SAS/STAT® 14.2 User's Guide
The SIM2D Procedure

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SAS/STAT® 14.2 User's Guide

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Chapter 105
The SIM2D Procedure

Contents

Overview: SIM2D Procedure . . . **8680**
- Introduction to Spatial Simulation . . . 8680

Getting Started: SIM2D Procedure . . . **8681**
- Preliminary Spatial Data Analysis . . . 8681
- Investigating Variability by Simulation . . . 8682

Syntax: SIM2D Procedure . . . **8688**
- PROC SIM2D Statement . . . 8690
- BY Statement . . . 8695
- COORDINATES Statement . . . 8696
- GRID Statement . . . 8697
- ID Statement . . . 8699
- RESTORE Statement . . . 8700
- SIMULATE Statement . . . 8701
- MEAN Statement . . . 8710

Details: SIM2D Procedure . . . **8712**
- Computational and Theoretical Details of Spatial Simulation . . . 8712
  - Introduction . . . 8712
  - Theoretical Development . . . 8712
  - Computational Details . . . 8715
- Output Data Set . . . 8715
- Displayed Output . . . 8716
- ODS Table Names . . . 8717
- ODS Graphics . . . 8717

Examples: SIM2D Procedure . . . **8718**
- Example 105.1: Simulation and Economic Feasibility . . . 8718
  - Simulating a Subregion for Economic Feasibility . . . 8718
  - Implementation Using PROC SIM2D . . . 8719
- Example 105.2: Variability at Selected Locations . . . 8723
- Example 105.3: Risk Analysis with Simulation . . . 8727

References . . . **8737**

Overview: SIM2D Procedure

The SIM2D procedure uses an LU decomposition technique to produce a spatial simulation for a Gaussian random field with a specified mean and covariance structure in two dimensions.

The simulation can be conditional or unconditional. If it is conditional, a set of coordinates and associated field values are read from a SAS data set. The resulting simulation honors these data values.

You can specify the mean structure as a quadratic function in the coordinates. Specify the semivariance by naming the form and supplying the associated parameters, or by using the contents of an item store file that was previously created by PROC VARIOGRAM.

PROC SIM2D can handle anisotropic and nested semivariogram models. Seven covariance models are supported: Gaussian, exponential, spherical, cubic, pentaspherical, sine hole effect, and Matérn. A single nugget effect is also supported.

You can specify the locations of simulation points 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.

The SIM2D procedure writes the simulated values for each grid point to an output data set. The SIM2D procedure 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 SIM2D, see the section "ODS Graphics" on page 8717.

Introduction to Spatial Simulation

The purpose of spatial simulation is to produce a set of partial realizations of a spatial random field (SRF) $Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2$ in a way that preserves a specified mean $\mu(\boldsymbol{s}) = E\left[Z(\boldsymbol{s})\right]$ and covariance structure $C_z(\boldsymbol{s}_1 - \boldsymbol{s}_2) = \mathrm{Cov}\left(Z(\boldsymbol{s}_1), Z(\boldsymbol{s}_2)\right)$. The realizations are partial in the sense that they occur only at a finite set of locations $(\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n)$. These locations are typically on a regular grid, but they can be arbitrary locations in the plane.

PROC SIM2D produces simulations for continuous processes in two dimensions by using the lower-upper (LU) decomposition method. In these simulations the possible values of the measured quantity $Z(\boldsymbol{s}_0)$ at location $\boldsymbol{s}_0 = (x_0, y_0)$ can vary continuously over a certain range. An additional assumption, needed for computational purposes, is that the spatial random field $Z(\boldsymbol{s})$ is Gaussian. The section "Details: SIM2D Procedure" on page 8712 provides more information about different types of spatial simulation and associated computational methods.

Spatial simulation is different from spatial prediction, where the emphasis is on predicting a point value at a given grid location. In this sense, spatial prediction is local. In contrast, spatial simulation is global; the emphasis is on the entire realization $(Z(\boldsymbol{s}_1), Z(\boldsymbol{s}_2), \ldots, Z(\boldsymbol{s}_n))$.

Given the correct mean $\mu(\boldsymbol{s})$ and covariance structure $C_z(\boldsymbol{s}_1 - \boldsymbol{s}_2)$, SRF quantities that are difficult or impossible to calculate in a spatial prediction context can easily be approximated by functions of multiple simulations.

Getting Started: SIM2D Procedure

Spatial simulation, just like spatial prediction, requires a model of spatial dependence, usually in terms of the covariance $C_z(\boldsymbol{h})$. For a given set of spatial data $Z(\boldsymbol{s}_i), i = 1, \ldots, n$, the covariance structure (both the form and parameter values) can be found by the VARIOGRAM procedure. This example uses the coal seam thickness data that are also used in the section "Getting Started: VARIOGRAM Procedure" on page 10027 in Chapter 124, "The VARIOGRAM Procedure."

In this example, the data consist of coal seam thickness measurements (in feet) taken over an area of 100×100 (10^6 ft^2). The coordinates are offsets from a point in the southwest corner of the measurement area, with the north and east distances in units of thousands of feet.

Preliminary Spatial Data Analysis

A semivariance analysis of the coal seam thickness thick data set is performed in "Getting Started: VARIOGRAM Procedure" on page 10027 in Chapter 124, "The VARIOGRAM Procedure." The analysis considers the spatial random field (SRF) $Z(\boldsymbol{s})$ of the Thick variable to be free of surface trends. The expected value $E[Z(\boldsymbol{s})]$ is then a constant $\mu(\boldsymbol{s}) = \mu$, which suggests that you can work with the original thickness data rather than residuals from a trend surface fit. In fact, a reasonable approximation of the spatial process generating the coal seam data is given by

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

where $\varepsilon(\boldsymbol{s})$ is a Gaussian SRF with Gaussian covariance structure

$$C_z(\boldsymbol{h}) = c_0 \exp\left(-\frac{h^2}{a_0^2}\right)$$

Of note, the term "Gaussian" is used in two ways in this description. For a set of locations $\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_n$, the random vector

$$\boldsymbol{Z}(\boldsymbol{s}) = \begin{bmatrix} Z(\boldsymbol{s}_1) \\ Z(\boldsymbol{s}_2) \\ \vdots \\ Z(\boldsymbol{s}_n) \end{bmatrix}$$

has a multivariate Gaussian or normal distribution $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. The (i,j) element of $\boldsymbol{\Sigma}$ is computed by $C_z(\boldsymbol{s}_i - \boldsymbol{s}_j)$, which happens to be a Gaussian functional form.

Any functional form for $C_z(\boldsymbol{h})$ that yields a valid covariance matrix $\boldsymbol{\Sigma}$ can be used. Both the functional form of $C_z(\boldsymbol{h})$ and the parameter values

$$\mu = 40.1173$$

$$c_0 = 7.4599$$

$$a_0 = 30.1111$$

are estimated by using PROC VARIOGRAM in section "Theoretical Semivariogram Model Fitting" on page 10036 in Chapter 124, "The VARIOGRAM Procedure." Specifically, the expected value μ is reported in the VARIOGRAM procedure OUTV output data set, and the parameters c_0 and a_0 are estimates derived from a weighted least squares fit.

The choice of a Gaussian functional form for $C_z(\boldsymbol{h})$ is simply based on the data, and it is not at all crucial to the simulation. However, it *is* crucial to the simulation method used in PROC SIM2D that $Z(\boldsymbol{s})$ be a Gaussian SRF. For details, see the section "Computational and Theoretical Details of Spatial Simulation" on page 8712.

Investigating Variability by Simulation

The variability of $Z(\boldsymbol{s})$, as modeled by

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

with the Gaussian covariance structure $C_z(\boldsymbol{h})$ found previously, is not obvious from the covariance model form and parameters. The variation around the mean of the surface is relatively small, making it difficult visually to pick up differences in surface plots of simulated realizations.

Instead, you can compute the mean for each location on a grid from a series of realizations in a simulation. Then, the standard deviation of all the simulated values at each grid location provides you with a measure of the variability of $Z(\boldsymbol{s})$ for the given covariance structure. You can also investigate variations at selected grid points in more detail, as shown in the "Example 105.2: Variability at Selected Locations" on page 8723.

The present example shows how to use ODS Graphics with PROC SIM2D to investigate the mean and standard deviation of simulated values. You use the thick data set which is available from the Sashelp library. In the data set, the Thick variable represents simulated observations of coal seam thickness. For your goal, you produce 5,000 realizations of a simulation with PROC SIM2D, where you specify the Gaussian model with the parameters found previously. You want the simulated data to pass through the simulated values, so first you define the data with the following data step:

```
title 'Using PROC SIM2D for Spatial Simulation';

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
;
```

Since this is a conditional simulation, you can specify the OBSERV option in the PLOTS option in PROC SIM2D to see the locations and values of the measured points in the area where you want to perform spatial simulations.

Furthermore, the SIM suboption in the PLOTS option specifies that you want to create a plot that shows the means of the simulated values across the region. The SIM suboption with no other arguments produces a plot that shows the contours of the simulated means in the foreground and the gradient of the simulated standard deviations in the background.

You obtain these PROC SIM2D results at the nodes of an output grid that you specify according to your application needs. In the present analysis, a convenient area that encompasses all the Thick data points is a square with a side length of 100,000 feet. You define a regular grid for your simulation in this area. Assume a distance of 2,500 feet between grid nodes in both directions for a smooth contour plot. Based on this choice, your square grid has 41 nodes on each side. This means that PROC SIM2D computes the simulated values at a total of 1,681 grid points. You use the GRID statement of the PROC SIM2D to specify this grid.

The SIMULATE statement specifies the parameters of your simulation across the output grid. In particular, the VAR= option specifies the conditional simulation variable. The number of realizations in the simulation is specified with the NUMREAL= option. The SEED= option specifies the seed for the simulation random number generator.

The spatial correlation model for the simulation is also specified in the SIMULATE statement. You specify the model type by using the FORM= option. The options SCALE= and RANGE= specify the covariance structure sill c_0 and range a_0 parameters, respectively, as discussed in the previous section.

Although it is not included in the original spatial structure, note that a minimal nugget effect is specified with the NUGGET= option to avoid singularity issues. Singularity can appear in the present example as a result of the combined use of the Gaussian covariance model and relatively short distances between nodes, data, or nodes and data in the simulation area.

These steps are implemented using the following DATA step and statements:

```
ods graphics on;

proc sim2d data=thick outsim=sim plot=(observ sim);
   coordinates xc=East yc=North;
   simulate var=Thick numreal=5000 seed=79931
      scale=7.4599 range=30.1111 nugget=1e-8 form=gauss;
   mean 40.1173;
   grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;
```

The table in Figure 105.1 shows the number of observations read and used in the conditional simulation. This table can provide you with useful information in case you have missing values in the input data.

Figure 105.1 Number of Observations for the thick Data Set

Using PROC SIM2D for Spatial Simulation

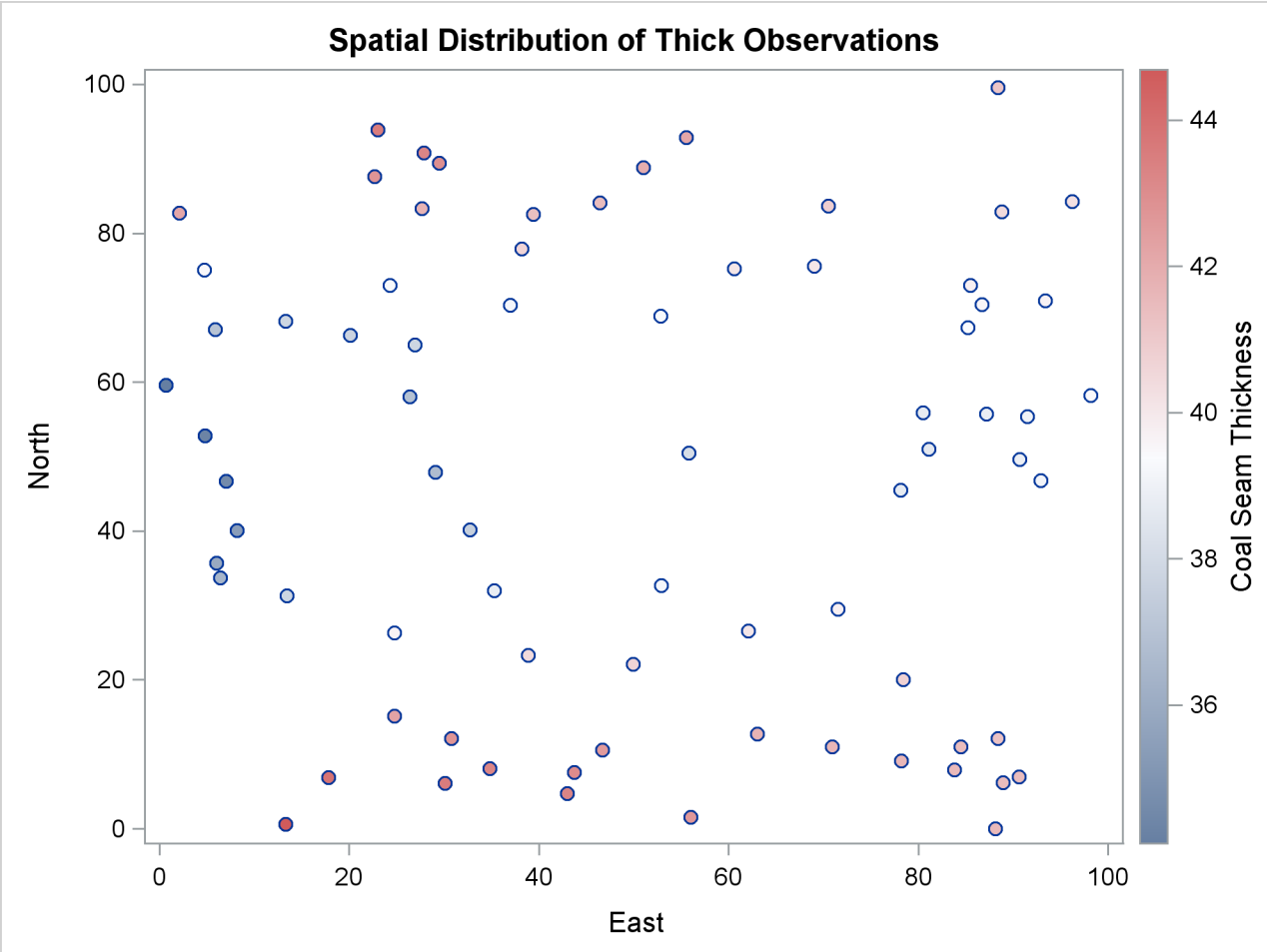
The SIM2D Procedure

Simulation: SIM1, Dependent Variable: Thick

Number of Observations Read	75
Number of Observations Used	75

The sample locations are then plotted in Figure 105.2. The figure clearly shows some small-scale variation that is typical of spatial data.

Figure 105.2 Scatter Plot of the Observations Spatial Distribution



PROC SIM2D also produces the table shown in Figure 105.3, which contains information about the type of simulation you run and the number of realizations requested.

