For example, to specify a non-nested model that uses a spherical covariance, an MDATA= data set might be given by the following statement:

```
data md1;
   input scale range form $;
   datalines;
   25 10 SPH
run;
```

The PROC KRIGE2D statement to use the MDATA= specification is of the form shown in the following:

```
proc krige2d data=...;
   predict var=....;
   model mdata=md1;
run;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc krige2d data=...;
   predict var=....;
   model scale=25 range=10 form=sph;
run;
```

The following MDATA= data set is an example of an anisotropic nested model:

```
data md1;
   input scale range form $ nugget angle ratio;
   datalines;
   20 8 S  5 35 0.7
   12 3 G  5 0  0.8
   4  1 G  5 45 0.5
   ;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc krige2d data=...;
   predict var=....;
   model scale=(20,12,4) range=(8,3,1) form=(S,G,G)
         angle=(35,0,45) ratio=(0.7,0.8,0.5) nugget=5;
run;
```

This example is somewhat artificial in that it is usually hard to detect different anisotropy directions and ratios for different nestings using an experimental semivariogram. Note that the NUGGET value is the same for all nestings. This is always the case; the nugget effect is a single additive term for all models. For further details, see the section "Details: VARIOGRAM Procedure" on page 7532 in the VARIOGRAM procedure.

NUGGET=*number*

specifies the nugget effect for the model. The nugget effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram (see the chapter on the VARIOGRAM procedure for details). For models without any nugget effect, this option is left out; the default is NUGGET=0.

RANGE=*range*

RANGE=*(range$_1$,...,range$_k$)*

specifies the range parameter in semivariogram models. If you have anisotropy, you must specify the range of the major anisotropy axis. In the case of a nested semivariogram model, you must specify a range for each nested structure.

The range parameter is the divisor in the exponent in all supported models except the power model. It has the units of distance, and it is related to the correlation scale for the underlying spatial process.

See the section "Theoretical Semivariogram Models" on page 2945 for details on how the RANGE= values are determined.

RATIO=*ratio*

RATIO=*(ratio$_1$,...,ratio$_k$)*

specifies the ratio of the length of the minor axis to the length of the major axis for anisotropic models. The value of the RATIO= option must be between 0 and 1. In the case of a nested semivariogram model, you can specify a ratio for each nesting. The default is RATIO=1.

SCALE=*scale*

SCALE=*(scale$_1$,...,scale$_k$)*

specifies the scale parameter in semivariogram models. In the case of a nested semivariogram model, you must specify a scale for each nesting.

The scale parameter is the multiplicative factor in all supported models; it has the same units as the variance of the VAR= variable in the preceding PREDICT statement.

See the section "Theoretical Semivariogram Models" on page 2945 for details on how the SCALE= values are determined.

SINGULAR=*number*

gives the singularity criteria for solving kriging systems. The larger the value of the SINGULAR= option, the easier it is for a kriging system to be declared singular. The default is SINGULAR=1E-7. See the section "Ordinary Kriging" on page 2962 for more detailed information.

Details: KRIGE2D Procedure

Theoretical Semivariogram Models

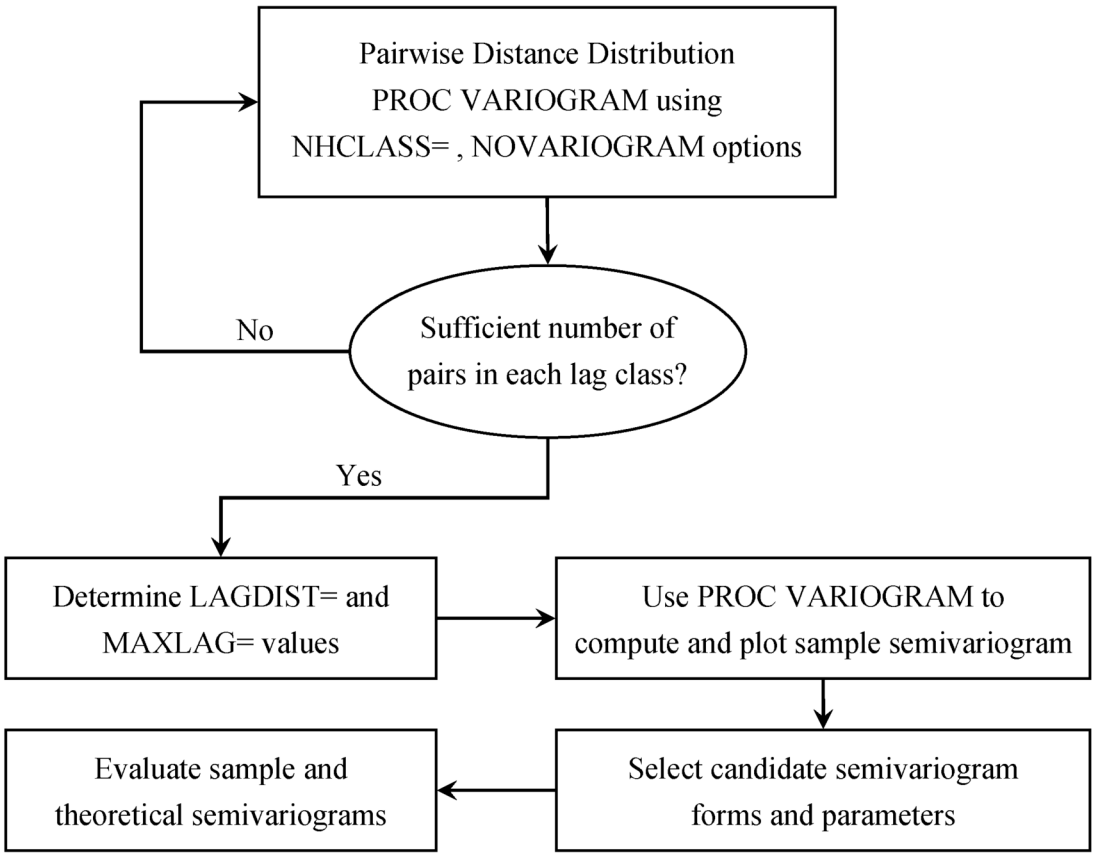
Consider a stochastic spatial process represented by the spatial random field (SRF; see Christakos 1992) $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2\}$. PROC VARIOGRAM computes the empirical (also known as sample or experimental) semivariance of $Z(\boldsymbol{s})$. Prediction of the spatial process $Z(\boldsymbol{s})$ at unsampled locations by techniques such as ordinary kriging requires a theoretical semivariogram or covariance.

When you use PROC VARIOGRAM and PROC KRIGE2D to perform spatial prediction, you must determine a suitable theoretical semivariogram based on the sample semivariogram. There are various methods of fitting semivariogram models, such as least squares, maximum likelihood, and robust methods (Cressie 1993, Section 2.6). A different approach is manual fitting, where a theoretical semivariogram is chosen based on visual inspection of the empirical estimate; see, for example, Hohn (1988, p. 25).

In some cases, a plot of the experimental semivariogram suggests that a single theoretical model is inadequate. Nested models, anisotropic models, and the nugget effect increase the scope of theoretical models available. All of these concepts are discussed in this section. The specification of the final theoretical model is provided by the syntax of PROC KRIGE2D.

Note the general flow of investigation. The empirical semivariogram is computed after a suitable choice is made for the LAGDISTANCE= and MAXLAGS= options in PROC VARIOGRAM, and possibly the NDIR= option or the DIRECTIONS statement for computations in more than one directions. Potential theoretical models (which can also incorporate nesting, anisotropy, and the nugget effect) are then plotted against the empirical semivariogram and evaluated. A suitable theoretical model is found by using the methodology presented in the section "Examples: VARIOGRAM Procedure" on page 7562 in the VARIOGRAM procedure. The flow of this process is illustrated in Figure 46.5.

Figure 46.5 Flowchart for Semivariogram Selection



Four theoretical models are supported by PROC KRIGE2D: the spherical, Gaussian, exponential, and power models—see also the section "Theoretical Semivariogram Models" on page 7532 in the VARIOGRAM procedure. For the first three types, the parameters a_0 and c_0, corresponding to the RANGE= and SCALE= options in the MODEL statement in PROC KRIGE2D, have the same dimensions and have similar effects on the shape of $\gamma_z(h)$, as illustrated in the following paragraph.

In particular, the dimension of c_0 is the same as the dimension of the variance of the spatial process $Z(\boldsymbol{s})$. The dimension of a_0 is length with the same units as h.

These four model forms are now examined in more detail.

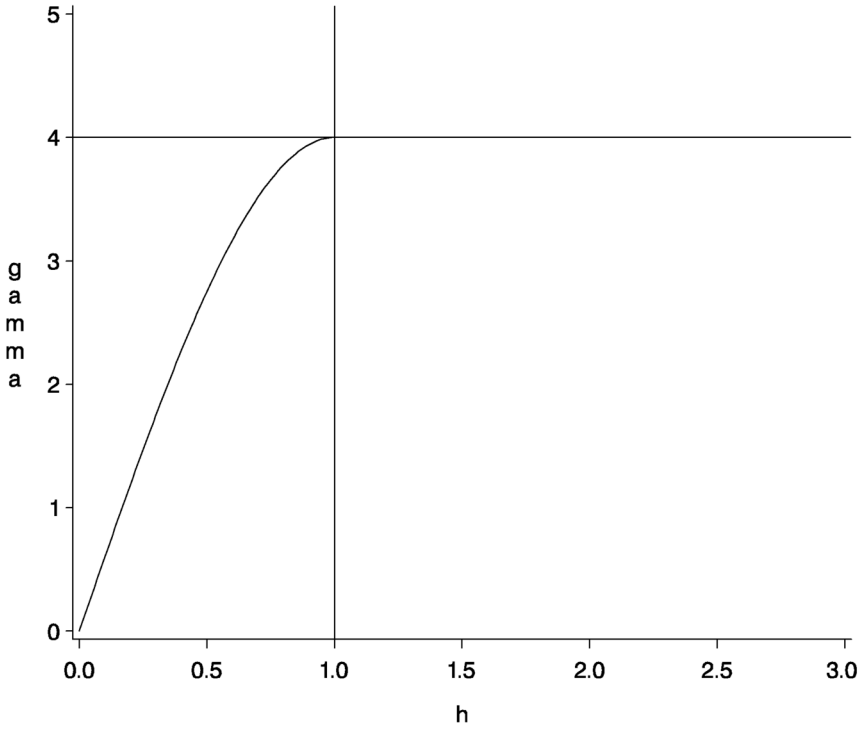
The Spherical Semivariogram Model

The form of the spherical model is

$$\gamma_z(h) = \begin{cases} c_0\left[\frac{3}{2}\frac{h}{a_0} - \frac{1}{2}\left(\frac{h}{a_0}\right)^3\right], & \text{for } h \le a_0 \\ c_0, & \text{for } h > a_0 \end{cases}$$

The shape is displayed in Figure 46.6, using range $a_0 = 1$ and scale $c_0 = 4$.

Figure 46.6 Spherical Semivariogram Model with Parameters $a_0 = 1$ and $c_0 = 4$



The vertical line at $h = 1$ shows the range a_0 of the model.

The horizontal line at 4.0 variance units (corresponding to $c_0 = 4$) is called the *sill.* In the case of the spherical model, $\gamma_z(h)$ actually reaches this value. For the following two model types, the sill is a horizontal asymptote.

