SAS/STAT® 14.2 User's Guide

The VARIOGRAM Procedure

This document is an individual chapter from *SAS/STAT® 14.2 User's Guide*.

The correct bibliographic citation for this manual is as follows: SAS Institute Inc. 2016. *SAS/STAT® 14.2 User's Guide*. Cary, NC: SAS Institute Inc.

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November 2016

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Chapter 124
The VARIOGRAM Procedure

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Overview: VARIOGRAM Procedure

The VARIOGRAM procedure computes empirical measures of spatial continuity for two-dimensional spatial data. These measures are a function of the distances between the sample data pairs. When the data are free of nonrandom (or systematic) surface trends, the estimated continuity measures are the empirical semivariance and covariance. The procedure also fits permissible theoretical models to the empirical semivariograms, so that you can use them in subsequent analysis to perform spatial prediction. You can produce plots of the empirical semivariograms in addition to plots of the fitted models. Both isotropic and anisotropic continuity measures are available.

PROC VARIOGRAM also provides the Moran's I and Geary's c spatial autocorrelation statistics, in addition to the Moran scatter plot to visualize spatial associations within a specified neighborhood around observations. The procedure produces the OUTVAR=, OUTPAIR=, and OUTDISTANCE= data sets that contain information about the semivariogram analysis. Also, the OUTACWEIGHTS= and the OUTMORAN= output data sets contain information about the autocorrelation analysis.

The VARIOGRAM 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 VARIOGRAM, see the section "ODS Graphics" on page 10111.

Introduction to Spatial Prediction

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

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

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

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

SAS/STAT software has two procedures that correspond to these steps for spatial prediction of two-dimensional data. The VARIOGRAM procedure is used in the first step (that is, calculating and modeling the dependence model), and the KRIGE2D procedure performs the kriging operations to produce the final predictions.

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

Getting Started: VARIOGRAM Procedure

PROC VARIOGRAM uses your data to compute the empirical semivariogram. This computation refers to the steps you take to derive the empirical semivariance from the data, and then to produce the corresponding semivariogram plot.

You can proceed further with the semivariogram analysis if the data are free of systematic trends. In that case, you can use the empirical outcome to determine a theoretical semivariogram model by using the automated methods provided by the VARIOGRAM procedure. The model characterizes the type of theoretical semivariance function you use to describe spatial dependence in your data set.

Graphical displays are requested by enabling ODS Graphics. For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS." For specific information about the graphics available in the VARIOGRAM procedure, see the section "ODS Graphics" on page 10111.

Preliminary Spatial Data Analysis

The thick data set is available from the Sashelp library. The data set simulates measurements of coal seam thickness (in feet) taken over an approximately square area. The Thick variable has the thickness values in the thick data set. 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.

It is instructive to see the locations of the measured points in the area where you want to perform spatial prediction. It is desirable to have the sampling locations scattered evenly throughout the prediction area. If the locations are not scattered evenly, the prediction error might be unacceptably large where measurements are sparse.

You can run PROC VARIOGRAM in this preliminary analysis to determine potential problems. In the following statements, the NOVARIOGRAM option in the COMPUTE statement specifies that only the descriptive summaries and a plot of the raw data be produced.

```
title 'Spatial Correlation Analysis with PROC VARIOGRAM';

ods graphics on;

proc variogram data=sashelp.thick plots=pairs(thr=30);
   compute novariogram nhc=20;
   coordinates xc=East yc=North;
   var Thick;
run;
```

PROC VARIOGRAM produces the table in Figure 124.1 that shows the number of Thick observations read and used. This table provides you with useful information in case you have missing values in the input data.

Figure 124.1 Number of Observations for the thick Data Set

Spatial Correlation Analysis with PROC VARIOGRAM

The VARIOGRAM Procedure

Dependent Variable: Thick

Number of Observations Read	75
Number of Observations Used	75

Then, the scatter plot of the observed data is produced as shown in Figure 124.2. According to the figure, although the locations are not ideally spread around the prediction area, there are not any extended areas

lacking measurements. The same graph also provides the values of the measured variable by using colored markers.

Figure 124.2 Scatter Plot of the Observations Spatial Distribution

The following is a crucial step. Any obvious surface trend must be removed before you compute the empirical semivariogram and proceed to estimate a model of spatial dependence (the theoretical semivariogram model). You can observe in Figure 124.2 the small-scale variation typical of spatial data, but a first inspection indicates no obvious major systematic trend.