Figure 105.3 Simulation Analysis Information

Simulation Information	
Simulation Grid Points	1681
Type	Conditional
Number of Realizations	5000

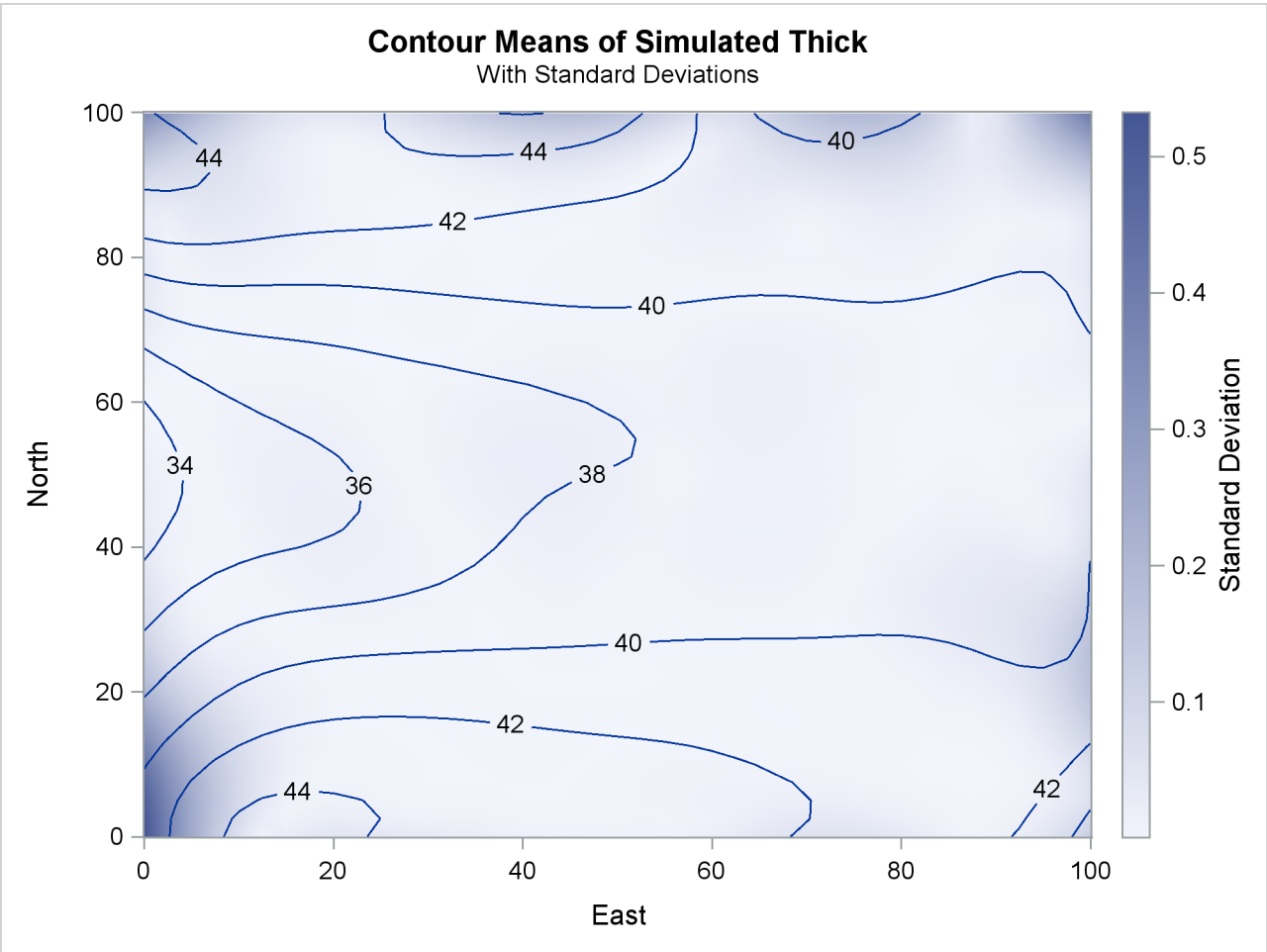
The table in Figure 105.4 displays the spatial correlation model information that is used by PROC SIM2D for the current simulation. If applicable, the table also provides the effective range. This is the distance r_ϵ at which the covariance is 5% of its value at zero. Here you specified the Gaussian model, for which the effective range r_ϵ is $\sqrt{3}a_0$.

Figure 105.4 Simulation Covariance Model Information

Covariance Model Information	
Type	Gaussian
Sill	7.4599
Range	30.1111
Effective Range	52.153955
Nugget Effect	1E-8

Eventually, the SIM2D procedure produces the requested simulation plot shown in Figure 105.5. The contours of the mean of the simulated values show the average of the simulated realizations at each grid node; the average is based on the given spatial structure characteristics. In this case, these means are also conditioned by the Thick observations across the region.

Figure 105.5 Contour Plot of Conditionally Simulated Coal Seam Thickness



Observe also the gradient that shows the standard deviation of the simulated values at each grid node. This gradient appears to be generally small throughout the region. A few exceptions are evident close to the region borders. In these areas the simulated realizations depend on a limited amount of neighboring data. The simulation at these locations relies mainly on the underlying spatial structure.

In addition to the simulation analysis, you can use the PROC SIM2D output to obtain statistical information about the simulated values at selected locations. Assume that you would like some basic statistics for the extreme southwest point at (East=0, North=0) and the point (East=75, North=75) toward the northeast corner of the region. You use the following DATA step to select the realizations for these points from the OUTSIM= output data set:

```
data selected;
   set sim(where=((gxc=0 and gyc=0) or (gxc=75 and gyc=75)));
   label gxc = "X-coord";
   label gyc = "Y-coord";
run;
```

Then, you use PROC SORT to sort the selected data set entries and PROC MEANS to produce the simulation statistics for the selected points. The following statements yield the mean, standard deviation, and maximum values of the 5,000 realizations of the Thick values at each one of the selected locations:

```
proc sort data=selected;
   by gxc gyc;
run;
proc means data=selected Mean Std Max;
   class gxc gyc;
   ways 2;
   where (  ((gxc =  0) & (gyc =  0))
          | ((gxc = 75) & (gyc = 75)));
   var SValue;
run;

ods graphics off;
```

The requested statistics for the grid points (East=0, North=0) and (East=75,North=75) are shown in Figure 105.6.

Figure 105.6 Simulation Statistics at Grid Points (East=0, North=0) and (East=75, North=75)

Using PROC SIM2D for Spatial Simulation

The MEANS Procedure

Analysis Variable : SVALUE Simulated Value at Grid Point					
X-coord	Y-coord	N Obs	Mean	Std Dev	Maximum
0	0	5000	40.6968472	0.5328597	42.6616357
75	75	5000	40.1090845	0.0024556	40.1197239

"Example 105.2: Variability at Selected Locations" on page 8723 shows you how to perform a simulation at a set of selected locations rather than on a domain-wide grid, and how to obtain more detailed statistics from the simulation.

Syntax: SIM2D Procedure

The following statements are available in the SIM2D procedure:

PROC SIM2D *options* ;
  BY *variables* ;
  COORDINATES *coordinate-variables* ;
  GRID *grid-options* ;
  ID *variable* ;
  RESTORE *store-options* ;
  SIMULATE *simulate-options* ;
  MEAN *mean-options* ;

The SIMULATE and MEAN statements are hierarchical; you can specify any number of SIMULATE statements, but you must specify at least one. If you specify a MEAN statement, it refers to the preceding SIMULATE statement. If you omit the MEAN statement, a zero-mean model is simulated.

You must specify a single COORDINATES statement to identify the x and y coordinate variables in the input data set when you perform a conditional simulation. You must also specify a single GRID statement to specify the grid information.

Table 105.1 outlines the *options* available in PROC SIM2D classified by function.

Table 105.1 Options Available in the SIM2D Procedure

Task	Statement	Option
Data Set Options		
Specify an input data set	PROC SIM2D	DATA=
Specify a grid data set	GRID	GDATA=
Specify labels for individual grid points or in 1-D	GRID	LABEL
Specify correlation model and parameters	SIMULATE	MDATA=
Write simulated values	PROC SIM2D	OUTSIM=
Specify plot display and options	PROC SIM2D	PLOTS
Specify a quadratic form data set	MEAN	QDATA=
Specify plot display and options	PROC SIM2D	PLOTS
Declaring the Role of Variables		
Specify variables to define analysis subgroups	BY	
Specify a variable with observation labels	ID	
Specify the conditioning variable	SIMULATE	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=
Specify the constant coefficient variable in the QDATA= data set	MEAN	CONST=
Specify the linear x coefficient variable in the QDATA= data set	MEAN	CX=

Table 105.1 *continued*

Task	Statement	Option
Specify the linear y coefficient variable in the QDATA= data set	MEAN	CY=
Specify the quadratic x coefficient variable in the QDATA= data set	MEAN	CXX=
Specify the quadratic y coefficient variable in the QDATA= data set	MEAN	CYY=
Specify the quadratic xy coefficient variable in the QDATA= data set	MEAN	CXY=
Controlling the Simulation		
Specify the number of grid points in one-dimensional cases	GRID	NPTS=
Specify the number of realizations	SIMULATE	NUMREAL=
Specify the seed value for the random generator	SIMULATE	SEED=
Controlling the Mean Quadratic Surface		
Specify the CONST term	MEAN	CONST=
Specify the linear x term	MEAN	CX=
Specify the linear y term	MEAN	CY=
Specify the quadratic x term	MEAN	CXX=
Specify the quadratic y term	MEAN	CYY=
Specify the quadratic cross term	MEAN	CXY=
Controlling the Semivariogram Model		
Specify an angle for an anisotropic model	SIMULATE	ANGLE=
Specify nested angles	SIMULATE	ANGLE=$(a_1, \ldots, a_k)$
Specify a functional form	SIMULATE	FORM=
Specify nested functional forms	SIMULATE	FORM=$(f_1, \ldots, f_k)$
Specify a nugget effect	SIMULATE	NUGGET=
Specify a range parameter	SIMULATE	RANGE=
Specify nested range parameters	SIMULATE	RANGE=$(r_1, \ldots, r_k)$
Specify a minor-major axis ratio for an anisotropic model	SIMULATE	RATIO=
Specify nested minor-major axis ratios	SIMULATE	RATIO=$(ra_1, \ldots, ra_k)$
Specify a scale parameter	SIMULATE	SCALE=
Specify nested scale parameters	SIMULATE	SCALE=$(s_1, \ldots, s_k)$
Specify item store with correlation information	RESTORE	IN=
Specify model and parameters from an item store	SIMULATE	STORESELECT

PROC SIM2D Statement

PROC SIM2D *options* **;**

The PROC SIM2D statement invokes the SIM2D procedure. Table 105.2 summarizes the *options* available in the PROC SIM2D statement.

Table 105.2 PROC SIM2D Statement Options

Option	Description
DATA=	Specifies an input data set
IDGLOBAL	Uses ascending observation numbers across BY groups
IDNUM	Uses the observation number for the observation labels
NARROW	Restricts the variables included in the OUTSIM= data set
NOPRINT	Suppresses the normal display of results
OUTSIM=	Writes simulated values to a SAS data set
PLOTS	Specifies plot display and options

You can specify the following *options* with the PROC SIM2D statement.

DATA=*SAS-data-set*

specifies a SAS data set that contains the x and y coordinate variables and the VAR= variables that are used in the SIMULATE statements. This data set is required if you specify the BY statement or the COORDINATES statement or if any of the SIMULATE statements are conditional—that is, if you specify the VAR= option in any of those. Otherwise, you do not need the DATA= option, and this option is ignored if you specify it.

IDGLOBAL

specifies that ascending observation numbers be used across BY groups for the observation labels in the appropriate output data sets and the OBSERVATIONS plot, instead of resetting the observation number in the beginning of each BY group. The IDGLOBAL option is ignored if no BY variables are specified. Also, if you specify the ID statement, then the IDGLOBAL option is ignored unless you also specify the IDNUM option in the PROC SIM2D statement.

IDNUM

specifies that the observation number be used for the observation labels in the appropriate output data sets and the OBSERVATIONS plot. The IDNUM option takes effect when you specify the ID statement; otherwise, it is ignored.

NARROW

restricts the variables included in the OUTSIM= data set. When you specify the NARROW option, only four variables are included. This option is useful when a large number of simulations are produced. Including only four variables reduces the memory required for the OUTSIM= data set. For details about the variables that are excluded with the NARROW option, see the section "Output Data Set" on page 8715.

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:** This option temporarily disables the Output Delivery System (ODS); see the section "ODS Graphics" on page 8717 for more information.

OUTSIM=*SAS-data-set*

specifies a SAS data set in which to store the simulation values, iteration number, simulate statement label, variable name, and grid location. For details, see the section "Output Data Set" on page 8715.

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) sim)
plots=(sim(fill=mean line=sd obs=grad) sim(fill=sd))
```

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

```
ods graphics on;

proc sim2d data=thick outsim=sim;
   coordinates xc=East yc=North;
   simulate var=Thick numreal=5000 seed=79931
      scale=7.4599 range=30.1111 form=gauss;
   mean 40.1173;
   grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 607 in Chapter 21, "Statistical Graphics Using ODS."

By default, no graphs are created; you must specify the PLOTS= option to make graphs.

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

ONLY

produces only plots that are specifically requested.

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 all appropriate plots and an additional simulation plot, specify PLOTS=(ALL SIM).

EQUATE
specifies that all appropriate plots be produced in a way in which 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 in conditional simulations. Only one observations plot is 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.

LABEL < (*label-option*) >
labels the observations. The label is the ID variable if the ID statement is specified; otherwise, it is the observation number. The *label-option* can be one of the following:

EQ=*number*
specifies that labels show for any observation whose value is equal to the specified *number*.

MAX=*number*
specifies that labels show for observations with values smaller than or equal to the specified *number*.

MIN=*number*
specifies that labels show for observations with values equal to or greater than the specified *number*.

If you specify multiple instances of the OBSERVATIONS option and you specify the LABEL suboption in any of those, then the resulting observations plot displays the observations labels. If more than one *label-option* is specified in multiple LABEL suboptions, then the prevailing *label-option* in the resulting OBSERVATIONS plot emerges by adhering to the choosing order: MIN, MAX, EQ.

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 displays the observations with missing values.

If you omit any of the GRADIENT, OUTLINE, and OUTLINEGRADIENT suboptions, the OUTLINEGRADIENT is the default suboption. If you specify multiple instances of the OBSERVATIONS option or multiple suboptions for OBSERVATIONS, then the resulting observations plot honors the last specified GRADIENT, OUTLINE, or OUTLINEGRADIENT suboption.

SIMULATION < (*sim-plot-options*) >

SIM < (*sim-plot-options*) >

specifies that simulation plots be produced. You can specify the SIM option multiple times in the same PLOTS option to request instances of plots with the following *sim-plot-options*:

ALPHA=*number*

specifies a parameter to obtain the confidence level for constructing confidence limits based on the simulation standard deviation. The value of *number* must be between 0 and 1, and the confidence level is $1-$*number*. The default is ALPHA=0.05; this corresponds to the confidence level of 95%. The ALPHA= suboption is used only for simulation plots in one dimension, and it is incompatible with the FILL and LINE suboptions.

CLONLY

specifies that only the confidence limits be shown in a simulation plot without the simulation mean. This suboption can be useful for identifying confidence limits when the simulation standard deviation is small at the simulation locations. CLONLY is used only for simulation band plots of simulations on a linear grid, and it is incompatible with the FILL and LINE suboptions.

CONNP

specifies that grid points that you provide as individual simulation locations be connected with a line on the area map. This suboption is ignored when you have a single grid point, a prediction grid in two dimensions, or when you also specify the NOMAP suboption. The CONNP suboption is incompatible with the FILL and LINE suboptions.

FILL=NONE | MEAN | SD

produces a surface plot for either the values of the means or the standard deviations. FILL=SD is the default. However, if you omit the FILL suboption the behavior depends on the LINE suboption as follows: If you specify LINE=NONE or entirely omit the LINE suboption, then the FILL suboption is set to its default value. If LINE=PRED or LINE=SE, then the FILL suboption is set to the same value as the LINE suboption.

LINE=NONE | MEAN | SD

produces a contour line plot for either the values of the means or the standard deviations. LINE=MEAN is the default. However, if you omit the LINE suboption the behavior depends on the FILL suboption as follows: If you specify FILL=NONE or entirely omit the FILL suboption, then the LINE suboption is set to its default value. If FILL=PRED or FILL=SE, then the LINE suboption is set to the same value as the FILL suboption.

NOMAP
specifies that the simulation plot be produced without a map of the domain where you have observations. The NOMAP suboption is used in the case of simulation in one dimension or at individual points. It is ignored in the case of unconditional simulation, and it is incompatible with the FILL and LINE suboptions.

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 displays the means surface and the observations. The conditional simulation honors the observed values, so the means surface at the observation locations has the same color as the corresponding observations.

LINEGRAD
is the same as OBS=GRAD except that a border is shown around each observation. This option is useful for identifying the location of observations where the standard deviations 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 when you have a grid in two dimensions, and OBS=LINEGRAD is the default used in the area map when you specify a conditional simulation in one dimension.

SHOWD
specifies that the horizontal axis in scatter plots of linear simulation grids show the distance between grid points instead of the grid points' coordinates. When the area map is displayed, the simulation locations are also connected with a line. In all other grid configurations the SHOWD suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

SHOWP
specifies that the grid points in band plots of linear simulation grids be shown as marks on the band plot. In all other grid configurations the SHOWP suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

TYPE=BAND | BOX
requests a particular type of plot when you have a linear grid, regardless of the default SIM plot behavior in this case. The TYPE suboption is incompatible with the FILL and LINE suboptions.

If you specify multiple instances of the ALPHA, FILL, LINE, OBS, or TYPE suboptions in the same SIM option, then the resulting simulation plot honors the last value specified for any of the

suboptions. Any combination where you specify FILL=NONE and LINE=NONE is not available. When the simulation grid is in two dimensions, only the FILL, LINE, and OBS suboptions apply. If you specify incompatible suboptions in the same SIM plot, then the plot instance is skipped.

The SIM option produces a surface or contour line plot for grids in two dimensions and a band plot or box plot for grids in one dimension or individual points. In two dimensions the plot illustrates the means and standard deviations of the simulation realizations at each grid point. By default, when you specify a linear grid with fewer than 10 points, PROC SIM2D produces a SIM box plot that depicts the simulation distribution at each point. For 10 or more points in a linear grid, the SIM plot is a band plot of the simulation means and the confidence limits at the 95% confidence level. You can override the default behavior in linear grids with the TYPE suboption. Simulation at individual locations always produces a SIM box plot.