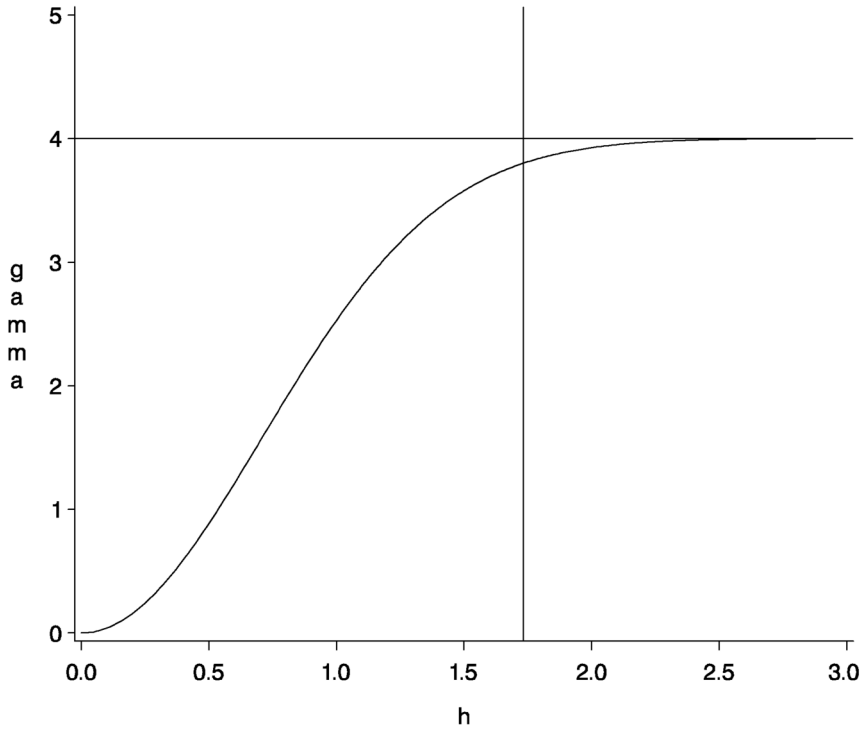
The Gaussian Semivariogram Model

The form of the Gaussian model is

$$\gamma_z(h) = c_0 \left[1 - \exp\left(-\frac{h^2}{a_0^2} \right) \right]$$

The shape is displayed in Figure 46.7, using range $a_0 = 1$ and scale $c_0 = 4$.

Figure 46.7 Gaussian Semivariogram Model with Parameters $a_0 = 1$ and $c_0 = 4$



The vertical line at $h = r_\epsilon = \sqrt{3}a_0$ shows the *effective* (or *practical*) *range* as defined by Deutsch and Journel (1992), or the *range* ϵ defined by Christakos (1992). The effective range is the h-value where the covariance is approximately 5% of its value at zero.

The horizontal line at 4.0 variance units (corresponding to $c_0 = 4$) is the sill; $\gamma_z(h)$ approaches the sill asymptotically.

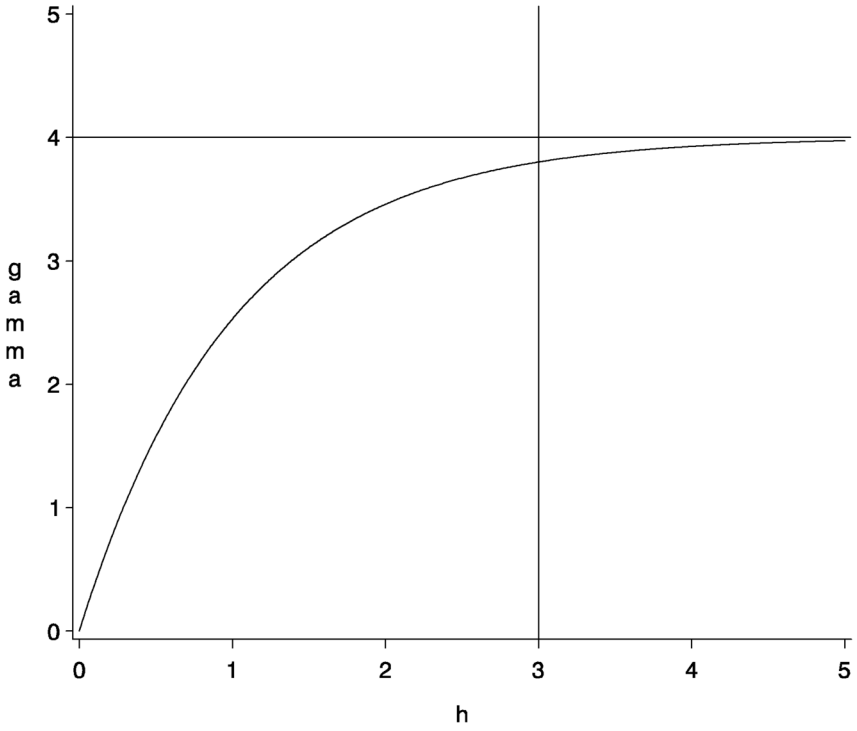
The Exponential Semivariogram Model

The form of the exponential model is

$$\gamma_z(h) = c_0 \left[1 - \exp\left(-\frac{h}{a_0} \right) \right]$$

The shape is displayed in Figure 46.8, using range $a_0 = 1$ and scale $c_0 = 4$.

Figure 46.8 Exponential Semivariogram Model with Parameters $a_0 = 1$ and $c_0 = 4$



The vertical line at $h = r_\epsilon = 3a_0$ is the *effective* (or *practical*) *range*, or the *range* ϵ (that is, the h-value where the covariance is approximately 5% of its value at zero).

The horizontal line at 4.0 variance units (corresponding to $c_0 = 4$) is the sill, as in the previous model types.

It is noted from Figure 46.7 and Figure 46.8 that the major distinguishing feature of the Gaussian and exponential forms is the shape in the neighborhood of the origin $h = 0$. In general, small lags are important in determining an appropriate theoretical form based on a sample semivariogram.

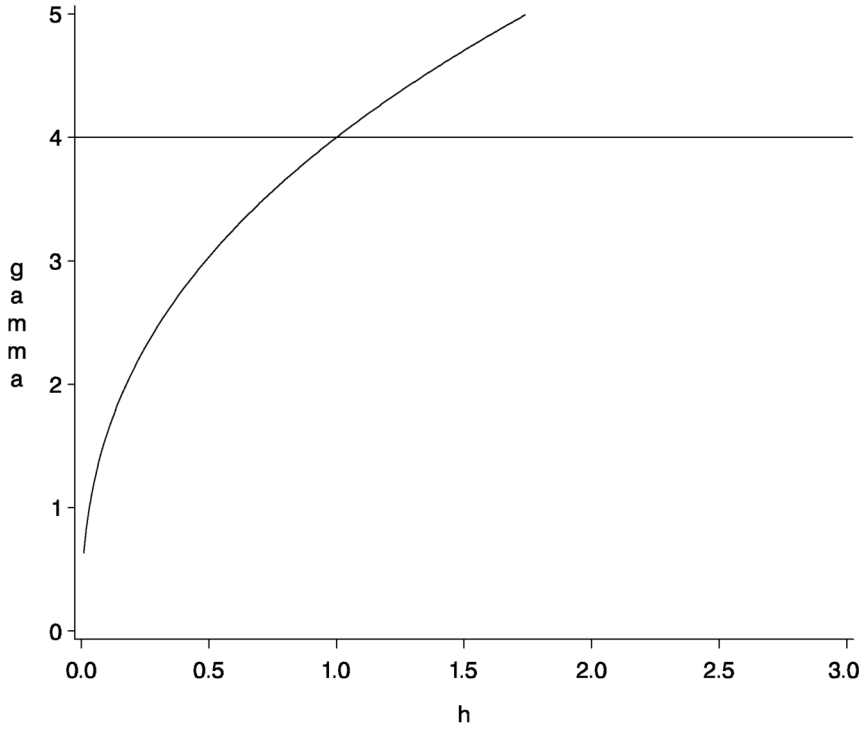
The Power Semivariogram Model

The form of the power model is

$$\gamma_z(h) = c_0 h^{a_0}$$

For this model, the parameter a_0 is a dimensionless quantity, with typical values $0 < a_0 < 2$. Note that the value of $a_0 = 1$ yields a straight line. The parameter c_0 has dimensions of the variance, as in the other models. There is no sill for the power model. The shape of the power model with $a_0 = 0.4$ and $c_0 = 4$ is displayed in Figure 46.9.

Figure 46.9 Power Semivariogram Model with Parameters $a_0 = 0.4$ and $c_0 = 4$



Nested Models

For a given set of spatial data, a plot of an experimental semivariogram might not seem to fit any of the individual theoretical models. In such a case, you might obtain a more accurate fit if you consider your covariance model to be the sum of two or more covariance structures. Such covariance models are called *nested* models. Nesting is common in geologic applications where there are correlations at different length scales. At small lag distances h, the smaller scale correlations dominate, while the large scale correlations dominate at larger lag distances.

Nested models are permissible covariances if they are the sum of permissible models. Therefore, you can include in a sum any combination of the models presented in the preceding subsections and produce permissible covariance models. As an illustration, consider two semivariogram models: an exponential and a spherical:

$$\gamma_{z,1}(h) = c_{0,1} \exp(-\frac{h}{a_{0,1}})$$

and

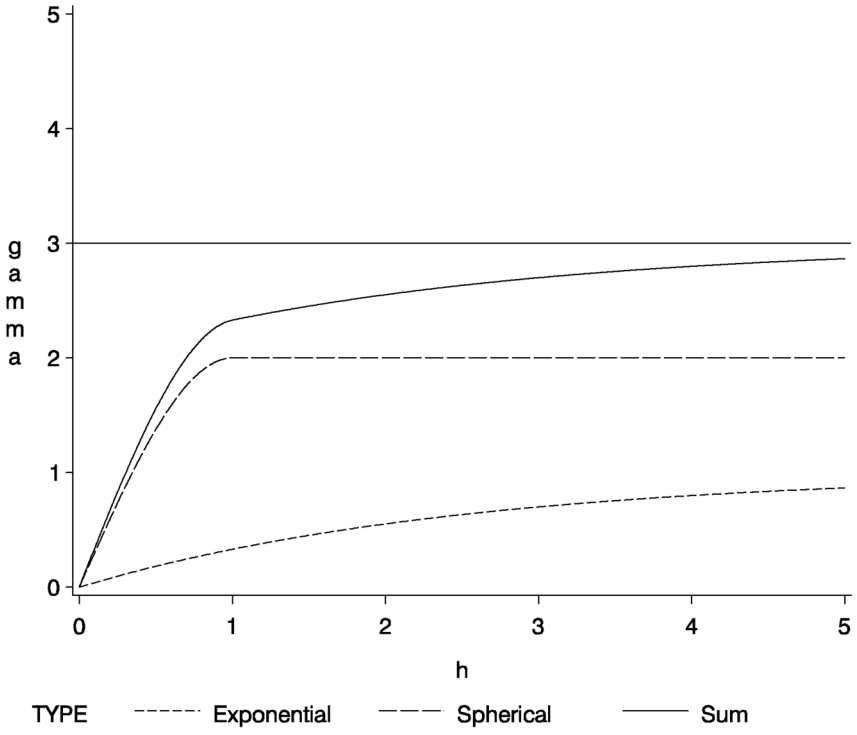
$$\gamma_{z,2}(h) = \left\{ \begin{array}{ll} c_{0,2}\left[\frac{3}{2}\frac{h}{a_{0,2}} - \frac{1}{2}(\frac{h}{a_{0,2}})^3\right], & \text{for } h \le a_{0,2} \\ c_{0,2}, & \text{for } h > a_{0,2} \end{array} \right\}$$

with $c_{0,1} = 1, a_{0,1} = 2.5, c_{0,2} = 2$, and $a_{0,2} = 1$. If both of these correlation structures are present in a spatial process $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D\}$, then the semivariance $\gamma_z(h)$ of this process can be expressed as

$$\gamma_z(h) = \gamma_{z,1}(h) + \gamma_{z,2}(h)$$

In this case, the experimental semivariogram $\gamma_z(h)$ for the process $Z(\boldsymbol{s})$ resembles the semivariogram of the sum of $\gamma_{z,1}(h)$ and $\gamma_{z,2}(h)$. This is illustrated in Figure 46.10.