Assuming, therefore, that the data are free of surface trends, you can work with the original thickness rather than residuals obtained from a trend removal process. The following analysis also assumes that the spatial characterization is independent of the direction of the line that connects any two equidistant pairs of data; this is a property known as isotropy. See "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122 for a more detailed approach to trend analysis and the issue of anisotropy.

Following the previous exploratory analysis, you then need to classify each data pair as a member of a distance interval (lag). PROC VARIOGRAM performs this grouping with two required options for semivariogram computation: the LAGDISTANCE= and MAXLAGS= options. These options are based on your assessment of how to group the data pairs within distance classes.

The meaning of the required LAGDISTANCE= option is as follows. Classify all pairs of points into intervals according to their pairwise distance. The width of each distance interval is the LAGDISTANCE= value. The meaning of the required MAXLAGS= option is simply the number of intervals you consider. The problem is that given only the scatter plot of the measurement locations, it is not clear what values to give to the LAGDISTANCE= and MAXLAGS= options.

Ideally, you want a sufficient number of distance classes that capture the extent to which your data are correlated and you want each class to contain a minimum of data pairs to increase the accuracy in your computations. A rule of thumb used in semivariogram computations is that you should have at least 30 pairs per lag class. This is an empirical arbitrary threshold; see the section "Choosing the Size of Classes" on page 10087 for further details.

In the preliminary analysis, you use the option NHCLASSES= in the COMPUTE statement to help you experiment with these numbers and choose values for the LAGDISTANCE= and MAXLAGS= options. Here, in particular, you request NHCLASSES=20 to preview a classification that uses 20 distance classes across your spatial domain. A zero lag class is always considered; therefore the output shows the number of distance classes to be one more than the number you specified.

Based on your selection of the NHCLASSES= option, the NOVARIOGRAM option produces a pairwise distances table from your observations shown in Figure 124.3, and the corresponding histogram in Figure 124.4. For illustration purposes, you also specify a threshold of minimum data pairs per distance class in the PAIRS option as THR=30. As a result, a reference line appears in the histogram so that you can visually identify any lag classes with pairs that fall below your specified threshold.

Figure 124.3 Pairwise Distance Intervals Table

Pairwise Distance Intervals				
Lag Class	Bounds		Number of Pairs	Percentage of Pairs
0	0.00	3.48	7	0.25%
1	3.48	10.45	81	2.92%
2	10.45	17.42	138	4.97%
3	17.42	24.39	167	6.02%
4	24.39	31.36	204	7.35%
5	31.36	38.33	210	7.57%
6	38.33	45.30	213	7.68%
7	45.30	52.27	253	9.12%
8	52.27	59.24	237	8.54%
9	59.24	66.20	280	10.09%
10	66.20	73.17	252	9.08%
11	73.17	80.14	230	8.29%
12	80.14	87.11	217	7.82%
13	87.11	94.08	154	5.55%
14	94.08	101.05	71	2.56%
15	101.05	108.02	41	1.48%
16	108.02	114.99	14	0.50%
17	114.99	121.96	5	0.18%
18	121.96	128.93	1	0.04%
19	128.93	135.89	0	0.00%
20	135.89	142.86	0	0.00%

The NOVARIOGRAM option also produces a table with useful facts about the pairs and the distances between the most remote data in selected directions, shown in Figure 124.5. In particular, the lag distance value is calculated based on your selection of the NHCLASSES= option. The last three table entries report the overall maximum distance among your data pairs, in addition to the maximum distances in the main axes directions—that is, the vertical (N–S) axis and the horizontal (E–W) axis. This information is also provided in the inset of Figure 124.4. When you specify a threshold in the PAIRS suboption of the PLOTS option, as in this example, the threshold also appears in the table. Then, the line that follows indicates the highest lag class with the following property: each one of the distance classes that lie farther away from this lag features a pairs population below the specified threshold.

With the preceding information you can determine appropriate values for the LAGDISTANCE= and MAXLAGS= options in the COMPUTE statement. In particular, the classification that uses 20 distance classes is satisfactory, and you can choose LAGDISTANCE=7 after following the suggestion in Figure 124.5.

Figure 124.4 Distribution of Pairwise Distances

Figure 124.5 Pairs Information Table

Pairs Information	
Number of Lags	21
Lag Distance	6.97
Minimum Pairs Threshold	30
Highest Lag With Pairs > Threshold	15
Maximum Data Distance in East	97.50
Maximum Data Distance in North	99.60
Maximum Data Distance	139.38

The MAXLAGS= option needs to be specified based on the spatial extent to which your data are correlated. Unless you know this size, in the present omnidirectional case you can assume the correlation extent to be roughly equal to half the overall maximum distance between data points.