In cases of conditional simulation in one dimension or at individual points an area map is produced that shows the observations and the grid points. Band plots of linear grids display the grid points as a line on the map. When you specify individual simulation locations, the grid points are indicated with marks on the area map. The area map appears on the side of conditional simulation band plots or box plots, unless you specify the NOMAP suboption. You can also label individual grid points or the ends of linear grid segments with the LABEL option of the GRID statement.

SEMIVARIOGRAM < (*semivar-plot-option*) >

SEMIVAR < (*semivar-plot-option*) >

specifies that the semivariogram used for the simulation be produced. You can use the following *semivar-plot-option*:

MAXD=*number*

specifies a positive value for the upper limit of the semivariogram horizontal axis of distance. The SEMIVARIOGRAM plot extends by default to a distance that depends on the correlation model range. You can use the MAXD= option to adjust the default maximum distance value for the plot.

The SEMIVARIOGRAM option produces a plot for each correlation model that you specify for your simulation tasks. In an anisotropic case, the plot is not produced if you assign different anisotropy angles for different model components. The only exception is when you specify zonal components at right angles with the nonzonal model components. Also, the SEMIVARIOGRAM option is ignored for models that consist of purely zonal components.

BY Statement

BY *variables* **;**

You can specify a BY statement with PROC SIM2D to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

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

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SIM2D 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).

In PROC SIM2D it makes sense to use the BY statement only in conditional simulations where observations are involved. In particular, using the BY statement assumes that you have specified an input data set with the DATA= option in the PROC SIM2D statement. In PROC SIM2D if you omit the VAR= option in the SIMULATE statement, then this is a request for unconditional simulation even if you have specified the DATA= option in the PROC SIM2D statement. Therefore, it is possible to specify the BY statement and request mixed types of simulations by specifying multiple SIMULATE statements in the same PROC SIM2D step.

A special case occurs when you omit the DATA= option in the PROC SIM2D statement, your unconditional simulation correlation model input comes from an item store in the RESTORE statement, and this store has its own BY groups. The SIM2D procedure exhibits then a BY-like behavior, even though you specified no BY statement. This behavior enables you to distinguish the simulation tasks that depend on models in the different store BY groups.

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

COORDINATES Statement

COORDINATES *coordinate-variables* **;**

The two options in the COORDINATES statement give the name of the variables in the DATA= data set that contains the values of the *x* and *y* coordinates of the conditioning data. You must specify the COORDINATES statement when you specify an input data set with the DATA= option in the PROC SIM2D statement.

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

You can abbreviate the COORDINATES statement as COORD.

XCOORD=(*variable-name***)**

XC=(*variable-name***)**

gives the name of the variable that contains the *x* coordinate of the data in the DATA= data set.

YCOORD=(*variable-name***)**

YC=(*variable-name***)**

gives the name of the variable that contains the *y* coordinate of the data locations in the DATA= data set.

GRID Statement

GRID *grid-options* < / *option* > **;**

The GRID statement specifies the grid of spatial locations at which to perform the simulations. A single GRID statement is required and is applied to all SIMULATE statements. Specify the grid in one of the following three ways:

- Specify the x and y coordinates explicitly for a grid in two dimensions.
- Specify the NPTS= option in addition to the x and y coordinates to define a grid of individual points or in one dimension.
- Specify the coordinates by using a SAS data set for a grid of individual points or in one dimension.

The GRID statement has the following *grid-options*:

NPTS=*number* | **ALL**

controls specification of a grid in one dimension or a grid of individual simulation locations.

When you specify the NPTS=*number* option and the coordinates of two points in the GRIDDATA= data set or in both the X= and Y= options, you request a linear simulation grid. Its direction is across the line defined by the specified points. The grid size is equal to the *number* of points that you specify in the NPTS= option, where *number* ≥ 2.

When you specify the NPTS=ALL option and the coordinates for any number of points in the GRIDDATA= data set or in each of the X= and Y= options, the SIM2D procedure performs simulation only at the specified individual locations. Use the NPTS=ALL option to examine a set of individual points anywhere on the XY plane or to specify a custom grid in one dimension.

If the number of x coordinates and the number of y coordinates in the X= and Y= options, respectively, are different, then the NPTS= option is ignored; in that case, a two-dimensional grid is used according to the specified X= and Y= options.

If you specify a simulation grid with any number of points other than two in the GRIDDATA= data set, then the option NPTS=ALL has the same effect as omitting the NPTS= option.

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.

Use the X= and Y= options of the GRID statement to specify a grid in one or two dimensions, or a grid of individual simulation 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;
```

In the following example, the first GRID statement produces a grid in two dimensions. The second statement produces simulation output only for the four individual points at the locations (1,0), (2,5), (3,7), and (4,10) on the XY plane.

```
GRID X=1 TO 4 Y=0,5,7,10;

GRID X=1 TO 4 Y=0,5,7,10 NPTS=ALL;
```

In the next example, the first GRID statement specifies a 2-by-2 grid in two dimensions. The second GRID statement specifies a linear grid of eight points. The grid is in the direction of the line defined by the specified points (2,8) and (3,5) on the XY plane and it extends between these two points.

```
GRID X=2,3 Y=8,5;

GRID x=2,3 Y=8,5 NPTS=8;
```

The last example shows a GRID statement that specifies a linear grid made of seven points across the Y axis. In this case, the syntax is sufficient to fully define a linear grid without the NPTS= option.

```
GRID X=5 Y=3 TO 9;
```

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

GRIDDATA=*SAS-data-set*

GDATA=*SAS-data-set*

specifies a SAS data set that contains the *x* and *y* grid coordinates. Use the GRIDDATA= option of the GRID statement to specify a grid in one dimension or a grid of individual simulation locations.

XCOORD=(*variable-name***)**

XC=(*variable-name***)**

gives the name of the variable that contains the *x* coordinate of the grid locations in the GRIDDATA= data set.

YCOORD=(*variable-name***)**

YC=(*variable-name***)**

gives the name of the variable that contains the *y* coordinate of the grid locations in the GRIDDATA= data set.

You can specify the following *option* in the GRID statement after a slash (/):

LABEL < (*suboption*) > = (*character-list*)

specifies labels to tag grid points in simulation plots when you use grids in one dimension. You can specify one or more such labels as quoted strings in the *character-list*.

When the number of labels in the *character-list* exceeds the number of points in your grid, the labels in the list are used sequentially and any labels in excess are ignored. When the number of labels in the *character-list* is smaller than the number of points in your grid, the behavior is as follows:

- If an area map is included in the simulation plot, then blank labels are assigned to the remaining nonlabeled grid points on the map.
- For the simulation band and box plots, the coordinates of nonlabeled grid points are automatically assigned as their labels.

If the grid points are collinear and the horizontal axis displays distance, then two labels appear by default in the simulation plot. These are assigned to the first and the last points of the grid to help identify the ends of the linear grid segment on the plot map. This label pair is shown only when the plot includes an area map. Specifically, the two labels appear when you request simulation band plots, or simulation box plots for which you specify the SIM(SHOWD) suboption, if applicable. The two labels do not appear if you specify explicitly the NOMAP suboption in the PLOTS=SIM option.

The two labels have default values, unless you choose to specify your own labels with the LABEL= option. If you specify more than two labels in the *character-list* under these conditions, then only the first and last labels in the list are used; any additional labels in between are ignored.

The LABEL= option has the following *suboption*:

ALL

specifies that all individual points in the grid are assigned sequentially the labels you specify in the LABEL(ALL)= option when the SIM(SHOWD) suboption is applicable and specified in a simulation box plot. In all other cases, the ALL suboption is ignored.

The ALL suboption enables you to override the default behavior when the SIM(SHOWD) suboption is specified (the default behavior is to display labels only for the first and last grid points). As a result, you can use the ALL suboption to label grid points in both conditional and unconditional simulation tasks regardless of whether you specify the NOMAP suboption in the PLOTS=SIM option.

The LABEL= option is ignored when you produce simulation plots of grids in two dimensions.

ID Statement

ID *variable* **;**

The ID statement specifies which variable to include for identification of the observations in the labels and tool tips of the OBSERVATIONS plot and the tool tips of the SIM plot. The ID statement has an effect only when you perform conditional simulation.

In the SIM2D procedure you can specify only one ID variable in the ID statement. If no ID statement is given, then PROC SIM2D uses the observation number in the plots.

RESTORE Statement

RESTORE IN=*store-name* < / *option* > **;**

The RESTORE statement specifies an item store that provides spatial correlation model input for the PROC SIM2D simulation tasks. An item store is a binary file defined by the SAS System. You cannot modify the contents of an item store. The SIM2D procedure can use only item stores created by PROC VARIOGRAM.

Item stores enable you to use saved correlation models without having to repeat specification of these models in the SIMULATE statement. In principle, an item store contains the chosen model from a model fitting process in PROC VARIOGRAM. If more than one model form is fitted, then all successful fits are included in the item store. In this case, you can choose any of the available models to use for simulation with the STORESELECT(MODEL=) option in the SIMULATE statement. Successfully fitted models might include questionable fits, which are so flagged when you specify the INFO option to display model names.

The *store-name* is a usual one- or two-level SAS name, as for SAS data sets. If you specify a one-level name, then the item store resides in the WORK library and is deleted at the end of the SAS session. Since item stores are often used for postprocessing tasks, typical usage specifies a two-level name of the form *libname.membername*.

When you specify the RESTORE statement, the default output contains some general information about the input item store. This information includes the store name, label (if assigned), the data set that was used to create the store, BY group information, the procedure that created the store, and the creation date.

You can specify the following *option* in the RESTORE statement after a slash (/):

INFO < **(** *info-options* **)** >

specifies that additional information about the input item store be printed. This information is provided in two ODS tables. One table displays the variables in the item store, in addition to the mean and standard deviation for each of them. These statistics are based on the observations that were used to produce the store results. The second table shows the model on top of the list of all fitted models for each direction angle in the item store. The INFO option has the following *info-options*:

DETAILS

DET

specifies that more detailed information be displayed about the input item store. This option produces the full list of models for each direction angle in the item store, in addition to the model equivalence class. For more information about classes of equivalence, see the section "Classes of Equivalence" on page 10099 in Chapter 124, "The VARIOGRAM Procedure." The DETAILS option is ignored if the input item store contains information about a single fitted model.

ONLY

specifies that only information about the input item store without any simulation tasks be displayed.

Each variable in an item store has a mean value that is passed to PROC SIM2D and used in simulations. If the mean in the item store is a missing value, then a zero mean is used by default. Specify the "MEAN Statement" on page 8710 to override the mean information in the item store. For example, if you want to use only the correlation model in the item store and exclude the accompanying mean, then explicitly specify a zero mean in the "MEAN Statement" on page 8710.

When you specify an input item store with the RESTORE statement in PROC SIM2D, all the DATA= input data set variables must match input item store variables. If there are BY groups in the input DATA= set or in the input RESTORE variables, then PROC SIM2D handles the different cases as follows:

- If both PROC SIM2D has BY groups and the RESTORE statement has BY groups, then the analysis variables must match. This matching assumes implicitly that in each BY group of PROC SIM2D and the item store, the corresponding set of observations and correlation model comes from the same random field. This assumption is valid if you use the same data set, first in PROC VARIOGRAM to fit a model and save it in the item store, and then in PROC SIM2D to run simulations with the resulting correlation models.
- If PROC SIM2D has BY groups but the item store does not, then the item store is accepted only if the procedure and the item store analysis variables match. In this case, the same item store model choice iterates across the BY groups of the input data. You are advised to proceed with caution: each BY group in the input DATA= set corresponds to a different realization of a random field. Hence, by using the same correlation model for simulation purposes, you implicitly assume that all these different realizations are instances of the same random field.
- If PROC SIM2D has an input DATA= set and no BY groups but the item store has BY groups, then the item store is rejected
- If PROC SIM2D has no input DATA= set and the item store has BY groups, then PROC SIM2D runs unconditional simulations for the models in the store BY groups. See also the BY statement for more about the behavior in this case.

SIMULATE Statement

SIMULATE *simulate-options* **;**

The SIMULATE statement specifies details on the simulation and the covariance model used in the simulation. You can specify the following *simulate-options* with a SIMULATE statement, which can be abbreviated by SIM.

Table 105.3 summarizes the *options* available in the SIMULATE statement.

Table 105.3 SIMULATE Statement Options

Option	Description
Simulate-Options	
NUMREAL=	Specifies the number of realizations to produce
VAR=	Specifies the conditioning variable
Covariance Model Specification	
ANGLE=	Specifies the angle of the major axis
FORM=	Specifies the functional form
MDATA=	Specifies the input data set containing parameter values
NUGGET=	Specifies the nugget effect for the model
RANGE=	Specifies the range parameter

Table 105.3 *continued*

Option	Description
RATIO=	Specifies the ratio of the minor axis to the major axis
SCALE=	Specifies the scale (or *sill*) parameter
SEED=	Specifies the seed to use for the random number generator
SINGULAR=	Gives the singularity criterion
SMOOTH=	Specifies the smoothness parameter
STORESELECT	Uses information from an input item store for prediction

NUMREAL=*number*

NUMR=*number*

NR=*number*

specifies the number of realizations to produce for the spatial process specified by the covariance model. As a result, the number of observations in the OUTSIM= data set contributed by a given SIMULATE statement is the product of the NUMREAL= value and the number of grid points. This can cause the OUTSIM= data set to become large even for moderate values of the NUMREAL= option.

VAR=(*variable-name***)**

specifies the single numeric variable used as the conditioning variable in the simulation. In other words, the simulation is conditional on the values of the VAR= variable found in the DATA= data set. If you omit the VAR= option or if all observations of the VAR= variable are missing values, then the simulation is *unconditional*. Since multiple SIMULATE statements are allowed, you can perform both unconditional and conditional simulations with a single PROC SIM2D statement.

Covariance Model Specification

You can specify a semivariogram or covariance model in three ways:

- You specify the required parameters SCALE, RANGE, FORM, and SMOOTH (if you specify the MATERN form), and possibly the optional parameters NUGGET, ANGLE, and RATIO, explicitly in the SIMULATE statement.
- You specify an MDATA= data set. This data set contains variables that correspond to the required parameters SCALE, RANGE, FORM, and SMOOTH (if you specify the MATERN form), and, optionally, variables for the NUGGET, ANGLE, and RATIO parameters.
- You can specify an input item store in the RESTORE statement. The item store contains one or more correlation models for one or more direction angles. You can specify these models in the STORESELECT option of the SIMULATE statement to run a simulation.

The three methods are mutually exclusive: you specify all parameters explicitly, they are all are read from the MDATA= data set, or you select a model and its parameters from an input item store. The following *simulate-options* are related to model specification:

ANGLE=*angle* | **(***angle1, . . . , anglek***)**
specifies the angle of the major axis for anisotropic models, measured in degrees clockwise from the N–S axis. The default is ANGLE=0.

In the case of a nested semivariogram model with k nestings, you have the following two ways to specify the anisotropy major axis: you can specify only one *angle* which is then applied to all nested forms, or you can specify one angle for each of the k nestings.

NOTE: The syntax makes it possible to specify different angles for different forms of the nested model, but this practice is rarely used.

FORM=*form* | **(***form1, . . . , formk***)**
specifies the functional form (type) of the semivariogram model. Use the syntax with the single *form* to specify a non-nested model. Use the syntax with forms *formi*, $i = 1, \ldots, k$, to specify a nested model with k structures. Each of the forms can be any of the following:

CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |
PENTASPHERICAL | SINEHOLEEFFECT | SPHERICAL
CUB | EXP | GAU | MAT | PEN | SHE | SPH
specify the functional form (type).

For example, the syntax

```
FORM=GAU
```

specifies a model with a single Gaussian structure. Also, the syntax

```
FORM=(EXP,SHE,MAT)
```

specifies a nested model with an exponential, a sine hole effect, and a Matérn structure. Finally

```
FORM=(EXP,EXP)
```

specifies a nested model with two structures both of which are exponential.

NOTE: In the documentation, models are named either by using their full names or by using the first three letters of their structures. Also, the names of different structures in a nested model are separated by a hyphen (-). According to this convention, the previous examples illustrate how to specify a GAU, an EXP-SHE-MAT, and an EXP-EXP model, respectively, with the FORM= option.

All the supported model forms have two parameters specified by the SCALE= and RANGE= options, except for the MATERN model which has a third parameter specified by the SMOOTH= option. A FORM= value is required, unless you specify the MDATA= option or the STORESELECT option.

Computation of the MATERN covariance is numerically demanding. As a result, simulations that use Matérn covariance structures can be time-consuming.

MDATA=*SAS-data-set*

specifies the input data set that contains parameter values for the covariance or semivariogram model. The MDATA= option cannot be combined with any of the FORM= or STORESELECT options.

The MDATA= data set must contain variables named SCALE, RANGE, and FORM, and it can optionally contain variables NUGGET, ANGLE, and RATIO. If you specify the MATERN form, then you must also include a variable named SMOOTH in the MDATA= data set.

The FORM variable must be a character variable, and it can assume only the values allowed in the explicit FORM= syntax described previously. The RANGE, SCALE and SMOOTH 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 covariance or semivariogram model. For example, to specify a non-nested model that uses a spherical covariance, an MDATA= data set might contain the following statements:

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

The PROC SIM2D statement to use the MDATA= specification is of the form shown in the following:

```
proc sim2d data=...;
   sim var=.... mdata=md1;
run;
```

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

```
proc sim2d data=...;
   sim var=.... scale=25 range=10 form=sph;
run;
```

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

```
data md2;
   input scale range form $ nugget angle ratio smooth;
   datalines;
   20 8 SPH  5 35 .7   .
   12 3 MAT  5 0  .8 2.8
   4  1 GAU  5 45 .5   .
;


proc sim2d data=...;
   sim var=.... mdata=md2;
run;
```

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

```
proc sim2d data=...;
   sim var=.... scale=(20,12,4) range=(8,3,1) form=(SPH,MAT,GAU)
           angle=(35,0,45) ratio=(.7,.8,.5) nugget=5 smooth=2.8;
run;
```

This example is somewhat artificial in that it is usually hard to detect different anisotropy directions and ratios for different nestings by using an experimental semivariogram. **NOTE:** The NUGGET variable 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 "The Nugget Effect" on page 5038 in Chapter 68, "The KRIGE2D Procedure."

The example also shows that if you specify a MATERN form in the nested model, then the SMOOTH variable must be specified for all nestings in the MDATA= data set. You simply specify the SMOOTH value as missing for nestings other than MATERN.

The SIMULATE statement can be given a label. This is useful for identification in the OUTSIM= data set when multiple SIMULATE statements are specified. For example:

```
proc sim2d data=...;
   gauss1: sim var=.... form=gau;
   mean ....;
   gauss2: sim var=.... form gau;
   mean ....;
   exp1: sim var=.... form=exp;
   mean ....;
   exp2: sim var=.... form=exp;
   mean ....;
run;
```

In the OUTSIM= data set, the values "GAUSS1," "GAUSS2," "EXP1," and "EXP2" for the LABEL variable help to identify the realizations that correspond to the four SIMULATE statements. If you do not provide a label for a SIMULATE statement, a default label of SIM*n* is given, where *n* is the number of unlabeled SIMULATE statements seen so far.

NUGGET=*number*

specifies the nugget effect for the model. This effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram (see the section "The Nugget Effect" on page 5038 in Chapter 68, "The KRIGE2D Procedure," for details). For models without any nugget effect, the NUGGET= option is left out. The default is NUGGET=0.

RANGE=*range* | **(***range1, . . . , rangek***)**

specifies the range parameter in the semivariogram models. In the case of a nested semivariogram model with *k* nestings, you must specify a range for each nesting.

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

See the section "Theoretical Semivariogram Models" on page 5031 in Chapter 68, "The KRIGE2D Procedure," for details about how the RANGE= values are determined.

RATIO=*ratio* | (*ratio1, . . . , ratiok*)
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 with k nestings, you can specify a ratio for each nesting. The default is RATIO=1.

SCALE=*scale* | (*scale1, . . . , scalek*)
specifies the scale (or *sill*) parameter in semivariogram models. In the case of a nested semivariogram model with k nestings, 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.

See the section "Theoretical Semivariogram Models" on page 5031 in Chapter 68, "The KRIGE2D Procedure," for details about how the SCALE= values are determined.

SEED=*seed-value*
specifies the seed to use for the random number generator. The SEED= option *seed-value* has to be an integer.

SINGULAR=*number*
gives the singularity criterion for solving the set of linear equations involved in the computation of the mean and covariance of the conditional distribution associated with a given SIMULATE statement. The larger the value of the SINGULAR= option, the easier it is for the covariance matrix system to be declared singular. The default is SINGULAR=1E–8.

For more details about the use of the SINGULAR= option, see the section "Computational and Theoretical Details of Spatial Simulation" on page 8712.

SMOOTH=*smooth* | (*smooth1, . . . , smoothm*)
specifies the smoothness parameter $\nu > 0$ in the Matérn type of semivariance structures. The special case $\nu = 0.5$ is equivalent to the exponential model, whereas $\nu \to \infty$ gives the Gaussian model.

When you specify m different MATERN forms in the FORM= option, you must also provide m smoothness values in the SMOOTH option. If you must specify more than one smoothness value, the values are assigned sequentially to the MATERN nestings in the order the nestings are specified. If you specify more smoothness values than necessary, then values in excess are ignored.

STORESELECT(*ssel-options***)**
SSEL(*ssel-options***)**
specifies that information from an input item store be used for the prediction. You cannot combine the STORESELECT option with any of the FORM= or MDATA= options. The STORESELECT option has the following *ssel-options*:

TYPE=*field-type*
specifies whether to perform isotropic or anisotropic simulation. You can choose the *field-type* from one of the following:

ISO
specifies isotropic field for the simulation.

ANIGEO | GEO
specifies a field with geometric anisotropy for the simulation.

ANIZON(*zonal-form1, . . . , zonal-formn***)**
ZON(*zonal-form1, . . . , zonal-formn***)**

specifies a field with zonal anisotropy for the simulation. Each *zonal-formi*, $i = 1, \ldots, n$, can be any of the following:

CUB | EXP | GAU | MAT | PEN | SHE | SPH
specify a form for the simulation.

Each *zonal-formi*, $i = 1, \ldots, n$, is a structure in the purely zonal component of the correlation model in the direction angle of the minor anisotropy axis. For this reason, when you specify the TYPE=ANIZON suboption you must also specify the nonzonal component of the correlation model in the MODEL= suboption of the STORESELECT option. Assume the nonzonal component has k structures; these are common across all directions and each one has the same scale in all directions. In that sense, you use the TYPE=ANIZON suboption to specify only the n zonal anisotropy structures of an input store $(k + n)$-structure nested model in the direction angle of the minor anisotropy axis.

Given this specification, $k+n$ must be up to the maximum number of nested model structures that is supported by the item store. See also the MODEL= suboption of the STORESELECT option.

In conclusion, you can use an input item store for prediction with zonal anisotropy if you know that every structure in the nonzonal model component has the same scale across all directions. When this condition does not apply for the item store models, specify the model parameters explicitly in the SIMULATE statement.

Computation of the MATERN covariance is numerically demanding. As a result, predictions that use Matérn covariance structures can be time-consuming.

If you omit the TYPE= option, the default behavior is TYPE=ISO when the input item store contains information for only one angle or for the omnidirectional case. If you specify an item store with information for more than one direction, then the default behavior is TYPE=ANIGEO.

When you specify TYPE=ISO to request isotropic analysis in the presence of an item store with information for multiple directions, you must specify the ANGLEID= suboption of the STORESELECT option with one argument. This argument specifies which of the direction angles information to use for the isotropic analysis.

When you indicate the presence of anisotropy with the TYPE=ANIGEO or TYPE=ANIZON suboptions of the STORESELECT option, the following conditions apply:

- You must specify the ANGLEID= suboption of the STORESELECT option to designate the major and minor anisotropy axes. See the ANGLEID= suboption of the STORESELECT option for details.
- – For TYPE=ANIGEO, ensure that you have the same scale in all anisotropy directions.
  – For TYPE=ANIZON, ensure that the nonzonal component scale is the same in all anisotropy directions.

  If you import a nested model, these rules also apply to each one of the nested structures.
- Model ranges in the major anisotropy axis must be longer than ranges in the minor anisotropy axis.
- Any Matérn covariance structure must maintain its smoothness parameter value in all anisotropy directions.

ANGLEID=*angleid1* | (*angleid1, angleid2*)

specifies which direction angles in the input item store be used for simulation. The angles are identified by the corresponding number in the AngleID column of the "Store Models Information" table, or by the AngleID parameter in the table title when you specify the INFO(DETAILS) option in the RESTORE statement.

If you request isotropic prediction in the TYPE= suboption of the STORESELECT option and the item store has omnidirectional contents or information about only one angle, then the ANGLEID= option is ignored. The simulation input comes from the omnidirectional information. In the case of a single angle, you still perform isotropic simulation and the model parameters are provided by the model in the single direction angle in the item store. However, if the item store contains information for more than one angle, then you must specify one angle ID in *angleid1*. The model information from the corresponding angle is then used in your isotropic simulation.

When you specify an anisotropic simulation in the TYPE= option of the STORESELECT option, you need to have information about two perpendicular direction angles. One of them is the major and the other is the minor anisotropy axis. You must always specify the major anisotropy axis angle ID in *angleid1* and the minor anisotropy axis angle ID in *angleid2*. This means that the range parameters of the model forms in the angle designated by the *angleid1* need to be larger than the corresponding ranges of the forms in the angle designated by the *angleid2*. Conveniently, if the item store has only two angles, then you only need to specify the ID *angleid1* of the major anisotropy axis angle. If the item store has only one angle, then you cannot perform anisotropic simulation with input from the item store.

NOTE: You can perform geometric anisotropic analysis even if the item store does not contain information about a direction that is perpendicular to the one specified by *angleid1*. This is possible due to the geometry of the ellipse. In particular, when you specify the major axis with *angleid1* and an angle ID for a second direction with a corresponding smaller range, then PROC SIM2D automatically computes the minor anisotropy axis range and the necessary range ratio parameter.

Anisotropic analysis is not possible when you specify instances of the same angle in the input item store. It is possible that PROC VARIOGRAM produces an item store where two or more directions can be the same if their corresponding correlation models were obtained for different angle tolerances or bandwidths in the VARIOGRAM procedure. Consequently, you cannot specify anisotropic simulation if the input store contains only two angles that are the same or if you specify *angleid1* and *angleid2* that correspond to equal angles.

MODEL=*form* | (*form1, . . . , formk*)

specifies the theoretical semivariogram model selection to use for the simulation. Use any combination of one, two, or three forms to describe a model in the input item store because up to three nested structures are supported. Each *formi*, $i = 1, \ldots, k$, can be any of the following:

CUB | EXP | GAU | MAT | PEN | SHE | SPH

specify the selection model.

Computation of the MATERN covariance is numerically demanding. As a result, simulations that use Matérn covariance structures can be time-consuming.

All fitted models that are stored in the input item store contain information about their component parameters and also about the nugget effect if any. The SIM2D procedure retrieves this

information when you make a model selection in the MODEL= option, and you do not need to individually specify a nugget effect or any other parameter of the model.

By default, the model that is ranked first among the models for a given angle in the item store is used for the simulation task. If more than one model is available in the item store, then you can specify the MODEL= option to use a different model for the simulation.

In an anisotropic simulation, the default selection is the model that is ranked first in the direction angle of the major anisotropy axis. If you specify the TYPE=ANIGEO option, then a model that consists of identical structures needs to be present in the selected minor anisotropy axis angle in the item store. If you specify the TYPE=ANIZON option, then a model with the exact same first k structures must be present in the selected minor anisotropy axis angle, and it must feature at least one more structure as a zonal component. The zonal component is specified separately in the TYPE=ANIZON suboption of the STORESELECT option. Consequently, remember that in zonal anisotropy the MODEL= suboption designates only the nonzonal component of the correlation model in the minor anisotropy axis direction. In all, if there are k common structures and n structures in the purely zonal component, then $k + n$ must be up to the maximum number of nested model structures that is supported by the item store.

SVAR=*store-var* | (*store-varlist*)

specifies one *store-var* item store variable or a list *store-varlist* of variables that are present in the item store. This option selects one or more item store variables whose correlation models you want to use in the current simulation task.

If you are performing a conditional simulation, then PROC SIM2D searches the input item store for the variable that is specified in the VAR= option of the SIMULATE statement. Then, the procedure selects the appropriate correlation model for the task. In this case, if you specify the SVAR= option, it is ignored. However, when you request an unconditional simulation and specify input from an item store, then you must also use SVAR= to specify a source for your correlation model.

In comparison to the other two ways of specifying a correlation model in PROC SIM2D, the STORESELECT option is quite different because you can avoid explicit specification of all parameter values of a model. When you specify the STORESELECT option, then the corresponding scale, range, nugget effect, and smoothness (if appropriate) parameter values are invoked as saved attributes of the model that you select from the item store.

In the case of anisotropy, you specify the angles indirectly with the ANGLEID= option of the STORESELECT option, and the ratios are computed implicitly by using the selected model ranges. Explore how to specify valid anisotropical models imported from an input item store with the two examples that follow.

In the first example, assume the input item store InStoreGeo contains exponential models in the angles $\theta_1 = 0°$, $\theta_2 = 45°$, and $\theta_3 = 90°$. You know in advance that all models have the same scale $c_1 = c_2 = c_3$ across these directions and that the respective ranges are $a_1 = 15$, $a_2 = 20$, and $a_3 = 25$ in distance units. Hence, you have a case of geometric anisotropy where the major anisotropy axis is in the direction of angle θ_3 and the minor anisotropy axis is in the direction of angle θ_1. The following statements in PROC SIM2D use the information in the item store InStoreGeo to perform simulation under the assumption of geometric anisotropy:

```
proc sim2d data=...;
   restore in=InStoreGeo;
   simulate storeselect(model=exp type=anigeo angleid=(3,1));
run;
```

For the second example, assume a case of zonal anisotropy. Consider the input item store InStoreZon, which contains models in the two angles, $\theta_1 = 30°$ and $\theta_2 = 120°$. Specifically, in θ_1 you have an exponential-spherical model: the exponential structure has scale $c_{1E} = 3$ and range $a_{1E} = 10$; the spherical structure has scale $c_{1S} = 1$ and range $a_{1S} = 6$. In direction θ_2 you have an exponential model with scale $c_{1E} = 3$ and range $a_{1E} = 12$. Hence, the zonal anisotropy major axis is in the direction of the lowest total variance, which is in angle θ_2; then, the minor axis is in the direction of angle θ_1. The following statements in PROC SIM2D use the information in the store InStoreZon to perform simulation under the assumption of zonal anisotropy:

```
proc sim2d data=...;
   restore in=InStoreZon;
   simulate storeselect(model=exp type=anizon(sph) angleid=(2,1));
run;
```

MEAN Statement

MEAN *spec1*, . . . , *spec6* **;**

MEAN QDATA=*SAS-data-set* **CONST=***var1* **CX=***var2* **CY=***var3*
CXX=*var4* **CYY=***var5* **CXY=***var6* **;**

MEAN QDATA=*SAS-data-set* **;**

A mean function $\mu(s)$ that is a quadratic in the coordinates can be written as

$$\mu(s) = \mu(x, y) = \beta_0 + \beta_1 x + \beta_2 y + \beta_3 x^2 + \beta_4 y^2 + \beta_5 xy$$

The MEAN statement specifies the quadratic surface to use as the mean function for the simulated SRF. There are two ways to specify the MEAN statement. The MEAN statement allows the specification of the coefficients $\beta_0, \ldots, \beta_5$ either explicitly or through a QDATA= data set.

An example of an explicit specification is the following:

```
mean 1.4 + 2.5*x + 3.6*y + 0.47*x*x + 0.58*y*y + 0.69*x*y;
```

In this example, all terms have a nonzero coefficient. Any term with a zero coefficient is simply left out of the specification. For example,

```
mean 1.4;
```

is a valid quadratic form with all terms having zero coefficients except the constant term.

An equivalent way of specifying the mean function is through the QDATA= data set. For example, the MEAN statement

```
mean 1.4 + 2.5*x + 3.6*y + 0.47*x*x + 0.58*y*y + 0.69*x*y;
```

can be alternatively specified by the following DATA step and MEAN statement:

```
data q1;
   input c1 c2 c3 c4 c5 c6;
   datalines;
   1.4 2.5 3.6 0.47 0.58 0.69
;

proc sim2d data=....;
   simulate ...;
   mean qdata=q1 const=c1 cx=c2 cy=c3 cxx=c4 cyy=c5 cxy=c6;
run;
```

The QDATA= data set specifies the data set containing the coefficients. The parameters CONST=, CX=, CY=, CXX=, CYY=, and CYX= specify the variables in the QDATA= data set that correspond to the constant, linear y, linear y, and so on. For any coefficient not specified in this list, the QDATA= data set is checked for the presence of variables with default names of CONST, CX, CY, CXX, CYY, and CXY. If these variables are present, their values are taken as the corresponding coefficients. Hence, you can rewrite the previous example as follows:

```
data q1;
   input const cx cy cxx cyy cxy;
   datalines;
   1.4 2.5 3.6 0.47 0.58 0.69
;

proc sim2d data=....;
   simulate ...;
   mean qdata=q1;
run;
```

If a given coefficient does not appear in the list or in the data set with the default name, a value of zero is assumed.

If you run a simulation task with input from a RESTORE statement, then by default the simulation uses the mean of the item store variable in the simulation. You can override this default behavior if you explicitly specify the MEAN statement with a different mean function.

Details: SIM2D Procedure

Computational and Theoretical Details of Spatial Simulation

Introduction

There are a number of approaches to simulating spatial random fields or, more generally, simulating sets of dependent random variables. These include sequential indicator methods, turning bands, and the Karhunen-Loeve expansion. See Christakos (1992, Chapter 8) and Deutsch and Journel (1992, Chapter V) for details.

A particularly simple method available for Gaussian spatial random fields is the LU decomposition method. This method is computationally efficient. For a given covariance matrix, the $\mathrm{LU} = \mathbf{LL}'$ decomposition is computed once, and the simulation proceeds by repeatedly generating a vector of independent $N(0,1)$ random variables and multiplying by the $\mathbf{L}$ matrix.

One problem with this technique is memory requirements; memory is required to hold the full data and grid covariance matrix in core. While this is especially limiting in the three-dimensional case, you can use PROC SIM2D, which handles only two-dimensional data, for moderately sized simulation problems.

Theoretical Development

It is a simple matter to produce an $N(0,1)$ random number, and by stacking k $N(0,1)$ random numbers in a column vector, you can obtain a vector with independent standard normal components $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$. The meaning of the terms *independence* and *randomness* in the context of a deterministic algorithm required for the generation of these numbers is subtle; see Knuth (1981, Chapter 3) for details.

Rather than $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$, what is required is the generation of a vector $\mathbf{Z} \sim N_k(\mathbf{0}, \mathbf{C})$—that is,

$$\mathbf{Z} = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_k \end{bmatrix}$$

with covariance matrix

$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1k} \\ C_{21} & C_{22} & \cdots & C_{2k} \\ & \ddots & & \\ C_{k1} & C_{k2} & \cdots & C_{kk} \end{pmatrix}$$

If the covariance matrix is symmetric and positive definite, it has a Cholesky root $\mathbf{L}$ such that $\mathbf{C}$ can be factored as

$$\mathbf{C} = \mathbf{LL}'$$

where $\mathbf{L}$ is lower triangular. See Ralston and Rabinowitz (1978, Chapter 9, Section 3-3) for details. This vector $\mathbf{Z}$ can be generated by the transformation $\mathbf{Z} = \mathbf{LW}$. Here is where the assumption of a Gaussian SRF is crucial. When $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$, then $\mathbf{Z} = \mathbf{LW}$ is also Gaussian. The mean of $\mathbf{Z}$ is

$$E(\mathbf{Z}) = \mathbf{L}(E(\mathbf{W})) = \mathbf{0}$$

and the variance is

$$\mathrm{Var}(\mathbf{Z}) = \mathrm{Var}(\mathbf{LW}) = E(\mathbf{LWW'L'}) = \mathbf{L}E(\mathbf{WW'})\mathbf{L'} = \mathbf{LL'} = \mathbf{C}$$

Consider now an SRF $Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2$, with spatial covariance function $C(\boldsymbol{h})$. Fix locations $\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_k$, and let $\mathbf{Z}$ denote the random vector

$$\mathbf{Z} = \begin{bmatrix} Z(\boldsymbol{s}_1) \\ Z(\boldsymbol{s}_2) \\ \vdots \\ Z(\boldsymbol{s}_k) \end{bmatrix}$$

with corresponding covariance matrix

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

Since this covariance matrix is symmetric and positive definite, it has a Cholesky root, and the $Z(\boldsymbol{s}_i), i = 1, \ldots, k$, can be simulated as described previously. This is how the SIM2D procedure implements unconditional simulation in the zero-mean case. More generally,

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

where $\mu(\boldsymbol{s})$ is a quadratic form in the coordinates $\boldsymbol{s} = (x, y)$ and the $\varepsilon(\boldsymbol{s})$ is an SRF that has the same covariance matrix $\mathbf{C}_z$ as previously. In this case, the $\mu(\boldsymbol{s}_i), i = 1, \ldots, k$, is computed once and added to the simulated vector $\varepsilon(\boldsymbol{s}_i), i = 1, \ldots, k$, for each realization.

For a conditional simulation, this distribution of

$$\mathbf{Z} = \begin{bmatrix} Z(\boldsymbol{s}_1) \\ Z(\boldsymbol{s}_2) \\ \vdots \\ Z(\boldsymbol{s}_k) \end{bmatrix}$$

must be conditioned on the observed data. The relevant general result concerning conditional distributions of multivariate normal random variables is the following. Let $\mathbf{X} \sim N_m(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}$$

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

The subvector $\mathbf{X}_1$ is $k \times 1$, $\mathbf{X}_2$ is $n \times 1$, $\boldsymbol{\Sigma}_{11}$ is $k \times k$, $\boldsymbol{\Sigma}_{22}$ is $n \times n$, and $\boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}'_{21}$ is $k \times n$, with $k + n = m$. The full vector $\mathbf{X}$ is partitioned into two subvectors, $\mathbf{X}_1$ and $\mathbf{X}_2$, and $\boldsymbol{\Sigma}$ is similarly partitioned into covariances and cross covariances.

With this notation, the distribution of $\mathbf{X}_1$ conditioned on $\mathbf{X}_2 = \boldsymbol{x}_2$ is $N_k(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\Sigma}})$, with

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\boldsymbol{x}_2 - \boldsymbol{\mu}_2)$$

and

$$\tilde{\boldsymbol{\Sigma}} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}$$

See Searle (1971, pp. 46–47) for details. The correspondence with the conditional spatial simulation problem is as follows. Let the coordinates of the observed data points be denoted $\tilde{\boldsymbol{s}}_1, \tilde{\boldsymbol{s}}_2, \ldots, \tilde{\boldsymbol{s}}_n$, with values $\tilde{z}_1, \tilde{z}_2, \ldots, \tilde{z}_n$. Let $\tilde{\mathbf{Z}}$ denote the random vector

$$\tilde{\mathbf{Z}} = \begin{bmatrix} Z(\tilde{\boldsymbol{s}}_1) \\ Z(\tilde{\boldsymbol{s}}_2) \\ \vdots \\ Z(\tilde{\boldsymbol{s}}_n) \end{bmatrix}$$

The random vector $\tilde{\mathbf{Z}}$ corresponds to $\mathbf{X}_2$, while $\mathbf{Z}$ corresponds to $\mathbf{X}_1$. Then $\left(\mathbf{Z} \mid \tilde{\mathbf{Z}} = \tilde{\mathbf{z}}\right) \sim N_k(\tilde{\boldsymbol{\mu}}, \tilde{\mathbf{C}})$ as in the previous distribution. The matrix

$$\tilde{\mathbf{C}} = \mathbf{C}_{11} - \mathbf{C}_{12}\mathbf{C}_{22}^{-1}\mathbf{C}_{21}$$

is again positive definite, so a Cholesky factorization can be performed.

The dimension n for $\tilde{\mathbf{Z}}$ is simply the number of nonmissing observations for the VAR= variable; the values $\tilde{z}_1, \tilde{z}_2, \ldots, \tilde{z}_n$ are the values of this variable. The coordinates $\tilde{\boldsymbol{s}}_1, \tilde{\boldsymbol{s}}_2, \ldots, \tilde{\boldsymbol{s}}_n$ are also found in the DATA= data set, with the variables that correspond to the x and y coordinates identified in the COORDINATES statement. **Note:** All VAR= variables use the same set of conditioning coordinates; this fixes the matrix $\mathbf{C}_{22}$ for all simulations.

The dimension k for $\mathbf{Z}$ is the number of grid points specified in the GRID statement. Since there is a single GRID statement, this fixes the matrix $\mathbf{C}_{11}$ for all simulations. Similarly, $\mathbf{C}_{12}$ is fixed.

The Cholesky factorization $\tilde{\mathbf{C}} = \mathbf{LL}'$ is computed once, as is the mean correction

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu}_1 + \mathbf{C}_{12}\mathbf{C}_{22}^{-1}(\boldsymbol{x}_2 - \boldsymbol{\mu}_2)$$

The means $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are computed using the grid coordinates $\boldsymbol{s}_1, \boldsymbol{s}_2, \ldots, \boldsymbol{s}_k$, the data coordinates $\tilde{\boldsymbol{s}}_1, \tilde{\boldsymbol{s}}_2, \ldots, \tilde{\boldsymbol{s}}_n$, and the quadratic form specification from the MEAN statement. The simulation is now performed exactly as in the unconditional case. A $k \times 1$ vector of independent standard $N(0,1)$ random variables is generated and multiplied by $\mathbf{L}$, and $\tilde{\boldsymbol{\mu}}$ is added to the transformed vector. This is repeated N times, where N is the value specified for the NR= option.

Computational Details

In the computation of $\tilde{\boldsymbol{\mu}}$ and $\boldsymbol{\Sigma}$ described in the previous section, the inverse $\boldsymbol{\Sigma}_{22}^{-1}$ is never actually computed; an equation of the form

$$\boldsymbol{\Sigma}_{22}\mathbf{A} = \mathbf{B}$$

is solved for $\mathbf{A}$ by using a modified Gaussian elimination algorithm that takes advantage of the fact that $\boldsymbol{\Sigma}_{22}$ is symmetric with constant diagonal $C_z(0)$ that is larger than all off-diagonal elements. The SINGULAR= option pertains to this algorithm. The value specified for the SINGULAR= option is scaled by $C_z(0)$ before comparison with the pivot element.

Memory Usage

For conditional simulations, the largest matrix held in core memory at any one time depends on the number of grid points and data points. Using the previous notation, the data-data covariance matrix $\mathbf{C}_{22}$ is $n \times n$, where n is the number of nonmissing observations for the VAR= variable in the DATA= data set. The grid-data cross covariance $\mathbf{C}_{12}$ is $n \times k$, where k is the number of grid points. The grid-grid covariance $\mathbf{C}_{11}$ is $k \times k$. The maximum memory required at any one time for storing these matrices is

$$\max\left(k(k+1), n(n+1) + 2(n \times k)\right) \times \text{sizeof(double)}$$

There are additional memory requirements that add to the total memory usage, but usually these matrix calculations dominate, especially when the number of grid points is large.

Output Data Set

The SIM2D procedure produces a single output data set: the OUTSIM=*SAS-data-set*. The OUTSIM= data set contains all the needed information to uniquely identify the simulated values.

The OUTSIM= data set contains the following variables:

- LABEL, which is the label for the current SIMULATE statement
- VARNAME, which is the name of the conditioning variable for the current SIMULATE statement
- MODSVAR, which is the name of the input item store variable associated with the current correlation model in an unconditional simulation

- _ITER_, which is the iteration number within the current SIMULATE statement
- GXC, which is the *x* coordinate for the current grid point
- GYC, which is the *y* coordinate for the current grid point
- SVALUE, which is the value of the simulated variable

If you specify the NARROW option in the PROC SIM2D statement, the LABEL and VARNAME variables are not included in the OUTSIM= data set. This option is useful in the case where the number of data points, grid points, and realizations are such that they generate a very large OUTSIM= data set. The size of the OUTSIM= data set is reduced when these variables are not included.

In unconditional simulation tasks where no input data set is specified, the VARNAME variable is excluded from the OUTSIM= data set. In unconditional simulation tasks where you have specified an input data set, the VARNAME variable is included but given a missing value. In the case of mixed conditional and unconditional simulations (that is, when multiple SIMULATE statements are specified, among which one or more contain a VAR= specification and one or more have no VAR= specification), the VARNAME variable is included but is given a missing value for those observations that correspond to an unconditional simulation.

The MODSVAR variable is included in the OUTSIM= data set only when you specify an input item store with the RESTORE statement, and it indicates the presence of that store. This variable helps you identify the output of different unconditional simulations when the model input comes from an item store; it is not suggesting that a simulation task is conditioned upon it.

Specifically, the MODSVAR variable has a missing value for conditional simulation tasks. The variable also has a missing value for unconditional simulations for which you specify a correlation model explicitly, either with the FORM= option or with the MDATA= data set in the SIMULATE statement. In all other cases, the MODSVAR variable indicates the input item store variable that is associated with the store model used for the current unconditional simulation task.

Displayed Output

In addition to the output data set, the SIM2D procedure produces output objects as well. The SIM2D 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 that shows the spatial distribution of the observations of the current VAR variable in the SIMULATE statement, in the case of conditional simulations. The observations are displayed by default with circled markers whose color indicates the VAR value at the corresponding location.
- a default table for each SIMULATE statement that summarizes the simulation specifications.
- a default table for each SIMULATE statement that shows the covariance model parameters for the corresponding simulation.
- plots of simulation outcome at each point of the specified output grid or at specified individual locations. You can produce more than one of these plots for every SIMULATE statement with styles that you can specify by using the available suboptions of the PLOTS=SIM option.

- a "Store Info" table with basic information about the input item store. This table is produced by default when you specify the RESTORE statement.
- a "Store Variables Information" table that describes the analysis variables of an input item store. The table is produced by default when you specify an item store with the RESTORE statement.
- a "Store Models Information" table with detailed information about the models and direction angles that are contained in an input item store. The table is produced by default when you specify an item store with the RESTORE statement.

ODS Table Names

Each table created by PROC SIM2D 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 105.4.

Table 105.4 ODS Tables Produced by PROC SIM2D

ODS Table Name	Description	Statement	Option
ModelInfo	Parameters of the covariance model used in current simulation	PROC	Default output
NObs	Number of observations read and used	PROC	Default output
SimuInfo	General information about the simulation	PROC	Default output
StoreInfo	Input item store identity information	RESTORE	Default output
StoreModelInfo	Input item store direction angles and models information	RESTORE	INFO
StoreVarInfo	Input item store variables and their statistics	RESTORE	INFO

ODS Graphics

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

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 607 in Chapter 21, "Statistical Graphics Using ODS."

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section "A Primer on ODS Statistical Graphics" on page 606 in Chapter 21, "Statistical Graphics Using ODS."

For additional control of the graphics that are displayed, see the PLOTS option in the section "PROC SIM2D Statement" on page 8690.

ODS Graph Names

PROC SIM2D 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. You must also specify the PLOTS= option indicated in Table 105.5.

Table 105.5 Graphs Produced by PROC SIM2D

ODS Graph Name	Plot Description	Statement	Option
SimulationPlot	Outlines of the observation locations, and either a contour plot of the simulated means and surface of the standard deviation in areal grids, or a band plot of the simulated means or box plot of the simulation distribution in linear grids or individual locations	PROC	PLOTS=SIM
ObservationsPlot	Scatter plot of observed data and colored markers indicating observed values	PROC	PLOTS=OBSERV
Semivariogram	Plots of the semivariogram models used for all simulation tasks	PROC	PLOTS=SEMIVAR

Examples: SIM2D Procedure

Example 105.1: Simulation and Economic Feasibility

You can use simulations to investigate the expected behavior of a stochastic process. Simulations with PROC SIM2D can indicate spatial characteristics in your study that might be important for decision making or general assessment. The present example and the one in section "Example 105.3: Risk Analysis with Simulation" on page 8727 are two instances of this type of analysis in different fields.

Continuing with the coal seam thickness example from the section "Getting Started: SIM2D Procedure" on page 8681, this example asks a rather complicated question of economic nature. For illustration, an (approximate) answer is provided, which requires the use of simulation.

Simulating a Subregion for Economic Feasibility

The coal seam must be of a minimum thickness, called a *cutoff value*, for a mining operation to be profitable. Suppose that, for a subregion of the measured area, the cost of mining is higher than in the remaining areas due to the geology of the overburden. This higher cost results in a higher thickness cutoff value for the subregion. Suppose also that it is determined from a detailed cost analysis that at least 60% of the subregion must exceed a seam thickness of 39.7 feet for profitability.

How can you use the SRF model (μ and $C_z(\boldsymbol{s})$) and the measured seam thickness values $Z(\boldsymbol{s}_i), i = 1, \ldots, 75$, to determine, in some approximate way, whether at least 60% of the subregion exceeds this minimum?

Spatial prediction does not appear to be helpful in answering this question. Although it is easy to determine whether a predicted value at a location in the subregion is above the 39.7-feet cutoff value, it is not clear how to incorporate the standard error associated with the predicted value. The standard error is what characterizes the stochastic nature of the prediction (and the underlying SRF). It is clear that it must be included in any realistic approach to the problem.

A conditional simulation, on the other hand, seems to be a natural way of obtaining an approximate answer. By simulating the SRF on a sufficiently fine grid in the subregion, you can determine the proportion of grid points in which the mean value over realizations exceeds the 39.7-feet cutoff and compare it with the 60% value needed for profitability.

It is desirable in any simulation study that the quantity being estimated (in this case, the proportion that exceeds the 39.7-feet cutoff) not depend on the number of simulations performed. For example, suppose that the maximum seam thickness is simulated. It is likely that the maximum value increases as the number of simulations performed increases. Hence, a simulation is not useful for such an estimate. A simulation is useful for determining the *distribution* of the maximum, but there are general theoretical results for such distributions, making such a simulation unnecessary. See Leadbetter, Lindgren, and Rootzen (1983) for details.

In the case of simulating the proportion that exceeds the 39.7-feet cutoff, it is expected that this quantity will settle down to a fixed value as the number of realizations increases. At a fixed grid point, the quantity being compared with the cutoff value is the mean over all simulated realizations; this mean value settles down to a fixed number as the number of realizations increases. In the same manner, the proportion of the grid where the mean values exceed the cutoff also becomes constant. This can be tested using PROC SIM2D.

A crucial, nonprovable assumption in applying SRF theory to the coal seam thickness data is that the values $Z(\boldsymbol{s}_i), i = 1, \ldots, 75$, represent a *single* realization from the set of all possible realizations consistent with the SRF model (μ and $C_z(\boldsymbol{h})$). A conditional simulation repeatedly produces other possible simulated realizations consistent with the model and data. However, the only concern of the mining company is this single unique realization. It is not concerned about similar coal fields to be mined sometime in the future; it might never see another coal field remotely similar to this one, or it might not be in business in the future.

Hence the proportion found by generating repeated simulated realizations must somehow relate back to the unique realization that is the coal field (seam thickness). This is done by interpreting the proportion found from a simulation to the spatial mean proportion for the unique realization. The term "spatial mean" is simply an appropriate integral over the fixed (but unknown) spatial function $z(\boldsymbol{s})$. (The SRF is denoted $Z(\boldsymbol{s})$; a particular realization, a deterministic function of the spatial coordinates, is denoted $z(\boldsymbol{s})$.)

This interpretation requires an ergodic assumption, which is also needed in the original estimation of $C_z(\boldsymbol{s})$. See Cressie (1993, pp. 53–58) for a discussion of ergodicity and Gaussian SRFs.

Implementation Using PROC SIM2D

The subregion to be considered is the southeast corner of the field, which is a square region with a length of 40 distance units (in thousands of feet). First, you input the thickness data as the following DATA step shows:

```
title 'Simulating a Subregion for Economic Feasibility';

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
;
```

PROC SIM2D is run on the entire data set for conditioning, while the simulation grid covers only this subregion. It is convenient to be able to vary the seed, the grid increment, and the number of simulations performed. The following macro implements the computation of the percent area that exceeds the cutoff value by using the seed, the grid increment, and the number of simulated realizations as macro arguments.

Within the macro, the data set produced by PROC SIM2D is transposed with PROC TRANSPOSE so that each grid location is a separate variable. The MEANS procedure averages then the simulated value at each grid point over all realizations. It is this average that is compared to the cutoff value. The last DATA step does the comparison, uses an appropriate loop to determine the percent of the grid locations that exceed this cutoff value, and writes the results to the listing file in the form of a report. This sequence is implemented with the following statements:

```
/* Construct macro for conditional simulation ------------------*/
%let cc0=7.4599;
%let aa0=30.1111;
%let ngt=1e-8;
%let form=gauss;
%let cut=39.7;

%macro area_sim(seed=,nr=,ginc=);
   %let ngrid=%eval(40/&ginc+1);
   %let tgrid=%eval(&ngrid*&ngrid);

   proc sim2d data=thick outsim=sim1;
      coordinates xc=east yc=north;
      simulate var=thick numreal=&nr seed=&seed
               scale=&cc0 range=&aa0 nugget=&ngt form=&form;
```

```
      mean 40.1173;
      grid x=60 to 100 by &ginc
           y= 0 to  40 by &ginc;
   run;

   proc transpose data=sim1 out=sim2 prefix=sims;
      by _iter_;
      var svalue;
   run;

   proc means data=sim2 noprint n mean;
      var sims1-sims&tgrid;
      output out=msim n=numsim mean=ms1-ms&tgrid;
   run;

   data _null_;
      file print;
      array simss ms1-ms&tgrid;
      set msim;
      cflag=0;
      do ss=1 to &tgrid;
         tempv=simss[ss];
         if simss[ss] > &cut then do;
            cflag + 1;
         end;
      end;

      area_per=100*(cflag/&tgrid);
      put // +5 'Conditional Simulation of Coal Seam'
                ' Thickness for Subregion';
      put / +5 'Subregion is South-East Corner 40 by 40 distance units';
      put / +5 "Seed:&seed" +2 "Grid Increment:&ginc";
      put / +5 "Total Number of Grid Points:&tgrid" +2
               "Number of Simulations:&nr";
      put / +5 "Percent of Subregion Exceeding Cutoff of %left(&cut) ft.:"
                +2 area_per 5.2;
   run;
%mend area_sim;
```

In the following statement, you invoke the macro three times. Each time, the macro is invoked with a different seed and combination of the grid increment and number of simulations. The macro is first invoked with a relatively coarse grid (grid increment of 10 distance units) and a small number of realizations (5). The output of this conditional simulation is shown in Output 105.1.1.

```
/* Execute macro for coarse grid -------------------------------*/
%area_sim(seed=12345,nr=5,ginc=10);
```

Output 105.1.1 Conditional Simulation of Coal Seam Thickness on a Coarse Grid

Simulating a Subregion for Economic Feasibility

```
Conditional Simulation of Coal Seam Thickness for Subregion

Subregion is South-East Corner 40 by 40 distance units

Seed:12345  Grid Increment:10

Total Number of Grid Points:25  Number of Simulations:5

Percent of Subregion Exceeding Cutoff of 39.7 ft.:  76.00
```

The next invocation, in the following statement, uses a finer grid and 50 realizations. The output of the second conditional simulation is shown in Output 105.1.2.

```
/* Execute macro for fine grid and fewer simulations ------------*/
%area_sim(seed=54321,nr=50,ginc=1);
```

Output 105.1.2 Conditional Simulation of Coal Seam Thickness on a Fine Grid

Simulating a Subregion for Economic Feasibility

```
Conditional Simulation of Coal Seam Thickness for Subregion

Subregion is South-East Corner 40 by 40 distance units

Seed:54321  Grid Increment:1

Total Number of Grid Points:1681  Number of Simulations:50

Percent of Subregion Exceeding Cutoff of 39.7 ft.:  76.09
```

The final invocation, in the following statement, uses the same grid increment and 500 realizations. The output of this conditional simulation is shown in Output 105.1.3.

```
/* Execute macro for fine grid and more simulations ------------*/
%area_sim(seed=655311,nr=500,ginc=1);
```

Output 105.1.3 Conditional Simulation of Coal Seam Thickness on a Fine Grid

Simulating a Subregion for Economic Feasibility

```
Conditional Simulation of Coal Seam Thickness for Subregion

Subregion is South-East Corner 40 by 40 distance units

Seed:655311  Grid Increment:1

Total Number of Grid Points:1681  Number of Simulations:500

Percent of Subregion Exceeding Cutoff of 39.7 ft.:  76.09
```

The results from the preceding simulations indicate that about 76% of the subregion exceeds the cutoff value.

NOTE: The number of grid points in the simulation increases with the square of the decrease in the grid increment, leading to long CPU processing times. Increasing the number of realizations results in a linear increase in processing times. Hence, using as coarse a grid as possible allows for more realizations and experimentation with different seeds.

Example 105.2: Variability at Selected Locations

This example exhibits a more detailed investigation of the variation of simulated Thick variable values. You use the same thick data set from the section "Getting Started: SIM2D Procedure" on page 8681, and you are interested in the simulated values statistics at two selected grid points.

Specifically, you perform a simulation asking for 5,000 realizations (iterations) at two points of the region defined in the section "Preliminary Spatial Data Analysis" on page 8681. These are the extreme southwest point and a point toward the northeast corner of the region. Since you want to avoid performing the simulation across the whole region, you need to produce a GDATA= data set to specify the coordinates of the selected points. These steps are implemented using the following DATA step and statements:

```
title 'Investigation of Random Field Variability';

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
;

data grid;
   input xc yc;
   datalines;
   0   0
   75  75
;
```

Then, you run PROC SIM2D with the same parameters and characteristics as those shown in the section "Preliminary Spatial Data Analysis" on page 8681. This time, however, you ask for simulated values only at the two locations you specified in the previous DATA step. The following statements execute the requested simulation:

```
proc sim2d data=thick outsim=sim1;
   coordinates xc=East yc=North;
   simulate var=Thick numreal=5000 seed=79931
            scale=7.4599 range=30.1111 form=gauss;
   mean 40.1173;
   grid gdata=grid xc=xc yc=yc;
run;
```

After the simulation is performed, summary statistics are computed for each of the specified grid points.

In particular, you use PROC UNIVARIATE and a BY statement to request the quantiles and the extreme observations at these locations, as the following statements show:

```
proc sort data=sim1;
   by gxc gyc;
run;

proc univariate data=sim1;
   var svalue;
   by gxc gyc;
   ods select Quantiles ExtremeObs;
   title 'Simulation Statistics at Selected Grid Points';
run;
```

The summary statistics for the first grid point (East=0, North=0) are presented in Output 105.2.1.

Output 105.2.1 Simulation Statistics at Grid Point (East=0, North=0)

Simulation Statistics at Selected Grid Points

The UNIVARIATE Procedure
Variable: SVALUE (Simulated Value at Grid Point)

X-coordinate of the grid point=0 Y-coordinate of the grid point=0

Quantiles (Definition 5)	
Level	**Quantile**
100% Max	42.4207
99%	41.8960
95%	41.5315
90%	41.3419
75% Q3	41.0324
50% Median	40.6701
25% Q1	40.2871
10%	39.9904
5%	39.7825
1%	39.4181
0% Min	38.6864

X-coordinate of the grid point=0 Y-coordinate of the grid point=0

Extreme Observations			
Lowest		**Highest**	
Value	**Obs**	**Value**	**Obs**
38.6864	2691	42.2952	1149
38.8611	1817	42.3114	3612
38.9013	3026	42.3305	3757
38.9467	2275	42.4177	135
38.9823	3100	42.4207	4536

Finally, Output 105.2.2 displays the summary statistics for the second grid point (East=75, North=75).

Output 105.2.2 Simulation Statistics at Grid Point (East=75, North=75)

Simulation Statistics at Selected Grid Points

The UNIVARIATE Procedure
Variable: SVALUE (Simulated Value at Grid Point)

X-coordinate of the grid point=75 Y-coordinate of the grid point=75

Quantiles (Definition 5)	
Level	**Quantile**
100% Max	40.1171
99%	40.1147
95%	40.1131
90%	40.1122
75% Q3	40.1108
50% Median	40.1092
25% Q1	40.1075
10%	40.1062
5%	40.1053
1%	40.1035
0% Min	40.1001

X-coordinate of the grid point=75 Y-coordinate of the grid point=75

Extreme Observations			
Lowest		**Highest**	
Value	**Obs**	**Value**	**Obs**
40.1001	7176	40.1167	8980
40.1007	6262	40.1167	9272
40.1011	7383	40.1169	5676
40.1016	7156	40.1170	6514
40.1017	5643	40.1171	5329

For each simulation location, a single realization might result in values that differ significantly from the random field mean at that location. However, the averages of progressively larger numbers of realizations tend to shorten this gap and reduce the simulation variability, as exhibited in the results for the two example locations in Output 105.2.1 and Output 105.2.2. At the limit of an infinite number of realizations, the simulation mean recovers the mean and covariance structure of the random field.

Example 105.3: Risk Analysis with Simulation

This example is in the field of environmental risk assessment. A square region of size 500 km × 500 km has been sampled for arsenic in drinking water. The logAsData data set consists of 138 simulated arsenic logarithm concentration observations represented by the logAs variable. Section "Example 124.1: Aspects of Semivariogram Model Fitting" on page 10112 in Chapter 124, "The VARIOGRAM Procedure," treats these observations as actual data in order to determine the spatial continuity structure for illustration in the examples.

A preliminary analysis indicates that the population exposure to the pollutant is currently at a relatively low level, as shown in the section "Example 68.1: Spatial Prediction of Pollutant Concentration" on page 5054 in Chapter 68, "The KRIGE2D Procedure," procedure. In particular, spatial prediction with kriging suggests that less than 1% of the region is affected by arsenic concentration in water that exceeds the World Health Organization (WHO) standard of 10 μg/lt.

You want to simulate the random field of the arsenic logarithm concentration so that you can gain insight into the characteristics of this field. Your objective is to assess whether the occurrence of above-threshold arsenic concentrations is a localized phenomenon, and whether you might expect more such occurrences across the region. For the simulation you need the outcome of the spatial continuity analysis in section "Example 124.1: Aspects of Semivariogram Model Fitting" on page 10112 in Chapter 124, "The VARIOGRAM Procedure." These results are the fitted semivariance models that are stored in the SemivAsStore item store by PROC VARIOGRAM.

Based on the discussion in the section "Example 105.1: Simulation and Economic Feasibility" on page 8718, you simulate the arsenic logarithm concentration on the premise of the ergodicity assumption. In brief, this assumption relates the mean and covariances of each individual realization to the corresponding values of the random field; see also the section "Ergodicity" on page 10079 in Chapter 124, "The VARIOGRAM Procedure." In the present case you are interested in the average of a large size of realizations, rather than individual ones. A single realization could suggest possible locations where the WHO regulatory standard might be violated. The average of multiple realizations has a smoothing effect on individual excessive-concentration episodes in single realizations. The smoothing enables you to see general characteristics of the arsenic concentration field behavior on the basis of its spatial correlation description.

For illustration, assume a rectangular grid of nodes with an equal spacing of 10 km between neighboring nodes in the north and east directions. Then, simulated values are produced at a total of $51 \times 51 = 2601$ locations.

You begin by reading the logAsData data set with the following DATA step:

```
title 'Risk Assessment with Simulation';

data logAsData;
   input East North logAs @@;
   label logAs='log(As) Concentration';
   datalines;
   193.0 296.6 -0.68153   232.6 479.1  0.96279   268.7 312.5 -1.02908
    43.6   4.9  0.65010   152.6  54.9  1.87076   449.1 395.8  0.95932
   310.9 493.6 -1.66208   287.8 164.9 -0.01779   330.0   8.0  2.06837
   225.7 241.7  0.15899   452.3  83.4 -1.21217   156.5 462.5 -0.89031
    11.5  84.4 -0.24496   144.4 335.7  0.11950   149.0 431.8 -0.57251
   234.3 123.2 -1.33642    37.8 197.8 -0.27624   183.1 173.9 -2.14558
   149.3 426.7 -1.06506   434.4  67.5 -1.04657   439.6 237.0 -0.09074
    36.4 175.2 -1.21211   370.6 244.0  3.28091   452.0  96.5 -0.77081
   247.0  86.8  0.04720   413.6 373.2  1.78235   253.5 291.7  0.56132
   129.7 111.9  1.34000   352.7  42.1  0.23621   279.3  82.7  2.12350
   382.6 290.7  0.86756   188.2 222.8 -1.23308   382.8 154.5 -0.94094
   304.4 309.2 -1.95158   337.5 387.2 -1.31294   490.7 189.8  0.40206
   159.0 100.1 -0.22272   245.5 329.2 -0.26082   372.1 379.5 -1.89078
   417.8  84.1 -1.25176   173.9 407.6 -0.24240   121.5 107.7  1.54509
   453.5 313.6  0.65895   143.5 346.7 -0.87196   157.4 125.5 -1.96165
   371.8 353.2 -0.59464   358.9 338.2 -1.07133     8.6 437.8  1.44203
   395.9 394.2 -0.24144   149.5  58.9  1.17459   453.5 420.6 -0.63951
   182.3  85.0  1.00005    21.0 290.1  0.31016    11.1 352.2 -0.88418
   131.2 238.4 -0.57184   104.9   6.3  1.12054   247.3 256.0  0.14019
   428.4 383.7  0.92448   327.8 481.1 -2.72543   199.2  92.8 -0.05717
   453.9 230.1  0.16571   205.0 250.6  0.07581   459.5 271.6  0.93700
   229.5 262.8  1.83590   370.4 228.6  2.96611   330.2 281.9  1.79723
   354.8 388.3 -3.18262   406.2 222.7  2.41594   254.4 393.1  2.03221
    96.7  85.2 -0.47156   407.2 256.8  0.66747   498.5 273.8  1.03041
   417.2 471.4 -1.42766   368.8 424.3 -0.70506   303.0  59.1  1.43070
   403.1 264.1  1.64554    21.2 360.8  0.67094   148.2  78.1  2.15323
   305.5 310.7 -1.47985   228.5 180.3 -0.68386   161.1 143.3  1.07901
    70.5 155.1  0.54652   363.1 282.6 -0.43051    86.0 472.5 -1.18855
   175.9 105.3 -2.08112    96.8 426.3  1.56592   475.1 453.1 -1.53776
   125.7 485.4  1.40054   277.9 201.6 -0.54565   406.2 125.0 -1.38657
    60.0 275.5 -0.59966   431.3 494.6 -0.36860   399.9 399.0 -0.77265
    28.8 311.1  0.91693   166.1 348.2 -0.49056   266.6  83.5  0.67277
    54.7 356.3  0.49596   433.5 460.3 -1.61309   201.7 167.6 -1.40678
   158.1 203.6 -1.32499    67.6 230.4  1.14672    81.9 250.0  0.63378
   372.0  50.7  0.72445    26.4 264.6  1.00862   300.1  91.7 -0.74089
   303.0 447.4  1.74589   108.4 386.2  1.12847    55.6 191.7  0.95175
    36.3 273.2  1.78880    94.5 298.3 -2.43320   366.1 187.3 -0.80526
   130.7 389.2 -0.31513    37.2 324.2  0.24489   295.5 211.8  0.41899
    58.6 206.2  0.18495   346.3 142.8 -0.92038   484.2 215.9  0.08012
   451.4 415.7  0.02773    58.9  86.5  0.17652   212.6 363.9  0.17215
   378.7 407.6  0.51516   265.9 305.0 -0.30718   123.2 314.8 -0.90591
    26.9 471.7  1.70285    16.5   7.1  0.51736   255.1 472.6  2.02381
   111.5 148.4 -0.09658   440.4 375.0  1.23285   406.4  19.5  1.01181
   321.2  65.8 -0.02095   466.4 357.1 -0.49272     2.0 484.6  0.50994
   200.9 205.1  0.43543    30.3 337.0  1.60882   297.0  12.7  1.79824
   158.2 450.7  0.05295   122.8 105.3  1.53936   417.8 329.7 -2.08124
;
```

For this simulation you use the spatial correlation information that is saved in the SemivAsStore item store in the section "Example 124.1: Aspects of Semivariogram Model Fitting" on page 10112 in Chapter 124, "The VARIOGRAM Procedure," with the following statements:

```
ods graphics on;

proc variogram data=logAsData plots=none;
   store out=SemivAsStore / label='LogAs Concentration Models';
   compute lagd=5 maxlag=40;
   coord xc=East yc=North;
   model form=auto(mlist=(exp,gau,mat) nest=1 to 2);
   var logAs;
run;
```

In PROC SIM2D you specify the container item store with the IN= option of the RESTORE statement. You request correlation input from an item store by specifying the STORESELECT option in the SIMULATE statement. You request 5,000 realizations for this simulation by specifying the number in the NUMREAL= option of the SIMULATE statement.

Assume that you first want to review the saved models in the item store. Use the INFO option of the RESTORE statement to produce a table with information about the top-ranking fitted model in the item store. Use the DET and ONLY suboptions of the INFO option to request details about all fitted models included in the item store. The ONLY suboption suppresses the simulation tasks and produces only the tables about the item store. You specify the following statements:

```
proc sim2d data=logAsData outsim=Outsim plots=none;
   restore in=SemivAsStore / info(det only);
   coordinates xc=East yc=North;
   simulate var=logAs numreal=5000 storeselect seed=39841;
   grid x=0 to 500 by 10 y=0 to 500 by 10;
run;
```

PROC SIM2D produces a table with general information about the input item store identity, as shown in Output 105.3.1.

Output 105.3.1 PROC SIM2D and Input Item Store General Information

Risk Assessment with Simulation

The SIM2D Procedure

Correlation Model Item Store Information	
Input Item Store	WORK.SEMIVASSTORE
Item Store Label	LogAs Concentration Models
Data Set Created From	WORK.LOGASDATA
By-group Information	No By-groups Present
Created By	PROC VARIOGRAM
Date Created	21OCT16:21:59:39

Output 105.3.2 displays the item store variables, in addition to the mean and standard deviation of their data set of origin. In this case, the logAs values come from the logAsData data set. By default, the SIM2D procedure uses the variable mean in the item store for the simulation, unless you explicitly specify the MEAN statement.

Output 105.3.2 Variables in the Input Item Store

Item Store Variables		
Variable	Mean	Std Deviation
logAs	0.084309	1.527707

The models in the SemivAsStore item store that have been fitted to the arsenic logarithm logAs empirical semivariance are shown in Output 105.3.3. The default item store model selection is the model on top of the list in Output 105.3.3.

Output 105.3.3 Angle and Models Information in the Input Item Store

Item Store Models For logAs	
Class	Model
1	Gau-Gau
	Gau-Mat
2	Exp-Gau
3	Exp-Mat
4	Mat
5	Gau
6	Exp
	Exp-Exp
	Mat-Exp
	Gau-Exp

You run again the SIM2D procedure without the INFO option in the RESTORE statement. This action prompts PROC SIM2D to run the simulation tasks that you specify with the SIMULATE statement. You specify the STORESELECT option in the SIMULATE statement without any suboptions, so that the simulation uses the default model selection in the SemivAsStore item store. You save the simulation output in the Outsim output data set. You also specify the SIM and the SEMIVAR suboptions in the PLOTS option of the PROC SIM2D statement to obtain output plots. You use the following statements:

```
proc sim2d data=logAsData outsim=Outsim plots=(sim semivar);
   restore in=SemivAsStore;
   coordinates xc=East yc=North;
   simulate var=logAs numreal=5000 storeselect seed=89702;
   grid x=0 to 500 by 10 y=0 to 500 by 10;
run;
```

NOTE: This step can take several minutes to run, and it produces a data set with over 10 million observations. When you run these statements, PROC SIM2D again produces a table about the input item store identity. This output is followed by a number of observations table and information about the simulation task, as shown in Output 105.3.4.

Output 105.3.4 Number of Observations and Simulation Information Tables

Risk Assessment with Simulation

The SIM2D Procedure

Simulation: SIM1, Dependent Variable: logAs

Number of Observations Read	138
Number of Observations Used	138

Simulation Information	
Simulation Grid Points	2601
Type	Conditional
Number of Realizations	5000

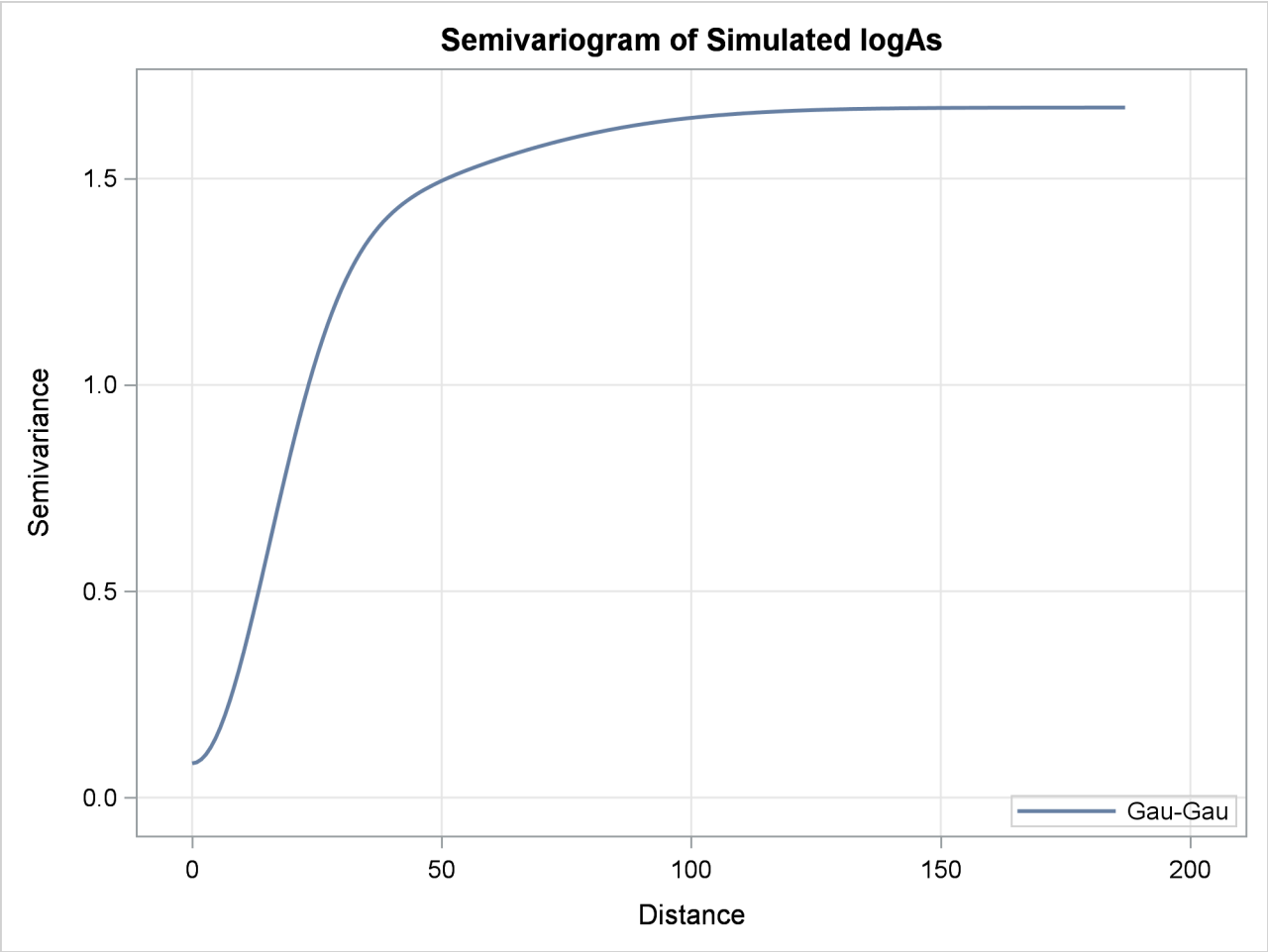
The SIM2D procedure uses the selected fitted Gaussian-Gaussian model in the SemivAsStore item store. Output 105.3.5 shows the saved parameter values of the model that are used in the simulation.

Output 105.3.5 Information about the Gaussian-Gaussian Model

Covariance Model Information	
Nested Structure 1 Type	Gaussian
Nested Structure 1 Sill	0.3276646
Nested Structure 1 Range	62.312728
Nested Structure 1 Effective Range	107.92881
Nested Structure 2 Type	Gaussian
Nested Structure 2 Sill	1.261545
Nested Structure 2 Range	21.459563
Nested Structure 2 Effective Range	37.169053
Nugget Effect	0.0830758

Output 105.3.6 shows a plot of the correlation model used in the simulation. Its parameters come from the stored information in the SemivAsStore item store.

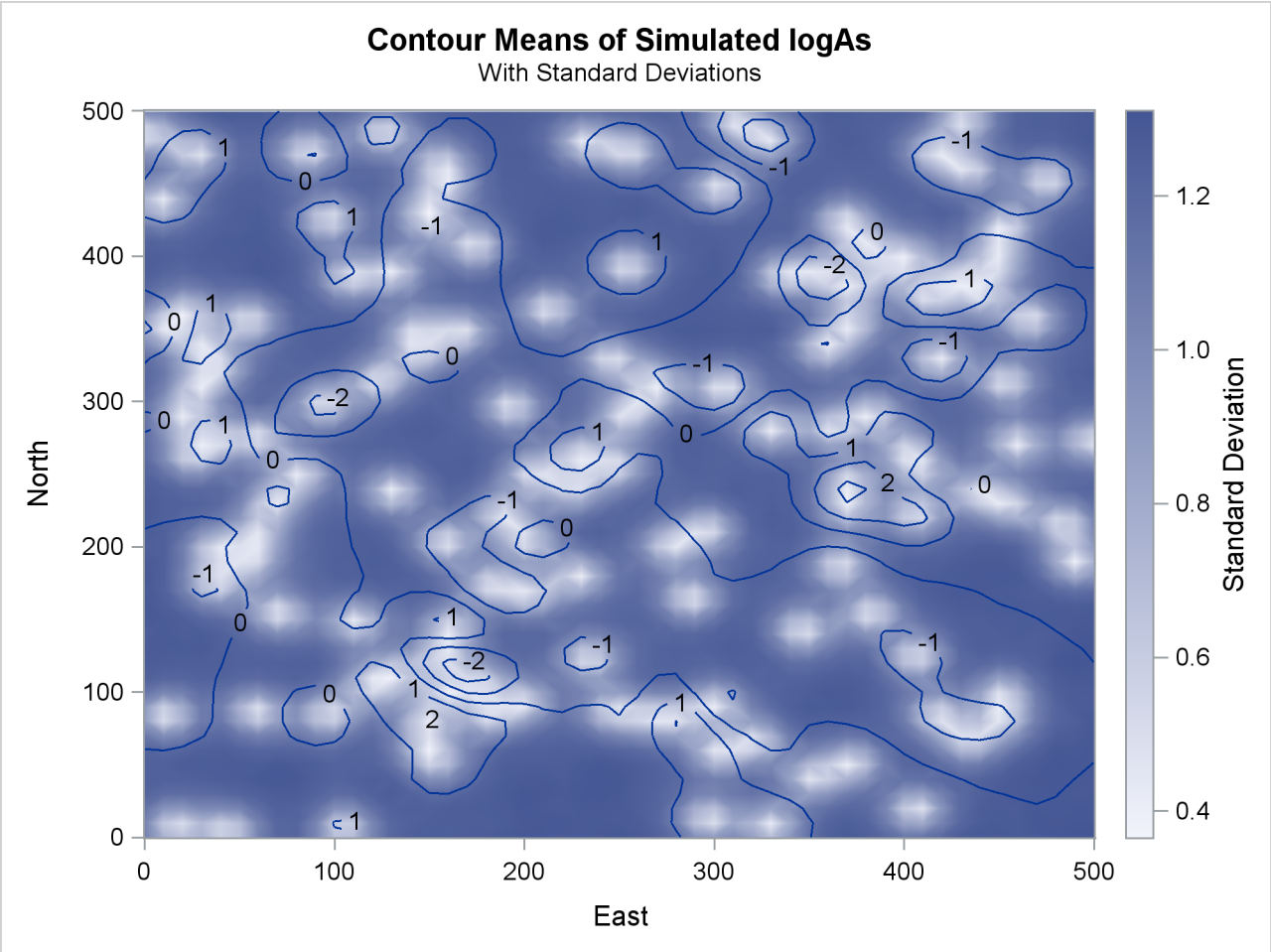
Output 105.3.6 Gaussian-Gaussian Semivariogram Model Used in Simulation



The PLOTS=SIM option produces contours of the mean value of the 5,000 realizations for each one of the output grid locations, and a surface of the associated standard deviation. The resulting plot is shown in Output 105.3.7. The mean value contours exhibit reduced variation compared to a SIM plot of one single realization. In fact, Output 105.3.7 is very similar to the prediction plot of the same Gaussian model in the section "Example 68.1: Spatial Prediction of Pollutant Concentration" on page 5054 in Chapter 68, "The KRIGE2D Procedure."

Clearly, there appears to be a small area of increased arsenic concentration values, which is located in the central-eastern part of the domain. The WHO threshold of 10 μg/lt for the maximum allowed arsenic concentration in water translates into about 2.3 in the log scale. The indicated area is the only one within the region where the simulated means exceed the value 3. In addition, there appear to be two smaller areas of simulated means values at or above 2 in the southern part of the region.

Output 105.3.7 Simulated Arsenic Logarithm Values with Gaussian-Gaussian Covariance



The simulation plot indicates that arsenic concentration values in excess of the WHO health standard is a rather localized phenomenon. If it were not so, then the plot would suggest that increased arsenic concentrations extend across larger areas. In turn, this means that individual realizations would tend to produce systematically higher arsenic concentrations at different neighboring locations, and their average would appear as higher logAs values in the SIM plot. Instead, you conclude that the Gaussian-Gaussian correlation that describes the spatial continuity for the arsenic logarithm observations leads to only localized occurrence of the WHO standard violation.

Now you want to find out whether additional localized occurrences might take place on the basis of the Gaussian-Gaussian spatial continuity behavior. The distribution of the simulation standard deviation values in Output 105.3.7 offers important feedback about this issue. Observe the areas in the plot where the means gradient indicates increasing values. The means contours create several pools where the values increase to simulated means higher than 1.

With the clear exceptions of the isolated area in the central-eastern part of the domain and the pool in the south-west that exhibit logAs values above 2, the simulation standard deviation seems to be around 1 or less in almost all other pools with logAs values above 1. Due to those relatively low standard deviations, this visual inspection suggests that even in individual realizations you might rarely expect the arsenic logarithm to exceed the threshold value of around 2.3.

However, in the few pools of logAs values above 1, there can be patches of increased standard deviation. In these cases, you suspect that arsenic concentration could exceed occasionally the WHO regulatory standard, even if the plot of the simulated means does not explicitly portray so.

Based on these remarks, you want to quantify the percentage of the region that could be affected by excessive arsenic concentration. You begin with a DATA step that takes as input the simulation Outsim output data set. The DATA step marks the simulated arsenic logarithm means values that are in excess of the WHO concentration threshold of 10 μg/lt, and saves the outcome into an indicator variable OverLimit. At the same time, the arsenic logarithm values are transformed back into arsenic concentration values so that they can be compared to the threshold value. The simulated means in the Outsim data set are stored in the svalue variable. You use the following statements:

```
data AsOverLimit;
   set Outsim;
   OverLimit = (exp(svalue) > 10) * 100;
run;
```

Then, you use the MEANS procedure to express the selected nodes population (where the WHO standard violation occurs) as a percentage of the entire domain area. You invoke PROC MEANS twice. The first time, you average over each realization in the PROC SIM2D output. For that purpose, you use the variable _ITER_ in the simulation sim1 output data set as a BY variable in PROC MEANS. You save the iteration-averaged indicator values in the PctOverLimit variable. The second time, PROC MEANS averages the PctOverLimit variable to obtain the percentage you want. You also specify the P5 and P95 options in the PROC MEANS statement to request the lower and upper confidence limits, respectively, in this computation. The interval between those limits expresses the 90% interval for the true area percentage based on the stochastic simulation. You use the following statements:

```
proc means data=AsOverLimit noprint;
   by _ITER_;
   var OverLimit;
   output out=OverLimitData mean=PctOverLimit;
run;
proc means data=OverLimitData mean p5 p95;
   var PctOverLimit;
   label PctOverLimit="Percent above threshold";
run;
```

The result is shown in Output 105.3.8. PROC MEANS accounts for all individual occurrences throughout the simulation where the WHO arsenic concentration threshold is exceeded. This happens at about 3.9% of the total area in 5,000 realizations. Compare this value to the less than 1% percentage in the PROC KRIGE2D prediction, as reported in the beginning of this section. On one hand, the prediction outcome tells you what goes on currently across the region within a degree of certainty given by the prediction error. On the other hand, the simulation provides you with an indicator that under the given spatial continuity estimate a relatively larger area is in potential danger of being affected by above-threshold arsenic concentration.

In fact, the 5% and 95% confidence limits in Output 105.3.8 show the area percentage limits within which you can expect excessive arsenic concentration. Based on the stochastic simulation, at the 90% confidence level the arsenic concentration in drinking water is expected to violate the WHO regulatory standard in anywhere from about 2.6% to 5.4% of the study region.

Output 105.3.8 Violation of Arsenic Concentration Threshold Using Gaussian-Gaussian Model

Risk Assessment with Simulation

The MEANS Procedure

Analysis Variable : PctOverLimit Percent above threshold		
Mean	5th Pctl	95th Pctl
3.9308727	2.6143791	5.4209919

You also want to compute the probability that individual areas in the region are expected to violate the WHO arsenic concentration standard. Start by identifying again the simulated arsenic logarithm means values in excess of the WHO concentration threshold of 10 μg/lt. The following DATA step saves the outcome into the variable LocalOverLimit:

```
data LocalAsOverLimit;
   set Outsim;
   LocalOverLimit = (exp(svalue) > 10);
run;
```

Then you use the SORT procedure to sort the information based on location coordinates. This intermediate step is necessary so that you can use the MEANS procedure with the LocalAsOverLimit data set. In the following statements, PROC MEANS computes the expected violations of the WHO standard for each location in the region across all realizations of the simulation:

```
proc sort data=LocalAsOverLimit;
   by gxc gyc;
run;
proc means data=LocalAsOverLimit noprint;
   by gxc gyc;
   var LocalOverLimit;
   output out=OverLimLoci mean=ProbOverLimit;
run;
```

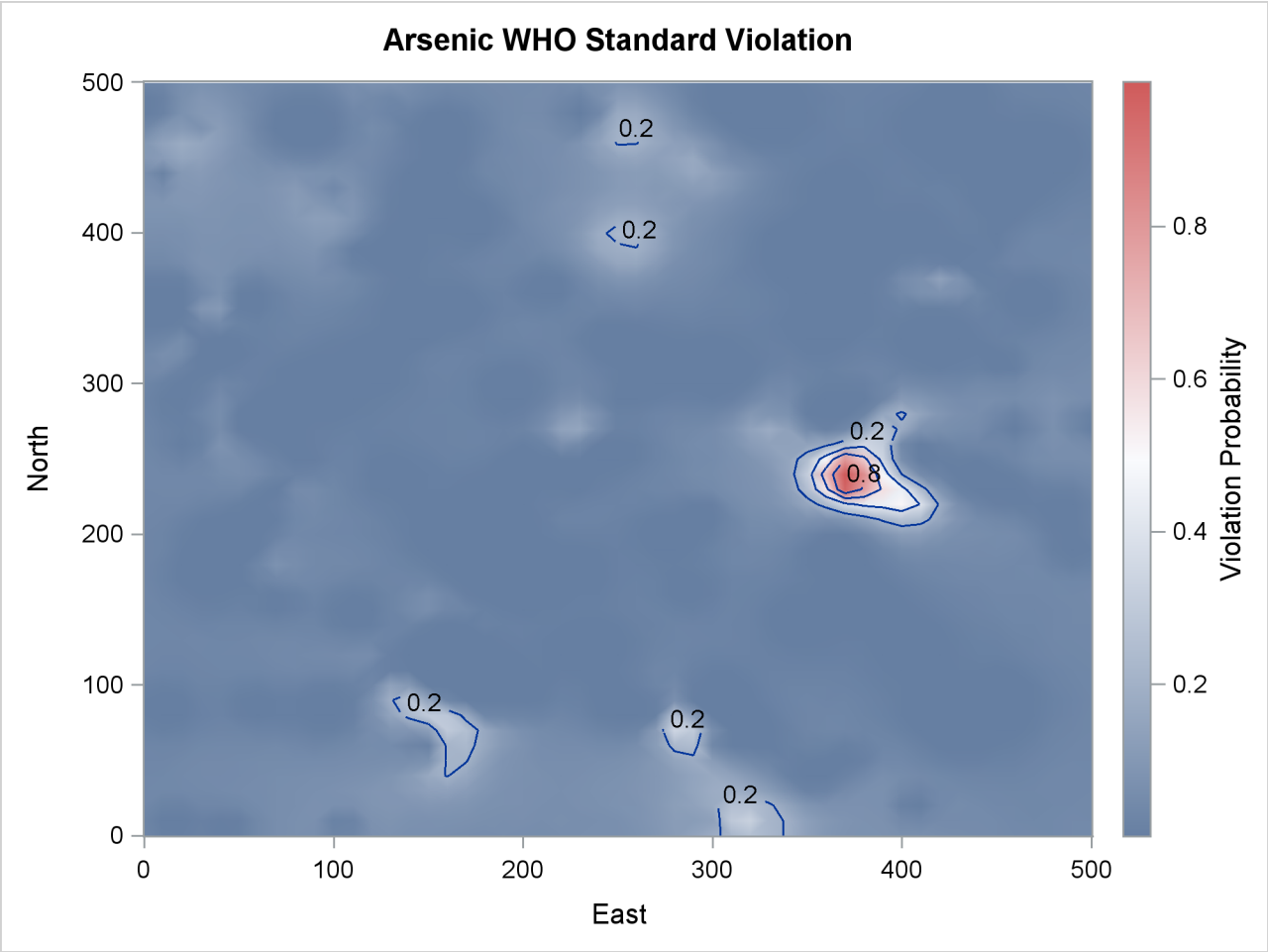
The output is the probability that the WHO standard is violated at each one of the simulation locations across the region. You create a plot of this probability with the help of the TEMPLATE and the SGRENDER procedures. You use the following statements:

```
proc template;
   define statgraph surfacePlot;
      dynamic _VARX _VARY _VAR _TITLE _LEGENDLABEL;
      BeginGraph;
      entrytitle _TITLE;
      layout overlay /
         xaxisopts = (offsetmax=0)
         yaxisopts = (offsetmax=0);
         contourplotparm x=_VARX y=_VARY z=_VAR /
                         nhint=10 name='probplot';
         continuouslegend 'probplot' / title=_LEGENDLABEL;
      endlayout;
      EndGraph;
   end;
run;

proc sgrender data=OverLimLoci template=surfacePlot;
   dynamic _VARX ='gxc'
           _VARY ='gyc'
           _VAR  ='ProbOverLimit'
           _TITLE='Arsenic WHO Standard Violation'
           _LEGENDLABEL='Violation Probability';
   label gyc='North' gxc='East';
run;

ods graphics off;
```

Output 105.3.9 shows the map of probability that the arsenic concentration WHO standard is violated in the region for the selected spatial correlation model of the pollutant. Based on the preceding analysis, the probability is very close to 1 in the area where the simulation mean values are above the standard limit. A few more areas that were indicated earlier in the analysis suggest a violation probability between 20% and 40%. The remaining areas in the region exhibit very low probability, which is notably nonzero at a few scattered locations. These findings suggest that throughout the simulation there have been realizations where the arsenic WHO standard was exceeded at locations whose simulated mean is well below that standard.

From the environmental risk assessment perspective, the preceding analysis can trigger a more detailed investigation into areas in the region where the health standard might be violated. Although the original observations in the logAsData data set indicate no existing problem in some of these areas, the present example illustrates that spatial analysis and simulation can raise flags of caution. This type of analysis can help to focus scientific, management, and policy efforts on these particular areas of the region and to monitor closely the pollutant concentration for potential health risks.

Output 105.3.9 Map of Violation of the Arsenic WHO Standard Probability



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Subject Index

computational details
SIM2D procedure, 8715
conditional and unconditional simulation
SIM2D procedure, 8680
conditional distributions of multivariate normal random variables
SIM2D procedure, 8713
covariance matrix
symmetric and positive definite (SIM2D), 8712
cubic semivariance model
SIM2D procedure, 8703

exponential semivariance model
SIM2D procedure, 8703

Gaussian assumption
SIM2D procedure, 8680
Gaussian random field
SIM2D procedure, 8680
Gaussian semivariance model
SIM2D procedure, 8703

Matérn semivariance model
SIM2D procedure, 8703
memory usage
SIM2D procedure, 8715

nugget effect
SIM2D procedure, 8705

ODS graph names
SIM2D procedure, 8718
ODS Graphics
SIM2D procedure, 8691
ODS table names
SIM2D procedure, 8717
output data sets
SIM2D procedure, 8691, 8715, 8716
OUTSIM= data set
SIM2D procedure, 8715, 8716

pentaspherical semivariance model
SIM2D procedure, 8703
plots (SIM2D procedure)
Observations, 8718
Semivariogram, 8718
Simulation, 8718

SIM2D procedure
Cholesky root, 8712
computational details, 8715
conditional and unconditional simulation, 8680
conditional distributions of multivariate normal random variables, 8713
conditional simulation, 8680, 8713
cubic semivariance model, 8703
examples, 8681, 8718, 8723, 8727
exponential semivariance model, 8703
Gaussian assumption, 8680
Gaussian random field, 8680
Gaussian semivariance model, 8703
LU decomposition, 8712
Matérn semivariance model, 8703
memory usage, 8715
nugget effect, 8705
ODS graph names, 8718
ODS Graphics, 8691
ODS table names, 8717
output data sets, 8691, 8715, 8716
OUTSIM= data set, 8715, 8716
pentaspherical semivariance model, 8703
quadratic form, 8713
simulation of spatial random fields, 8712–8715
sine hole effect semivariance model, 8703
spherical semivariance model, 8703
unconditional simulation, 8680, 8713
SIM2D procedure, plots
Observations, 8718
Semivariogram, 8718
Simulation, 8718
SIM2D procedure, tables
Model Information, 8717
Number of Observations, 8716
Simulation Information, 8717
Store Information, 8700, 8717, 8729
Store Model Information, 8700, 8717, 8730
Store Variables Information, 8700, 8717, 8730
simulation
at individual locations (SIM2D), 8697
conditional (SIM2D), 8680, 8713
correlation model (SIM2D), 8681, 8684, 8702, 8729
on one-dimensional grid (SIM2D), 8697
unconditional (SIM2D), 8680, 8713
simulation of spatial random fields
SIM2D procedure, 8712–8715
sine hole effect semivariance model

SIM2D procedure, 8703
spherical semivariance model
SIM2D procedure, 8703
symmetric and positive definite (SIM2D)
covariance matrix, 8712

tables (SIM2D procedure)
Model Information, 8717
Number of Observations, 8716
Simulation Information, 8717
Store Information, 8700, 8717, 8729
Store Model Information, 8700, 8717, 8730
Store Variables Information, 8700, 8717, 8730

Syntax Index

ANGLE= option
    SIMULATE statement (SIM2D), 8703

BY statement
    SIM2D procedure, 8695

COORDINATES statement
    SIM2D procedure, 8696

DATA= option
    PROC SIM2D statement, 8690

FORM= option
    SIMULATE statement (SIM2D), 8703

GRID statement
    SIM2D procedure, 8697
GRIDDATA= option
    GRID statement (SIM2D), 8698

ID statement
    SIM2D procedure, 8699
IDGLOBAL option
    PROC SIM2D statement, 8690
IDNUM option
    PROC SIM2D statement, 8690
INFO DETAILS option
    RESTORE statement (SIM2D), 8700
INFO ONLY option
    RESTORE statement (SIM2D), 8700
INFO option
    RESTORE statement (SIM2D), 8700

LABEL= option
    GRID statement (SIM2D), 8699

MDATA= option
    SIMULATE statement (SIM2D), 8704
MEAN statement
    SIM2D procedure, 8710

NARROW option
    PROC SIM2D statement, 8690
NOPRINT option
    PROC SIM2D statement, 8691
NPTS= option
    GRID statement (SIM2D), 8697
NUGGET= option
    SIMULATE statement (SIM2D), 8705
NUMREAL= option
    SIMULATE statement (SIM2D), 8702

OUTSIM= option
    PROC SIM2D statement, 8691

PLOTS option
    SIM2D procedure, PROC SIM2D statement, 8691
PLOTS(ONLY) option
    SIM2D procedure, PROC SIM2D statement, 8691
PLOTS=ALL option
    SIM2D procedure, PROC SIM2D statement, 8691
PLOTS=EQUATE option
    SIM2D procedure, PROC SIM2D statement, 8691
PLOTS=NONE option
    SIM2D procedure, PROC SIM2D statement, 8692
PLOTS=OBSERVATIONS option
    SIM2D procedure, PROC SIM2D statement, 8692
PLOTS=SEMIVARIOGRAM option
    SIM2D procedure, PROC SIM2D statement, 8695
PLOTS=SIM option
    SIM2D procedure, PROC SIM2D statement, 8693
PROC SIM2D statement, *see* SIM2D procedure

RANGE= option
    SIMULATE statement (SIM2D), 8705
RATIO= option
    SIMULATE statement (SIM2D), 8706
RESTORE statement (SIM2D), 8700

SCALE= option
    SIMULATE statement (SIM2D), 8706
SEED= option
    SIMULATE statement (SIM2D), 8706
SIM2D procedure, 8680
    syntax, 8688
SIM2D procedure, BY statement, 8695
SIM2D procedure, COORDINATES statement, 8696
    XCOORD= option, 8696
    YCOORD= option, 8696
SIM2D procedure, GRID statement, 8697
    GRIDDATA= option, 8698
    LABEL= option, 8699
    NPTS= option, 8697
    X= option, 8697
    XCCORD= option, 8698
    Y= option, 8697
    YCOORD= option, 8698
SIM2D procedure, ID statement, 8699
SIM2D procedure, MEAN statement, 8710

SIM2D procedure, PROC SIM2D statement, 8690
DATA= option, 8690
IDGLOBAL option, 8690
IDNUM option, 8690
NARROW option, 8690
NOPRINT option, 8691
OUTSIM= option, 8691
PLOTS option, 8691
PLOTS(ONLY) option, 8691
PLOTS=ALL option, 8691
PLOTS=EQUATE option, 8691
PLOTS=NONE option, 8692
PLOTS=OBSERVATIONS option, 8692
PLOTS=SEMIVARIOGRAM option, 8695
PLOTS=SIM option, 8693
SIM2D procedure, RESTORE statement, 8700
INFO DETAILS option, 8700
INFO ONLY option, 8700
INFO options, 8700
SIM2D procedure, SIMULATE statement, 8701
ANGLE= option, 8703
FORM= option, 8703
MDATA= option, 8704
NUGGET= option, 8705
NUMREAL= option, 8702
RANGE= option, 8705
RATIO= option, 8706
SCALE= option, 8706
SEED= option, 8706
SINGULAR= option, 8706
SMOOTH= option, 8706
STORESELECT ANGLEID= option, 8708
STORESELECT MODEL= option, 8708
STORESELECT option, 8706
STORESELECT SVAR= option, 8709
STORESELECT TYPE= option, 8706
VAR= option, 8702
SIMULATE statement (SIM2D), 8701
SINGULAR= option
SIMULATE statement (SIM2D), 8706
SMOOTH= option
SIMULATE statement (SIM2D), 8706
STORESELECT ANGLEID= option
SIMULATE statement (SIM2D), 8708
STORESELECT MODEL= option
SIMULATE statement (SIM2D), 8708
STORESELECT option
SIMULATE statement (SIM2D), 8706
STORESELECT SVAR= option
SIMULATE statement (SIM2D), 8709
STORESELECT TYPE= option
SIMULATE statement (SIM2D), 8706

VAR= option
SIMULATE statement (SIM2D), 8702

X= option
GRID statement (SIM2D), 8697
XCOORD= option
COORDINATES statement (SIM2D), 8696
GRID statement (SIM2D), 8698

Y= option
GRID statement (SIM2D), 8697
YCOORD= option
COORDINATES statement (SIM2D), 8696
GRID statement (SIM2D), 8698