Figure 46.10 Sum of Exponential and Spherical Structures at Different Scales



The sum of $\gamma_{z,1}(h)$ and $\gamma_{z,2}(h)$ in Figure 46.10 does not resemble any *single* theoretical semivariogram; however, its shape at $h = 1$ is similar to a spherical form. The asymptotic approach to a sill at three variance units, along with the shape around $h = 0$, indicates an exponential structure. Note that the sill value c_0 of the sum is the sum of the individual sills $c_{0,1} = 1$ and $c_{0,2} = 2$. In general, a nested model has a sill equal to the sum of the sills of its nested structures plus the nugget effect, if present.

Refer to Hohn (1988, p. 38ff) for further examples of nested correlation structures.

The Nugget Effect

For all the semivariogram models considered previously, the following property holds:

$$\gamma_z(0) = \lim_{h \downarrow 0} \gamma_z(h) = 0$$

However, a plot of the experimental semivariogram might indicate a discontinuity at $h = 0$; that is, $\gamma_z(h) \rightarrow c_n > 0$ as $h \rightarrow 0$, while $\gamma_z(0) = 0$. The quantity c_n is called the *nugget effect*; this term is from mining geostatistics where nuggets literally exist, and it represents variations at a much smaller scale than any of the measured pairwise distances—that is, at distances $h \ll h_{min}$, where

$$h_{min} = \min_{i,j} h_{ij} = \min_{i,j} | \boldsymbol{s}_i - \boldsymbol{s}_j |$$

There are conceptual and theoretical difficulties associated with a nonzero nugget effect; refer to Cressie (1993, Section 2.3.1) and Christakos (1992, Section 7.4.3) for details. There is no *practical* difficulty, however; you simply visually extrapolate the experimental semivariogram as $h \rightarrow 0$. The importance of availability of data at small lag distances is again illustrated.

As an example, an exponential semivariogram with a nugget effect c_n has the form

$$\gamma_z(h) = c_n + {\sigma_0}^2 \left[1 - \exp\left(-\frac{h}{a_0} \right) \right], h > 0$$

and

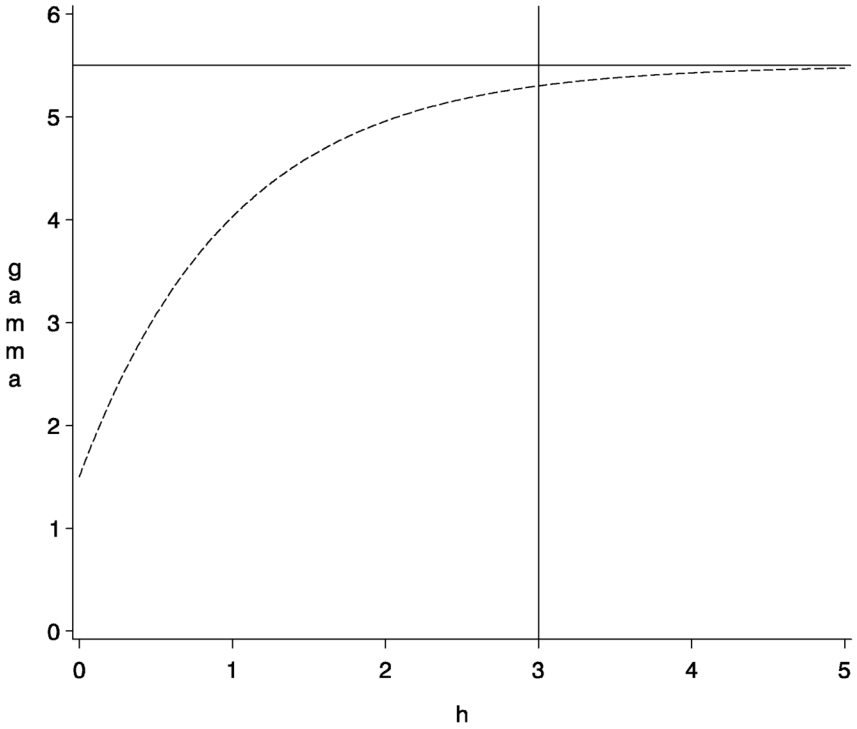
$$\gamma_z(0) = 0$$

where the factor ${\sigma_0}^2$ is called the *partial sill*, and the sill $c_0 = c_n + {\sigma_0}^2$.

This is illustrated in Figure 46.11 for the parameters $a_0 = 1$, ${\sigma_0}^2 = 4$, and nugget effect $c_n = 1.5$.

You can specify the nugget effect in PROC KRIGE2D with the NUGGET= option in the MODEL statement. It is a separate, additive term independent of direction; that is, it is isotropic. There is a way to approximate an anisotropic nugget effect; this is described in the following section.

Figure 46.11 Exponential Semivariogram Model with a Nugget Effect $c_n = 1.5$



Anisotropic Models

In all of the theoretical models considered previously, the lag distance h entered as a scalar value. This implies that the correlation between the spatial process at two point pairs P_1, P_2 is dependent *only* on the separation distance $h = | P_1 P_2 |$, not on the orientation of the vector $\boldsymbol{h}$. A spatial process described by an SRF $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2\}$ with this property is called isotropic, as is the associated covariance or semivariogram.

However, real spatial phenomena often show directional effects. Particularly in geologic applications, measurements along a particular direction might be highly correlated, while typically the perpendicular direction shows little or no correlation. Such processes are called anisotropic; see, for example, Journel and Huijbregts (1978, Section III.B.4).

When the correlation structure varies across different directions, you need different models for each direction so that you can account correctly for the continuity within the SRF. As you will see in the following subsections, techniques are applied to override the anisotropy effects for computational purposes. First, we examine characteristics of anisotropy.

The semivariogram sill is a measure of the process variability, hence the direction of the highest continuity is perpendicular to the direction where the highest sill occurs. If the sill is the same in all directions, then the direction with the highest range indicates highest continuity. The directions in which the spatial process $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D\}$ is most and least correlated are called the *major* and *minor* axis of anisotropy, respectively.

In some cases, these directions are known a priori. This can occur in mining applications where the geology of a region is known in advance. In most cases, however, nothing is known about possible anisotropy. Depending on the amount of data available, using several directions is usually sufficient to determine the presence of anisotropy and to find the approximate major/minor axis directions; see the discussion in the section "Anisotropy" on page 7539 in the VARIOGRAM procedure documentation. You can find a detailed example of anisotropy investigation in the section "Example 95.2: An Anisotropic Case Study with Surface Trend in the Data" on page 7566 in the VARIOGRAM procedure documentation.

Once you explore an anisotropic process and you identify the minor and major axis directions, you can compute the *anisotropy factor* parameter R which is defined as

$$R = \frac{{a_0}^{min}}{{a_0}^{max}}$$

where ${a_0}^{min}$ is the semivariogram range in the direction of the minor axis and ${a_0}^{max}$ is the semivariogram range in the direction of the major axis.

There are two types of anisotropy, depending on which semivariogram characteristics change in different directions. These types are the *geometric* and the *zonal* anisotropy, and either or both can be present. Both are examined in detail in the following subsections.

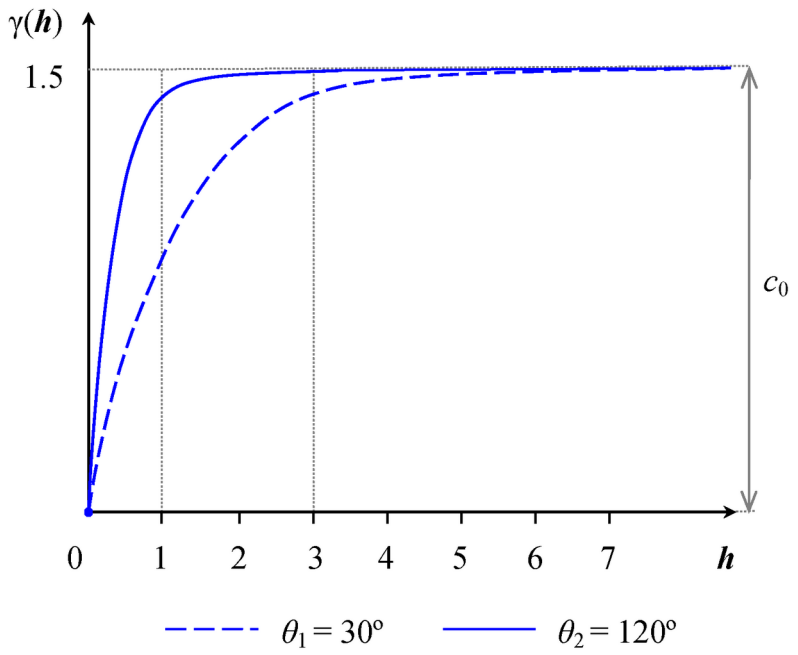
Geometric Anisotropy

Geometric anisotropy is the simplest type of anisotropy. It occurs when the same sill (or scale) parameter c_0 is present in all directions but the range a_0 changes with direction. Note also that in geometric anisotropy the same covariance form (or forms, if you use a nested model) is present in all directions.

Therefore, there is a single sill in geometric anisotropy, but the semivariogram reaches the sill in a shorter lag distance along a certain direction. This is illustrated in Figure 46.12, where an anisotropic exponential semivariogram is plotted. Assume that the two curves displayed in this figure have the same sill $c_0 = 1.5$ and are generated using the ranges $a_{0,1} = 3$ in the direction $\theta_1 = 30°$ (effective range is $r_{\epsilon,1} = 9$) and $a_{0,2} = 1$ in the direction $\theta_2 = 120°$ (effective range is $r_{\epsilon,2} = 3$).

As you can see from the figure, the ratio of the shorter to longer range is $R = 1/3$. The anisotropy factor R is the value to use in the RATIO= parameter in the MODEL statement in PROC KRIGE2D. Note that $R \leq 1$ for modeling geometric anisotropy. In fact, isotropy is a partial case of geometric anisotropy for which ${a_0}^{min} = {a_0}^{max}$ and $R = 1$.

Figure 46.12 Geometric Anisotropy with Major Axis in the Direction $\theta_1 = 30°$



The values of the RANGE= and ANGLE= parameters in the MODEL statement in PROC KRIGE2D are set based on the major anisotropy axis characteristics. Specifically, the RANGE= parameter is the value of the major axis range ${a_0}^{max} = a_{0,1}$, and the ANGLE= parameter is the angle θ_1 of the major axis measured clockwise from north (angles measured in this way are also known as *azimuths*). You can then specify the following MODEL statement in PROC KRIGE2D to approximate the covariance structure:

```
MODEL FORM=EXP RANGE=3 SCALE=1.5 ANGLE=30 RATIO=0.3333;
```

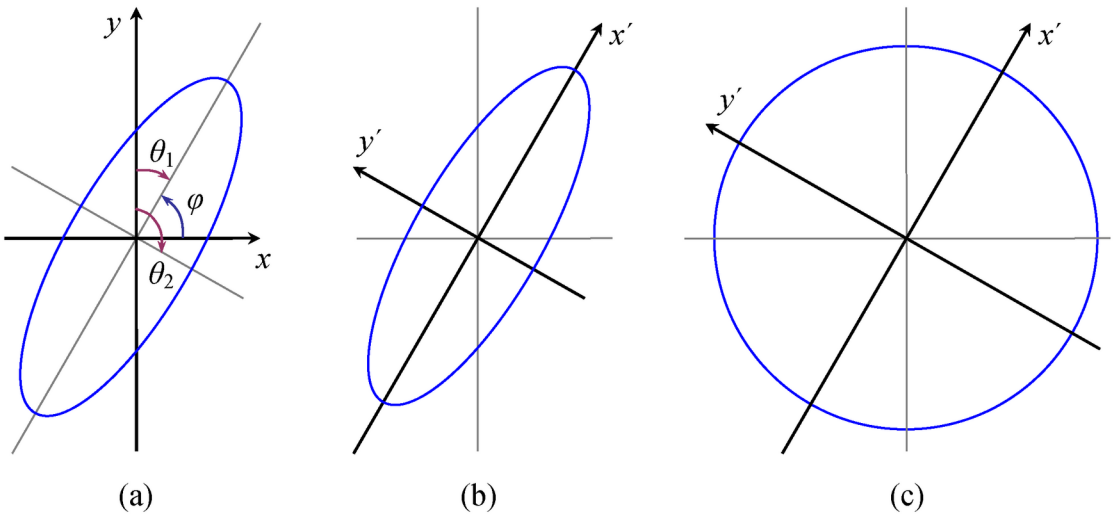
If you use a nested model, provide the type for each one of the nested structures with the FORM= option, and assign the individual SCALE= parameters so that they add up to the total sill (include in the sum the nugget effect, if present). In the typical case, all of your nested structures have the same anisotropy axes. This means that you specify the same ANGLE= parameter value for all structures. Each structure likely has its own values for the RANGE= and RATIO= parameters depending on the degree of its contribution to the nested model.

The terminology associated with geometric anisotropy is that of ellipses. To see how this comes about, consider the following hypothetical set of calculations. Let $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2\}$ be a geometrically anisotropic process, and assume there are sufficient data points to calculate an experimental semivariogram at a large number of angle classes $\theta \in \{0, \delta\theta, 2\delta\theta, \cdots, 180°\}$. At each of these angles θ, the experimental semivariogram is plotted and the range a_0 is recorded. A diagram in polar coordinates (a_0, θ) yields an ellipse with the major axis ${a_0}^{max}$ in the direction of the largest a_0 and the minor axis ${a_0}^{min}$ perpendicular to it. For the example in Figure 46.12, the ellipse is shown in Figure 46.13(a). Its major axis has size ${a_0}^{max}$ situated at angle θ_1 clockwise from north, and the minor axis has size ${a_0}^{min}$ oriented at angle θ_2 clockwise from north.

The KRIGE2D procedure handles geometric anisotropy by applying a reversible transformation in two steps that converts geometric anisotropy into isotropic conditions.

The first step is to align your coordinates axes with the anisotropy ellipse axes. Specifically, you choose to rotate by an angle φ the standard Cartesian orientation of the (x, y) coordinates system shown in Figure 46.13(a) so that the y axis coincides with the ellipse minor axis. The rotation result is illustrated in Figure 46.13(b). The second step is to elongate the minor axis so its length equals that of the major axis of the ellipse. You can see the result in Figure 46.13(c). The computational details are shown in the following.

Figure 46.13 Transformation Applied to Geometric Anisotropy



The transformation angle φ is measured in standard Cartesian orientation counterclockwise from the x axis (east). If the major axis azimuth is θ_1, then the Cartesian system of (x, y) needs to be rotated by $\varphi = 90^\circ - \theta_1$ so that the y axis can coincide with the ellipse minor axis; see Figure 46.13(a). Let us call the ellipse major axis x' and the minor axis y'. The transformation that converts any coordinates in the (x, y) system into (x', y') coordinates in terms of φ is given by the matrix:

$$\mathbf{H} = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ -\sin(\varphi) & \cos(\varphi) \end{pmatrix}$$

The elongation of the minor axis in the second step is performed with the matrix:

$$\mathbf{D}_R = \begin{pmatrix} 1 & 0 \\ 0 & 1/R \end{pmatrix}$$

Note that these two steps are sequential and their order cannot be reversed. For any point pair P_1 and P_2 with respective coordinates $\boldsymbol{s}_1 = (x_1, y_1)$ and $\boldsymbol{s}_2 = (x_2, y_2)$ in the (x, y) axes, their distance is given by:

$$| P_i P_j |_{(x,y)} = h = \sqrt{(\delta x)^2 + (\delta y)^2}$$

where the distance components $\delta x = x_2 - x_1$ and $\delta y = y_2 - y_1$. Based on the previous, the corresponding distances $\delta x'$ and $\delta y'$ in the (x', y') coordinates system are given by the vector:

$$\begin{pmatrix} \delta x' \\ \delta y' \end{pmatrix} = \mathbf{D}_R \, \mathbf{H} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix} = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ -\sin(\varphi)/R & \cos(\varphi)/R \end{pmatrix} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}$$

The transformed interpair distance is then:

$$\mid P_i P_j \mid_{(x',y')} = h' = \sqrt{(\delta x')^2 + (\delta y')^2}$$

As a result, the original anisotropic semivariogram in Figure 46.12 that was a function $\gamma(\boldsymbol{h}) = \gamma(h, \theta)$ of both h and θ is then transformed to an equivalent function $\hat{\gamma}(h')$ only of h':

$$\hat{\gamma}(h') = \gamma(\boldsymbol{h})$$

This single isotropic semivariogram $\hat{\gamma}(h')$ is then used for kriging purposes.

Note that the two steps used by PROC KRIGE2D in the previous analysis can be performed in a different manner, as well. For instance, you might equivalently choose to rotate the (x, y) Cartesian coordinates so that the y axis coincides with the ellipse major axis, rather than with the minor axis as was shown earlier. Also, you might prefer to compress the major axis rather than elongating the short one. In any case, you need to perform the appropriate computations for the transformation of your choice.

Zonal Anisotropy

In zonal anisotropy, the sill (or scale) parameter c_0 is different for different directions. It is not possible to transform such a structure into an isotropic semivariogram. Instead, nesting and geometric anisotropy are used together to approximate zonal anisotropy. Due to this process, you might also have to use different covariance forms in different directions, as shown in the following discussion.

The main idea when you deal with zonal anisotropy is to specify structures in the covariance model that contribute exclusively in particular directions and thus increase the sill only in these directions. After you have identified such a structure, you assign it a suitable range in the contributing direction. The contributing direction is the one of maximum continuity for this structure; hence it is the structure's major anisotropy axis with a range of ${a_0}^{max}$. For all other specified directions you want to use an infinite range that suggests that the structure sill is never reached in these directions.

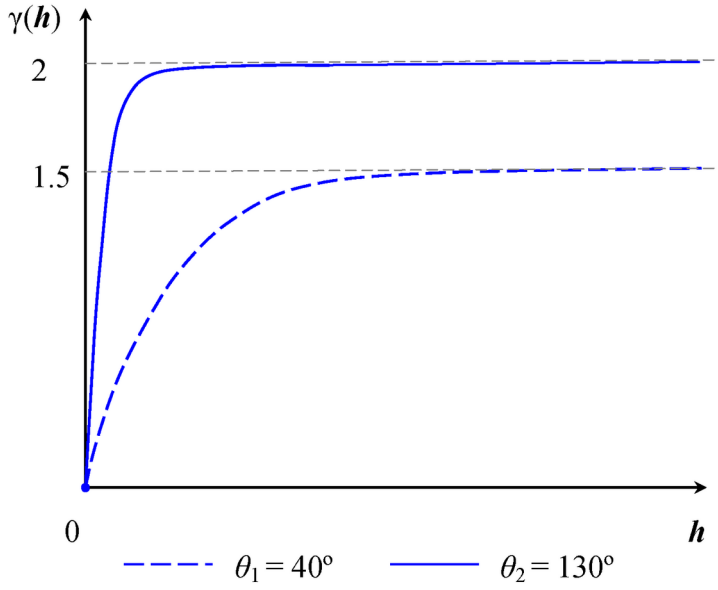
Practically, you can consider the structure range in any non-contributing direction to be a very large number compared to ${a_0}^{max}$. This means that the anisotropy factor R for this structure is a very large number, too. Accordingly, in PROC KRIGE2D you indicate the presence of zonal anisotropy and a covariance structure that contributes only in a particular direction by specifying the RATIO= parameter of this structure to a be large number. The two examples that follow illustrate different instances of zonal anisotropy and how to specify the corresponding covariance model parameters in PROC KRIGE2D.

Example 1

The first example shows that if you can model the direction with the highest sill as a nested model, you then treat the case as a composition of geometric anisotropy and an additional structure that acts only in the direction of the increased sill.

Consider a spatial process where the fitting of theoretical models in your experimental semivariogram produces a correlation structure like the one shown in Figure 46.14. In the direction $\theta_1 = 40°$, the covariance model has a single exponential structure $\gamma_1(\boldsymbol{h}) = \text{Exp}(a_{0,1E}, c_{0,1E})$ with range $a_{0,1E} = 2$ and sill $c_{0,1E} = 1.5$. In the direction $\theta_2 = 130°$, the covariance model $\gamma_2(\boldsymbol{h}) = \text{Exp}(a_{0,2E}, c_{0,2E}) + \text{Sph}(a_{0,2S}, c_{0,2S})$ has two nested structures: an exponential structure with range $a_{0,2E} = 0.5$ and sill $c_{0,2E} = 1.5$ and a spherical structure with range $a_{0,2S} = 1$ and sill $c_{0,2S} = 0.5$.

Figure 46.14 Zonal Anisotropy in Two Directions



The total sill in the direction θ_2 of the highest variance is the sum of the nested structures sills $c_{0,2E} + c_{0,2S} = 2$. You can consider that your process is characterized: (a) by a geometrically anisotropic exponential structure with common sill $c_{0,E} = 1.5$ across all directions and major axis range $a_{0,1E} = 2$ and (b) by a spherical structure which is a zonal anisotropy component that contributes only in the θ_2 direction. Based on the remarks in this section, the RATIO= parameter for the exponential structure is $R_E = 0.5/2 = 0.25$, whereas for the spherical structure you choose a large value, such as $R_S = 10^8$.

Then, you can approximate this structure in PROC KRIGE2D by specifying the two structures with the following MODEL statement:

```
MODEL FORM=(EXP,SPH) RANGE=(2,1) SCALE=(1.5,0.5)
      ANGLE=(40,130) RATIO=(0.25,1E8);
```

You can handle more elaborate cases in a similar way, where the covariance models in different directions might all be nested models. Your goal is to model the continuity by starting with a sum of isotropic or geometrically anisotropic structures whose total sill is the lowest sill in all directions. Then, in each of the directions with higher sills you add a zonal anisotropy component in the corresponding sum that compensates for the increased variability in that direction.

Example 2

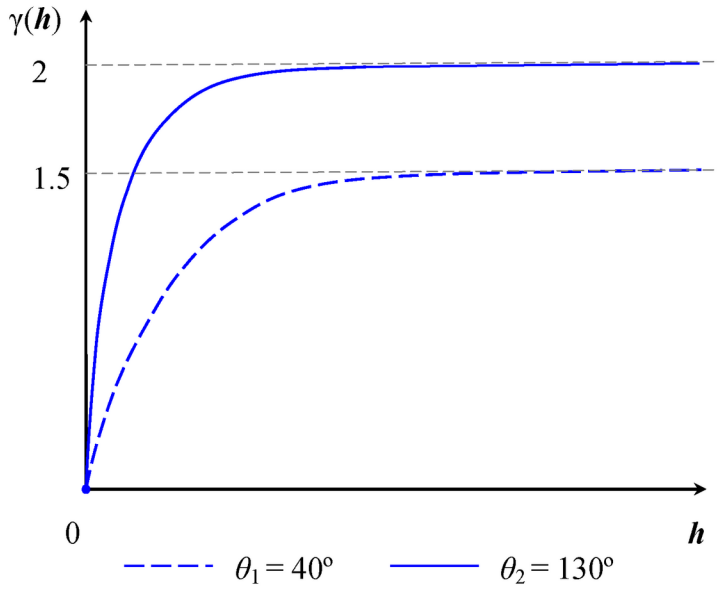
The second example provides important perspective of the physics in the zonal anisotropy analysis. It is an extreme case of the general guidelines for zonal anisotropy. You examine what happens when each of the directions can be modeled with a simple, nonnested model, and the sills for these models are clearly different.

Consider a spatial process with a spatial continuity description almost identical to the one in the previous example. In the direction θ_1, the covariance model has again a single exponential structure $\gamma_1(\boldsymbol{h}) = \text{Exp}(a_{0,1E}, c_{0,1E})$ with range $a_{0,1E} = 2$ and sill $c_{0,1E} = 1.5$. However, this time in the direction θ_2 you have fit the experimental semivariogram by using a single exponential structure $\gamma_2(\boldsymbol{h}) = \text{Exp}(a_{0,2E}, c_{0,2E})$ with range $a_{0,2E} = 1$ and sill $c_{0,2E} = 2$. These models are shown in Figure 46.15.

In this case you have a simplified situation with a single covariance structure in each direction, and neither structure contributes to the sill of the other direction. Hence, you could consider them both to be zonal anisotropy components, where there is no variation due to $\gamma_1(\boldsymbol{h})$ in the θ_2 direction and no variation due to $\gamma_2(\boldsymbol{h})$ in the θ_1 direction. As a result, both structures can be practically approximated by specifying two models with large RATIO= values. You could then use the following MODEL statement in PROC KRIGE2D to describe the covariance in this example:

```
MODEL FORM=(EXP,EXP) RANGE=(2,1) SCALE=(1.5,2)
      ANGLE=(40,130) RATIO=(1E8,1E8);
```

Figure 46.15 Zonal Anisotropy in Two Directions



However, note that the preceding representation of the spatial continuity accounts only for the specified directions of angles θ_1 and θ_2. Then, the lack of an underlying covariance structure in all other directions can be interpreted as zero continuity everywhere in the process except along the axes at angles θ_1 and θ_2. This would be a very unlikely occurrence in natural processes.

An acceptable alternative would be an attempt to represent the continuity by filling in the intermediate levels of the sill between its lowest and highest values. This would require that you provide zonal anisotropy components for as many directions as possible, thus monitoring closely the spatial continuity by means of the directional change of the process sill. However, in this way you are considering discretized directional intervals, so you are still missing a description for the spatial continuity in the intermediate directions within these intervals. This is also a more complicated approach which can be more tedious than the analysis in the previous example.

For that reason, it is strongly advised that in similar cases you should try to use the analysis illustrated in the previous example. In particular, you should try to model the highest sill direction as a nested structure, such that it comprises a geometrical anisotropy component with cumulative sill equal to the lower sill and a zonal anisotropy component that accounts for the sill difference.

Anisotropic Nugget Effect

Note that an isotropic nugget effect can be approximated by using nested models, with one of the nested structures having a small range. Applying a geometric anisotropy specification to this nested structure results in an anisotropic nugget effect.

Details of Ordinary Kriging

Introduction

There are three common characteristics often observed with spatial data (that is, data indexed by their spatial locations):

(i) slowly varying, large-scale variations in the measured values

(ii) irregular, small-scale variations

(iii) similarity of measurements at locations close together

As an illustration, consider a hypothetical example in which an organic solvent leaks from an industrial site and spreads over a large area. Assume the solvent is absorbed and immobilized into the subsoil above any groundwater level, so you can ignore any time dependence.

To find the areal extent and the concentration values of the solvent, you need measurements. Although the problem is inherently three-dimensional, if you measure total concentration in a column of soil or take a depth-averaged concentration, it can be handled reasonably well with two-dimensional techniques.

You usually assume that measured concentrations are higher closer to the source and decrease at larger distances from the source. On top of this smooth variation, there are small-scale variations in the measured concentrations, due perhaps to the inherent variability of soil properties.

You also tend to suspect that measurements made close together yield similar concentration values, while measurements made far apart can have very different values.

These physically reasonable qualitative statements have no explicit probabilistic content, and there are a number of numerical smoothing techniques, such as inverse distance weighting and splines, that make use of large-scale variations and "close distance-close value" characteristics of spatial data to interpolate the measured concentrations for contouring purposes.

While characteristics (i) and (iii) are handled by such smoothing methods, characteristic (ii), the small-scale residual variation in the concentration field, is not accounted for.

There can be situations, due to the use of the prediction map or the relative magnitude of the irregular fluctuations, where you cannot ignore these small-scale irregular fluctuations. In other words, the smoothed or predicted values of the concentration field alone are not a sufficient characterization; you also need the possible spread around these contoured values.

Spatial Random Fields

One method of incorporating characteristic (ii) into the construction of a contour map is to model the concentration field as a spatial random field (SRF). The mathematical details of SRF models are given in a number of texts, such as Cressie (1993) and Christakos (1992). The mathematics of SRFs is formidable. However, under certain simplifying assumptions, it produces classical linear predictors with very simple properties, allowing easy implementation for prediction purposes. These predictors, primarily ordinary kriging (OK), give both a prediction and a standard error of prediction at unsampled locations. This allows the construction of a map of both predicted values and level of uncertainty about the predicted values.

The key assumption in applying the SRF formalism is that the measurements come from a single realization of the SRF. However, in most geostatistical applications, the focus is on a single, unique realization. This is unlike most other situations in stochastic modeling in which there will be future experiments or observational activities (at least conceptually) under similar circumstances. This renders many traditional ideas of statistical inference ambiguous and somewhat counterintuitive.

There are additional logical and methodological problems in applying a stochastic model to a unique but partly unknown natural process; refer to the introduction in Matheron (1971) and Cressie (1993, Section 2.3). These difficulties have resulted in attempts to frame the prediction problem in a completely deterministic way (Isaaks and Srivastava 1988; Journel 1985). Also, some issues with kriging, and with spatial prediction methods in general, are related to the necessary assumption of ergodicity of the spatial process. This assumption is required to estimate the covariance or semivariogram from sample data. Details are provided in Cressie (1993, pp. 52–58).

Despite these difficulties, ordinary kriging remains a popular and widely used tool in modeling spatial data, especially in generating surface plots and contour maps. An abbreviated derivation of the OK predictor for point prediction and the associated standard error is discussed in the following section. Full details are given in Journel and Huijbregts (1978), Christakos (1992), and Cressie (1993).

Ordinary Kriging

Denote the SRF by $Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2$. Following the notation in Cressie (1993), the following model for $Z(\boldsymbol{s})$ is assumed:

$$Z(\boldsymbol{s}) = \mu + \varepsilon(\boldsymbol{s})$$

Here, μ is the fixed, unknown mean of the process, and $\varepsilon(\boldsymbol{s})$ is a zero mean SRF representing the variation around the mean.

In most practical applications, an additional assumption is required in order to estimate the covariance C_z of the $Z(\boldsymbol{s})$ process. This assumption is second-order stationarity:

$$C_z(\boldsymbol{s}_1, \boldsymbol{s}_2) = \mathrm{E}[\varepsilon(\boldsymbol{s}_1)\varepsilon(\boldsymbol{s}_2)] = C_z(\boldsymbol{s}_1 - \boldsymbol{s}_2) = C_z(\boldsymbol{h})$$

This requirement can be relaxed slightly when you are using the semivariogram instead of the covariance. In this case, second-order stationarity is required of the differences $\varepsilon(\boldsymbol{s}_1) - \varepsilon(\boldsymbol{s}_2)$ rather than $\varepsilon(\boldsymbol{s})$:

$$\gamma_z(\boldsymbol{s}_1, \boldsymbol{s}_2) = \frac{1}{2}\mathrm{E}[(\varepsilon(\boldsymbol{s}_1) - \varepsilon(\boldsymbol{s}_2))^2] = \gamma_z(\boldsymbol{s}_1 - \boldsymbol{s}_2) = \gamma_z(\boldsymbol{h})$$

By performing local kriging, the spatial processes represented by the previous equation for $Z(\boldsymbol{s})$ are more general than they appear. In local kriging, at an unsampled location $\boldsymbol{s}_0$, a separate model is fit using only data in a neighborhood of $\boldsymbol{s}_0$. This has the effect of fitting a separate mean μ at each point, and it is similar to the *kriging with trend* (KT) method discussed in Journel and Rossi (1989).

Given the N measurements $Z(\boldsymbol{s}_1), \ldots, Z(\boldsymbol{s}_N)$ at known locations $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_N$, you want to obtain a prediction of Z at an unsampled location $\boldsymbol{s}_0$. When the following three requirements are imposed on the predictor $\hat{Z}$, the OK predictor is obtained.

(i) $\hat{Z}$ is linear in $Z(\boldsymbol{s}_1), \cdots, Z(\boldsymbol{s}_N)$.

(ii) $\hat{Z}$ is unbiased.

(ii) $\hat{Z}$ minimizes the mean square prediction error $\mathrm{E}[(Z(\boldsymbol{s}_0) - \hat{Z}(\boldsymbol{s}_0))^2]$.

Linearity requires the following form for $\hat{Z}(\boldsymbol{s}_0)$:

$$\hat{Z}(\boldsymbol{s}_0) = \sum_{i=1}^{N} \lambda_i Z(\boldsymbol{s}_i)$$

Applying the unbiasedness condition to the preceding equation yields

$$\mathrm{E}[\hat{Z}(\boldsymbol{s}_0)] = \mu \Rightarrow \sum_{i=1}^{N} \lambda_i \mathrm{E}[Z(\boldsymbol{s}_i)] = \mu \Rightarrow \sum_{i=1}^{N} \lambda_i \mu = \mu \Rightarrow \sum_{i=1}^{N} \lambda_i = 1$$

Finally, the third condition requires a constrained linear optimization involving $\lambda_1, \cdots, \lambda_N$ and a Lagrange parameter $2m$. This constrained linear optimization can be expressed in terms of the function $L(\lambda_1, \cdots, \lambda_N, m)$ given by

$$L = \mathrm{E}\left[\left(Z(\boldsymbol{s}_0) - \sum_{i=1}^{N} \lambda_i Z(\boldsymbol{s}_i)\right)^2\right] - 2m\left(\sum_{i=1}^{N} \lambda_i - 1\right)$$

Define the $N \times 1$ column vector $\boldsymbol{\lambda}$ by

$$\boldsymbol{\lambda} = (\lambda_1, \cdots, \lambda_N)^T$$

and the $(N+1) \times 1$ column vector $\boldsymbol{\lambda_0}$ by

$$\boldsymbol{\lambda_0} = (\lambda_1, \cdots, \lambda_N, m)^T = \begin{pmatrix} \boldsymbol{\lambda} \\ m \end{pmatrix}$$

The optimization is performed by solving

$$\frac{\partial L}{\partial \boldsymbol{\lambda_0}} = \mathbf{0}$$

in terms of $\lambda_1, \cdots, \lambda_N$ and m.

The resulting matrix equation can be expressed in terms of either the covariance $C_z(\boldsymbol{h})$ or semivariogram $\gamma_z(\boldsymbol{h})$. In terms of the covariance, the preceding equation results in the following matrix equation:

$$\mathbf{C}\boldsymbol{\lambda_0} = \mathbf{C_0}$$

where

$$\mathbf{C} = \begin{pmatrix} C_z(\mathbf{0}) & C_z(\boldsymbol{s}_1 - \boldsymbol{s}_2) & \cdots & C_z(\boldsymbol{s}_1 - \boldsymbol{s}_N) & 1 \\ C_z(\boldsymbol{s}_2 - \boldsymbol{s}_1) & C_z(\mathbf{0}) & \cdots & C_z(\boldsymbol{s}_2 - \boldsymbol{s}_N) & 1 \\ & & \ddots & & \\ C_z(\boldsymbol{s}_N - \boldsymbol{s}_1) & C_z(\boldsymbol{s}_N - \boldsymbol{s}_2) & \cdots & C_z(\mathbf{0}) & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix}$$

and

$$\mathbf{C_0} = \begin{pmatrix} C_z(\boldsymbol{s}_0 - \boldsymbol{s}_1) \\ C_z(\boldsymbol{s}_0 - \boldsymbol{s}_2) \\ \vdots \\ C_z(\boldsymbol{s}_0 - \boldsymbol{s}_N) \\ 1 \end{pmatrix}$$

The solution to the previous matrix equation is

$$\hat{\boldsymbol{\lambda}}_\mathbf{0} = \mathbf{C}^{-1}\mathbf{C_0}$$

Using this solution for $\boldsymbol{\lambda}$ and m, the ordinary kriging prediction at r_0 is

$$\hat{Z}(\boldsymbol{s}_0) = \lambda_1 Z(\boldsymbol{s}_1) + \cdots + \lambda_N Z(\boldsymbol{s}_N)$$

with associated prediction error the square root of the variance

$${\sigma_z}^2(\boldsymbol{s}_0) = C_z(\mathbf{0}) - \boldsymbol{\lambda}'\mathbf{c_0} + m$$

where $\mathbf{c_0}$ is $\mathbf{C_0}$ with the 1 in the last row removed, making it an $N \times 1$ vector.

These formulas are used in the best linear unbiased prediction (BLUP) of random variables (Robinson 1991). Further details are provided in Cressie (1993, pp. 119–123).

Because of possible numeric problems when solving the previous matrix equation, Deutsch and Journel (1992) suggest replacing the last row and column of 1s in the preceding matrix $\mathbf{C}$ by $C_z(0)$, keeping the 0 in the $(N+1, N+1)$ position and similarly replacing the last element in the preceding right-hand vector $\mathbf{C_0}$ with $C_z(0)$. This results in an equivalent system but avoids numeric problems when $C_z(0)$ is large or small relative to 1.

Computational Resources

To generate a predicted value at a single grid point by using N data points, PROC KRIGE2D must solve the following kriging system:

$$\mathbf{C}\boldsymbol{\lambda_0} = \mathbf{C_0}$$

where the dimensions of $\mathbf{C}$ are $(N+1) \times (N+1)$, and the right-hand-side $\mathbf{C_0}$ has one column.

Holding the matrix and vector associated with this system in core requires approximately $8N^2/2$ bytes. The CPU time used in solving the system is proportional to N^3. For large N, this time dominates the $O(N^2)$ time to compute the elements of the covariance matrix $\mathbf{C}$ from the specified covariance or semivariogram model.

For local kriging, the kriging system is set up and solved for each grid point. Part of the setup process involves determining the neighborhood of each grid point. A fast K-D tree algorithm is used to determine neighborhoods. For G grid points, the dominant CPU time factor is setting up and solving the G kriging systems. The N in the algorithm of the section "Ordinary Kriging" on page 2962 is the number of data points in a given neighborhood, and it can differ for each grid point.

In global kriging, the entire input data set and all grid points are used to set up and solve the single system

$$\mathbf{C}\boldsymbol{\lambda_0} = \mathbf{C_0}$$

Again $\mathbf{C}$ has dimensions $(N+1) \times (N+1)$, but $\boldsymbol{\lambda_0}$ and $\mathbf{C_0}$ now have G columns, where G is the number of grid points. Memory requirements are approximately $8[(N^2/2) + GN]$ bytes. The CPU time used in solving the system is still dominated by the N^3 factorization of the left-hand side.

Output Data Sets

The KRIGE2D procedure produces two data sets: the OUTEST=*SAS-data-set* and the OUTNBHD=*SAS-data-set*. These data sets are described as follows.

OUTEST=*SAS-data-set*

The OUTEST= data set contains the kriging predictions and the associated standard errors. The OUTEST= data set contains the following variables:

- ESTIMATE, which is the kriging prediction for the current variable
- GXC, which is the x coordinate of the grid point at which the kriging prediction is made
- GYC, which is the y coordinate of the grid point at which the kriging prediction is made
- LABEL, which is the label for the current PREDICT/MODEL combination producing the kriging prediction. If you do not specify a label, default labels of the form Pred*j*.Model*k* are used.
- NPOINTS, which is the number of points used in the prediction. This number varies for each grid point if local kriging is performed.
- STDERR, which is the standard error of the kriging predict
- VARNAME, which is the variable name

OUTNBHD=*SAS-data-set*

When you specify the RADIUS= option or the NUMPOINTS= option in the PREDICT statement, local kriging is performed. Local kriging is simply ordinary kriging at a given grid location, using only those data points in a neighborhood defined by the RADIUS= value or the NUMPOINTS= value.

The OUTNBHD= data set contains one observation for each data point in each neighborhood. Hence, this data set can be large. For example, if the grid specification results in 1,000 grid points and each grid point has a neighborhood of 100 points, the resulting OUTNBHD= data set contains 100,000 points.

The OUTNBHD= data set contains the following variables:

- GXC, which is the x coordinate of the grid point
- GYC, which is the y coordinate of the grid point
- LABEL, which is the label for the current PREDICT/MODEL combination. If you do not specify a label, default labels of the form Pred*j*.Model*k* are used.

- NPOINTS, which is the number of points used in the prediction
- RADIUS, which is the radius used for each neighborhood
- VALUE, which is the value of the variable at the current data point
- VARNAME, which is the variable name of the current variable
- XC, which is the x coordinate of the current data point
- YC, which is the y coordinate of the current data point

Displayed Output

In addition to the output data sets, the KRIGE2D procedure produces output objects as well. The KRIGE2D procedure output objects are the following:

- a default "Number of Observations" table that displays the number of observations read from the input data set and the number of observations used in the analysis
- a map showing the spatial distribution of the observations of the current VAR variable in the PREDICT statement. The observations are displayed by default with circled markers whose color indicates the VAR value at the corresponding location.
- a default table for each PREDICT statement that sums up basic information about the kriging analysis
- a default table for each MODEL statement that shows the covariance model parameters for the corresponding PREDICT statement
- plots of the kriging prediction and the prediction standard error at each point of the specified output grid. The KRIGE2D procedure produces by default a plot of the kriging prediction and the corresponding prediction error for each MODEL statement of every PREDICT statement that you specify. You can produce more of these plots with styles that you can specify by using the available suboptions of the PLOTS=PREDICTION option.

ODS Table Names

Each table created by PROC KRIGE2D has a name associated with it, and you must use this name to reference the table when using ODS Graphics. These names are listed in Table 46.2.

Table 46.2 ODS Tables Produced by PROC KRIGE2D

ODS Table Name	Description	Statement	Option
KrigInfo	Kriging analysis general information	PROC	default output
ModelInfo	Parameters of the covariance model used in current kriging analysis	PROC	default output
NObs	Number of observations read and used	PROC	default output

ODS Graphics

This section describes the use of the Output Delivery System (ODS) for creating graphics with the KRIGE2D procedure.

To request these graphs, you must specify the ODS GRAPHICS statement. For additional control of the graphics that are displayed, see the PLOTS= option in the section "PROC KRIGE2D Statement" on page 2935. For more information about the ODS GRAPHICS statement, see Chapter 21, "Statistical Graphics Using ODS."

ODS Graph Names

PROC KRIGE2D assigns a name to each graph it creates by using ODS Graphics. You can use these names to reference the graphs when using ODS Graphics. The names are listed in Table 46.3.

Table 46.3 ODS Graphics Produced by PROC KRIGE2D

ODS Graph Name	Plot Description	Statement	Option
ObservationsPlot	Scatter plot of observed data and colored markers indicating observed values	PROC	PLOTS=OBSERV
PredictionPlot	Contour plots of the kriging prediction, surface of the prediction error, and outlines of the observation locations	PROC	PLOTS=PREDICTION

To request these graphs, you must specify the ODS GRAPHICS statement in addition to the statements indicated in Table 46.3. For more information about the ODS GRAPHICS statement, see Chapter 21, "Statistical Graphics Using ODS."

Examples: KRIGE2D Procedure

Example 46.1: Investigating the Effect of Model Specification on Prediction

In the section "Example 95.1: Theoretical Semivariogram Model Fitting" on page 7562 in the VARIOGRAM procedure, a particular theoretical semivariogram is chosen for the coal seam thickness data. The chosen semivariogram is Gaussian with a scale (sill) of $c_0 = 7.2881$, and a range of $a_0 = 30.6239$. This choice of the semivariogram is based on an automated fit by using PROC NLIN.

Another possible choice of model is the spherical semivariogram with the same scale (sill) of $c_0 = 7.5$ but with a range of $a_0 = 60$. This choice of range comes from a visual fit, which is based on a comparison of the plots of the regular and robust sample semivariograms and the spherical semivariogram for various scale (sill) and range values. While not as good as the Gaussian model, the fit is reasonable.

It is generally held that spatial prediction is robust against model specification, while the standard error computation is not so robust.

This example investigates the effect of using these different models on the prediction and associated standard errors. First, you use a DATA step to input the thickness data as in the following:

```
data thick;
   input East North Thick @@;
   label Thick='Coal Seam Thickness';
   datalines;
 0.7  59.6  34.1   2.1  82.7  42.2   4.7  75.1  39.5
 4.8  52.8  34.3   5.9  67.1  37.0   6.0  35.7  35.9
 6.4  33.7  36.4   7.0  46.7  34.6   8.2  40.1  35.4
13.3   0.6  44.7  13.3  68.2  37.8  13.4  31.3  37.8
17.8   6.9  43.9  20.1  66.3  37.7  22.7  87.6  42.8
23.0  93.9  43.6  24.3  73.0  39.3  24.8  15.1  42.3
24.8  26.3  39.7  26.4  58.0  36.9  26.9  65.0  37.8
27.7  83.3  41.8  27.9  90.8  43.3  29.1  47.9  36.7
29.5  89.4  43.0  30.1   6.1  43.6  30.8  12.1  42.8
32.7  40.2  37.5  34.8   8.1  43.3  35.3  32.0  38.8
37.0  70.3  39.2  38.2  77.9  40.7  38.9  23.3  40.5
39.4  82.5  41.4  43.0   4.7  43.3  43.7   7.6  43.1
46.4  84.1  41.5  46.7  10.6  42.6  49.9  22.1  40.7
51.0  88.8  42.0  52.8  68.9  39.3  52.9  32.7  39.2
55.5  92.9  42.2  56.0   1.6  42.7  60.6  75.2  40.1
62.1  26.6  40.1  63.0  12.7  41.8  69.0  75.6  40.1
70.5  83.7  40.9  70.9  11.0  41.7  71.5  29.5  39.8
78.1  45.5  38.7  78.2   9.1  41.7  78.4  20.0  40.8
80.5  55.9  38.7  81.1  51.0  38.6  83.8   7.9  41.6
84.5  11.0  41.5  85.2  67.3  39.4  85.5  73.0  39.8
86.7  70.4  39.6  87.2  55.7  38.8  88.1   0.0  41.6
88.4  12.1  41.3  88.4  99.6  41.2  88.8  82.9  40.5
```

```
   88.9   6.2  41.5  90.6   7.0  41.5  90.7  49.6  38.9
   91.5  55.4  39.0  92.9  46.8  39.1  93.4  70.9  39.7
   55.8  50.5  38.1  96.2  84.3  40.3  98.2  58.2  39.5
   ;
```

You run the KRIGE2D procedure on the original Gaussian model, as the following statements show:

```
proc krige2d data=thick outest=pred1 noprint;
   coordinates xc=East yc=North;
   predict var=Thick r=60;
   model scale=7.2881 range=30.6239 form=gauss;
   grid x=0 to 100 by 10 y=0 to 100 by 10;
run;
```

Then, you run the KRIGE2D procedure by using a spherical model with a modified range, using the following statements:

```
proc krige2d data=thick outest=pred2 noprint;
   coordinates xc=East yc=North;
   predict var=Thick r=60;
   model scale=7.5 range=60 form=spherical;
   grid x=0 to 100 by 10 y=0 to 100 by 10;
run;
```

Eventually, you perform the comparison and obtain the comparison results by using the COMPARE and the PRINT procedures as the following statements show:

```
data compare;
   merge pred1(rename=(estimate=g_prd stderr=g_std))
         pred2(rename=(estimate=s_prd stderr=s_std));
   prd_dif=g_prd-s_prd;
   std_dif=g_std-s_std;
run;

proc print data=compare;
   title 'Comparison of Gaussian and Spherical Models';
   title2 'Differences of Predictions and Standard Errors';
   var gxc gyc npoints g_prd s_prd prd_dif g_std s_std std_dif;
run;
```

The predicted values at each of the grid locations do not differ greatly for the two semivariogram models. However, the standard error of prediction for the spherical model is substantially larger than for the Gaussian model. A partial outcome from the first 50 prediction grid points of the comparison analysis is shown in Output 46.1.1.

Output 46.1.1 Comparison of Gaussian and Spherical Models

Comparison of Gaussian and Spherical Models
Differences of Predictions and Standard Errors: First 50 Observations

Obs	GXC	GYC	NPOINTS	g_prd	s_prd	prd_dif	g_std	s_std	std_dif
1	0	0	23	43.9702	42.6700	1.30018	0.63046	2.05947	−1.42901
2	0	10	28	41.7145	41.6780	0.03657	0.50937	2.03464	−1.52526
3	0	20	31	38.9756	39.7285	−0.75291	0.27275	1.93478	−1.66203
4	0	30	33	36.1591	37.2816	−1.12253	0.11363	1.54521	−1.43157
5	0	40	40	33.8340	35.4018	−1.56771	0.04291	1.37653	−1.33361
6	0	50	39	32.8464	34.3835	−1.53711	0.02561	1.22559	−1.19997
7	0	60	36	33.9556	34.3140	−0.35842	0.00168	0.54120	−0.53952
8	0	70	31	36.9217	37.6517	−0.73009	0.03428	1.20363	−1.16935
9	0	80	31	41.1035	41.1016	0.00192	0.04180	0.99544	−0.95364
10	0	90	28	43.6723	42.5216	1.15068	0.09125	1.57357	−1.48232
11	0	100	23	41.8818	42.6511	−0.76939	0.48854	2.20792	−1.71938
12	10	0	25	44.6825	44.1959	0.48655	0.07061	1.09743	−1.02683
13	10	10	31	42.8441	42.7496	0.09449	0.09701	1.46686	−1.36984
14	10	20	35	40.3026	40.3557	−0.05301	0.04555	1.54876	−1.50321
15	10	30	40	37.7583	37.7659	−0.00754	0.00766	0.94135	−0.93369
16	10	40	45	35.6487	35.5495	0.09918	0.00497	0.75917	−0.75420
17	10	50	45	35.0798	34.7083	0.37154	0.01284	1.05027	−1.03743
18	10	60	42	36.0688	35.4784	0.59034	0.01123	1.18270	−1.17147
19	10	70	37	38.1205	38.1052	0.01527	0.00272	0.89156	−0.88884
20	10	80	34	41.2811	41.0803	0.20080	0.02097	1.22754	−1.20657
21	10	90	30	43.2213	42.8904	0.33089	0.05290	1.49438	−1.44148
22	10	100	26	40.9801	43.1350	−2.15488	0.17057	1.93434	−1.76377
23	20	0	29	44.4724	44.4359	0.03655	0.05490	1.23618	−1.18128
24	20	10	36	43.3401	43.2958	0.04428	0.00417	0.95510	−0.95092
25	20	20	40	41.1299	40.9923	0.13757	0.00547	1.18538	−1.17991
26	20	30	44	38.6046	38.5335	0.07118	0.00765	1.08968	−1.08203
27	20	40	50	36.5357	36.5331	0.00258	0.02509	1.33589	−1.31080
28	20	50	50	36.1273	35.8019	0.32543	0.02075	1.31950	−1.29875
29	20	60	50	36.8110	36.5435	0.26748	0.00684	1.11476	−1.10791
30	20	70	40	38.4321	38.5186	−0.08647	0.00217	0.89419	−0.89202
31	20	80	37	41.0639	41.0482	0.01561	0.00645	1.18542	−1.17898
32	20	90	34	43.1765	43.1070	0.06948	0.00524	0.94924	−0.94400
33	20	100	27	42.7637	43.4689	−0.70513	0.06070	1.52094	−1.46024
34	30	0	36	43.4020	43.9436	−0.54159	0.03891	1.32240	−1.28348
35	30	10	40	43.1542	43.1454	0.00879	0.00175	0.72412	−0.72237
36	30	20	45	41.2410	41.2158	0.02520	0.00397	1.10233	−1.09836
37	30	30	53	38.9347	39.0203	−0.08556	0.00391	1.04491	−1.04100
38	30	40	58	37.2798	37.3441	−0.06425	0.00654	0.89225	−0.88571
39	30	50	58	36.7224	36.7485	−0.02611	0.00534	0.83405	−0.82871
40	30	60	56	37.2079	37.3339	−0.12594	0.00561	1.00195	−0.99634
41	30	70	49	38.8800	38.8913	−0.01132	0.00225	1.01429	−1.01204
42	30	80	44	41.0573	41.0664	−0.00910	0.00192	0.97336	−0.97145
43	30	90	37	43.0975	43.0463	0.05114	0.00168	0.51312	−0.51144
44	30	100	30	44.6255	43.3247	1.30077	0.12062	1.57134	−1.45072
45	40	0	37	42.8223	43.5137	−0.69134	0.01588	1.25685	−1.24097
46	40	10	41	42.8953	42.9167	−0.02144	0.00247	0.95163	−0.94916
47	40	20	53	41.1033	41.1816	−0.07829	0.00154	0.96204	−0.96049
48	40	30	61	39.3295	39.2949	0.03453	0.00366	1.05527	−1.05161
49	40	40	68	38.1841	37.9297	0.25443	0.01252	1.27124	−1.25872
50	40	50	68	37.3330	37.4359	−0.10284	0.02764	1.44559	−1.41796

Example 46.2: Data Quality and Prediction with Missing Values

Kriging methods depend primarily on your data. The quantity and quality of your observations are important factors in minimizing prediction errors and increasing accuracy in your prediction analysis.

A typical aspect of data quality is measurement accuracy. In principle, the accuracy level of your data is not a parameter in kriging prediction; kriging assumes by definition that your data are perfectly accurate (hard) measurements. Whether you accept this assumption depends on your application. For example, an instrumentation error of $\pm 1\%$ in the data values might be regarded as considerable in one case, whereas the same level of uncertainty might be trivial within a different framework. Your experience and judgment are crucial when you consider whether observations in a data set might be too noisy for kriging predictions to be useful.

A second aspect of data quality involves the spatial arrangement of your observations. You need to have a sufficient number of observations in order to perform spatial prediction. Also, a key element in minimizing prediction errors is an adequate sampling density. Interpretation of the expressions "sufficient number" and "adequate sampling" is again case-specific. In any event, you want enough measurements so that you can deduce the underlying spatial correlation in the working domain; see also the discussion in the section "Choosing the Size of Classes" on page 7547 in the VARIOGRAM procedure.

This example focuses on the effects of different sampling densities on the prediction analysis. The demonstration is a slight variation of the example in the section "Getting Started: KRIGE2D Procedure" on page 2929. Specifically, you use the same correlation structure and prediction grid. However, the thick data set, is modified as follows: three values in the central area of the grid are assumed missing, namely the observation values at locations $\boldsymbol{s}_1 = (x_1, y_1) = (55.8, 50.5)$, $\boldsymbol{s}_2 = (x_2, y_2) = (52.8, 68.9)$, and $\boldsymbol{s}_3 = (x_3, y_3) = (52.9, 32.7)$. These locations have been selected so that an extended area without observations is created in the domain. The following DATA step is the input for the modified thick data set:

```
data thick;
   input East North Thick @@;
   label Thick='Coal Seam Thickness';
   datalines;
    0.7  59.6  34.1   2.1  82.7  42.2   4.7  75.1  39.5
    4.8  52.8  34.3   5.9  67.1  37.0   6.0  35.7  35.9
    6.4  33.7  36.4   7.0  46.7  34.6   8.2  40.1  35.4
   13.3   0.6  44.7  13.3  68.2  37.8  13.4  31.3  37.8
   17.8   6.9  43.9  20.1  66.3  37.7  22.7  87.6  42.8
   23.0  93.9  43.6  24.3  73.0  39.3  24.8  15.1  42.3
   24.8  26.3  39.7  26.4  58.0  36.9  26.9  65.0  37.8
   27.7  83.3  41.8  27.9  90.8  43.3  29.1  47.9  36.7
   29.5  89.4  43.0  30.1   6.1  43.6  30.8  12.1  42.8
   32.7  40.2  37.5  34.8   8.1  43.3  35.3  32.0  38.8
   37.0  70.3  39.2  38.2  77.9  40.7  38.9  23.3  40.5
   39.4  82.5  41.4  43.0   4.7  43.3  43.7   7.6  43.1
   46.4  84.1  41.5  46.7  10.6  42.6  49.9  22.1  40.7
   51.0  88.8  42.0  52.8  68.9     .  52.9  32.7     .
```

```
   55.5  92.9  42.2  56.0   1.6  42.7  60.6  75.2  40.1
   62.1  26.6  40.1  63.0  12.7  41.8  69.0  75.6  40.1
   70.5  83.7  40.9  70.9  11.0  41.7  71.5  29.5  39.8
   78.1  45.5  38.7  78.2   9.1  41.7  78.4  20.0  40.8
   80.5  55.9  38.7  81.1  51.0  38.6  83.8   7.9  41.6
   84.5  11.0  41.5  85.2  67.3  39.4  85.5  73.0  39.8
   86.7  70.4  39.6  87.2  55.7  38.8  88.1   0.0  41.6
   88.4  12.1  41.3  88.4  99.6  41.2  88.8  82.9  40.5
   88.9   6.2  41.5  90.6   7.0  41.5  90.7  49.6  38.9
   91.5  55.4  39.0  92.9  46.8  39.1  93.4  70.9  39.7
   55.8  50.5     .  96.2  84.3  40.3  98.2  58.2  39.5
   ;

title 'Coal Seam Thickness Kriging';
ods graphics on;
```

Note that here you assume prior knowledge of the correlation structure model, because its parameters are based on the complete thick data set. A covariance model extracted from the incomplete set with the missing values would be a covariance model coming from a different data set; hence, it is likely to have different parameters.

After you define the modified data set, you run PROC KRIGE2D and request the OBSERVATIONS plot with the SHOWMISSING suboption. You also request two instances of the PREDICTION plot: one that displays the prediction surface and contours, and another that plots the kriging standard error surface and contours. In both of these PREDICTION plots you specify that the observations be shown as gradient markers with outlines. The following statements compute the kriged predictions and produce the requested graphics:

```
proc krige2d data=thick outest=predictions
             plots(only)=(observ(showmissing)
                          pred(fill=pred line=pred obs=linegrad)
                          pred(fill=se line=se obs=linegrad));
   coordinates xc=East yc=North;
   predict var=Thick r=60;
   model scale=7.2881 range=30.6239 form=gauss;
   grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;
```

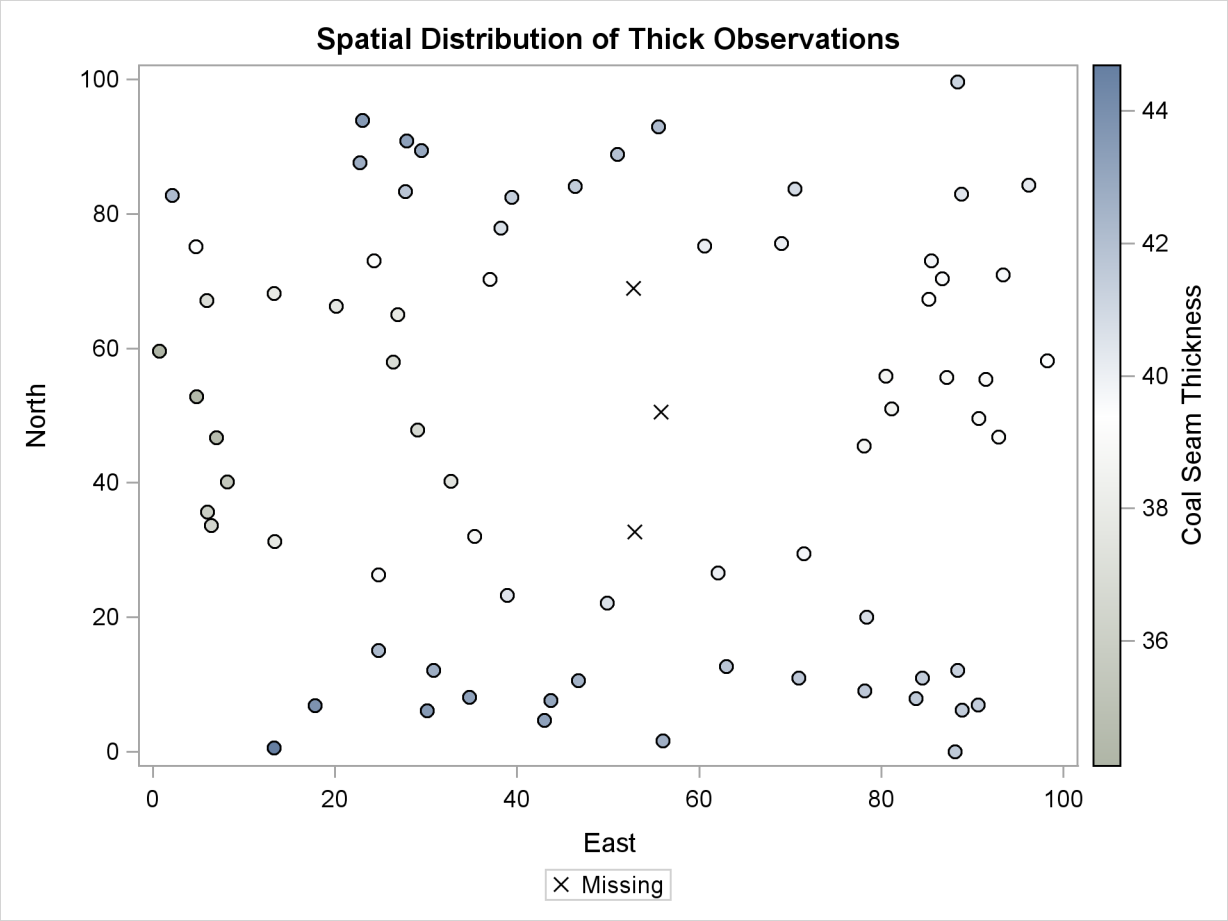
The number of observations table indicates the three missing values in Output 46.2.1.

Output 46.2.1 Number of Observations for the Modified thick Data Set

```
                    Coal Seam Thickness Kriging

                       The KRIGE2D Procedure
                     Dependent Variable: Thick

                Number of Observations Read          75
                Number of Observations Used          72
```

Output 46.2.2 is a map of the scatter plot of the modified observed data. The SHOWMISSING suboption produces marks in the observations plot that conveniently indicate the locations s_1, s_2, and s_3 of the missing values. Consequently, there is now an extended area without any Thick observed values in the central part of the domain.

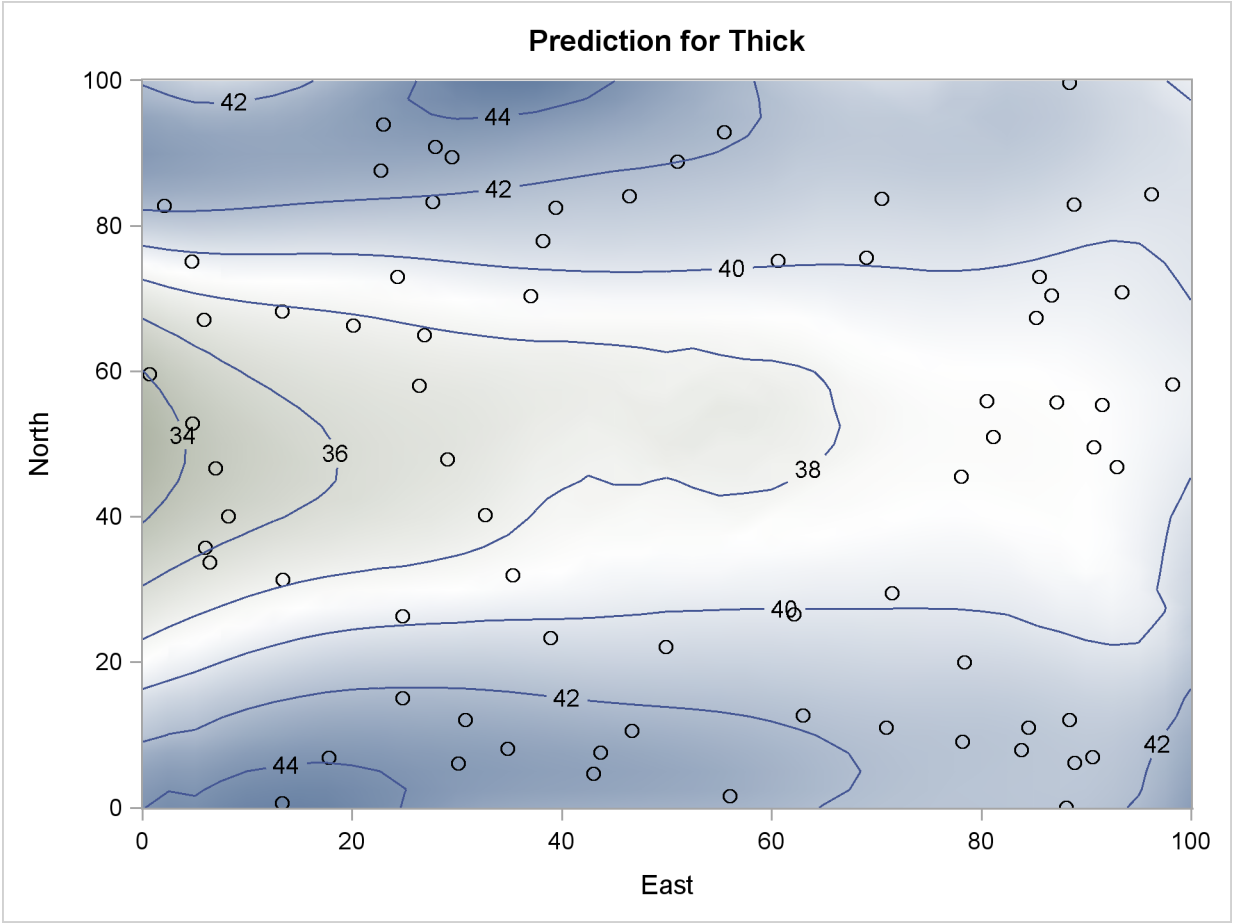
Output 46.2.2 Scatter Plot of the Observations Spatial Distribution



Predictions at grid points with few neighboring data points rely heavily on the underlying covariance structure. The covariance model has a range of about 30,000 feet, which suggests that within this range a grid point might have no data neighbors at all and still obtain a prediction value on the basis of the correlation structure alone. This type of behavior is demonstrated in the Output 46.2.3, which shows a circular region in the center of the plot where there are no data points. Predictions at the nodes in this area are mostly influenced by the covariance structure.

You can see the impact of this effect on the predictions if you compare the prediction contours in the Output 46.2.3 to the ones in Figure 46.4. Despite the contribution of the neighboring Thick data values to the predictions within the area of no observations, the outcome is clearly altered by the absence of observations at the locations s_1, s_2, and s_3.

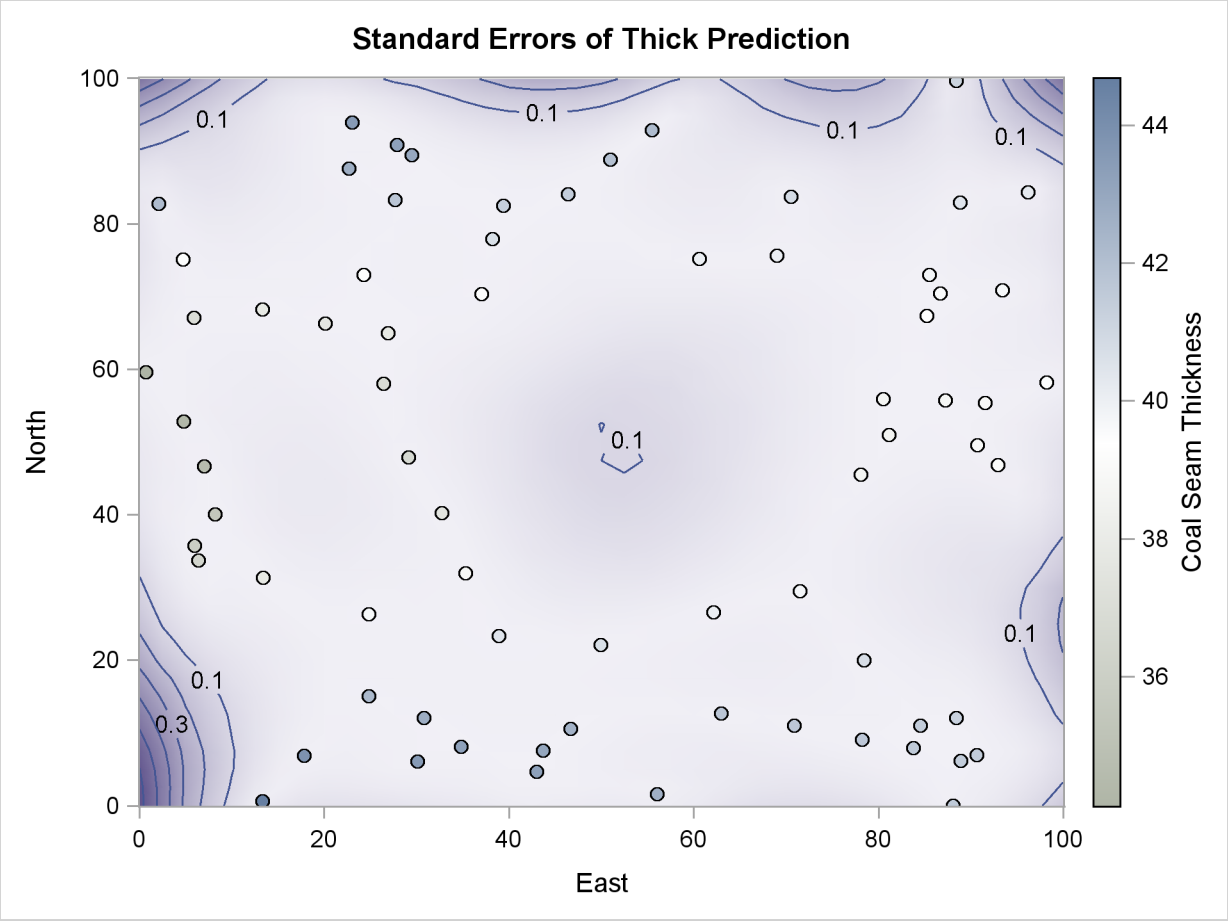
Output 46.2.3 Surface Plot and Contours of Kriged Coal Seam Thickness



A noticeable difference is also apparent in the plot of the prediction standard errors. Output 46.2.4 displays these errors, and you can compare it to the standard error surface in Figure 46.4. The comparison shows a slight difference in the color gradient within the area of the missing data values. Output 46.2.4 uses standard error contours to enhance the effect of this difference.

The lack of information from the removed data resulted in an increase of the prediction uncertainty at the grid nodes that are most remotely situated from any observation in the central part of the domain. According to Output 46.2.4, the standard error at these nodes is almost comparable to the error observed near the borders of the domain, where the nodes of the prediction grid have relatively fewer data neighbors than other nodes in the domain.

Output 46.2.4 Surface Plot and Contours of Prediction Standard Errors



Note that PREDICTION plots display only observations with nonmissing values, as the plots in Output 46.2.3 and Output 46.2.4 demonstrate.

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Syntax Index

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