The table in Figure 124.5 suggests that this number corresponds to 139,380 feet, which is most likely on or close to a diagonal direction (that is, the northeast–southwest or northwest–southeast direction). Hence, you can expect the correlation extent in this scale to be around $139.4/2 = 69,700$ feet. Consequently, consider lag classes up to this distance for the empirical semivariogram computations. Given your lag size selection, Figure 124.3 indicates that this distance corresponds to about 10 lags; hence you can set MAXLAGS=10.

Overall, for a specific NHCLASSES= choice of class count, you can expect your choice of MAXLAGS= to be approximately half the number of the lag classes (see the section "Spatial Extent of the Empirical Semivariogram" on page 10089 for more details).

After you have starting values for the LAGDISTANCE= and MAXLAGS= options, you can run the VARIOGRAM procedure multiple times to inspect and compare the results you get by specifying different values for these *options*.

Empirical Semivariogram Computation

Using the values of LAGDISTANCE=7 and MAXLAGS=10 computed previously, rerun PROC VARIOGRAM without the NOVARIOGRAM option in order to compute the empirical semivariogram. You specify the CL option in the COMPUTE statement to calculate the 95% confidence limits for the classical semivariance. The section "COMPUTE Statement" on page 10049 describes how to use the ALPHA= option to specify a different confidence level.

Also, you can request a robust version of the semivariance with the ROBUST option in the COMPUTE statement. PROC VARIOGRAM produces a plot that shows both the classical and the robust empirical semivariograms. See the details of the PLOTS option to specify different instances of plots of the empirical semivariogram. The following statements implement the preceding requests:

```
proc variogram data=sashelp.thick outv=outv;
   compute lagd=7 maxlag=10 cl robust;
   coordinates xc=East yc=North;
   var Thick;
run;
```

Figure 124.6 displays the PROC VARIOGRAM output empirical semivariogram table for the preceding statements. The table displays a total of eleven lag classes, even though you specified MAXLAGS=10. The VARIOGRAM procedure always includes a zero lag class in the computations in addition to the MAXLAGS classes you request with the MAXLAGS= option. Hence, semivariance is actually computed at MAXLAGS+1 lag classes; see the section "Distance Classification" on page 10083 for more details.

Figure 124.6 Output Table for the Empirical Semivariogram Analysis

Spatial Correlation Analysis with PROC VARIOGRAM

The VARIOGRAM Procedure

Dependent Variable: Thick

Empirical Semivariogram							
			Semivariance				
Lag Class	Pair Count	Average Distance	Robust	Classical	Standard Error	95% Confidence Limits	
0	7	2.64	0.028	0.034	0.018	0	0.069
1	82	7.29	0.210	0.394	0.061	0.273	0.514
2	138	14.16	1.008	1.179	0.142	0.901	1.458
3	169	21.08	3.018	2.799	0.304	2.202	3.396
4	205	27.93	4.811	4.602	0.455	3.711	5.493
5	213	35.17	5.990	5.928	0.574	4.802	7.054
6	214	42.20	8.104	7.518	0.727	6.094	8.943
7	250	48.78	7.533	7.221	0.646	5.955	8.487
8	247	56.16	8.066	7.195	0.647	5.926	8.464
9	281	62.89	8.279	6.845	0.577	5.713	7.976
10	250	69.93	8.144	6.358	0.569	5.243	7.472

Figure 124.7 shows both the classical and robust empirical semivariograms. In addition, the plot features the approximate 95% confidence limits for the classical semivariance. The figure exhibits a typical behavior of the computed semivariance uncertainty, where in general the variance increases with distance from the origin at Distance=0.

Figure 124.7 Classical and Robust Empirical Semivariograms for Coal Seam Thickness Data

The needle plot in the lower part of the Figure 124.7 provides the number of pairs that were used in the computation of the empirical semivariance for each lag class shown. In general, this is a pairwise distribution that is different from the distribution depicted in Figure 124.4. First, the number of pairs shown in the needle plot depends on the particular criteria you specify in the COMPUTE statement of PROC VARIOGRAM. Second, the distances shown for each lag on the Distance axis are not the midpoints of the lag classes as in the pairwise distances plot, but rather the average distance from the origin Distance=0 of all pairs in a given lag class.

Autocorrelation Analysis

You can use the autocorrelation analysis features of PROC VARIOGRAM to compute the autocorrelation Moran's I and Geary's c statistics and to obtain the Moran scatter plot. In the following statements, you ask for the Moran's I and Geary's c statistics under the assumption of randomization using binary weights, in addition to the Moran scatter plot:

```
proc variogram data=sashelp.thick outv=outv plots(only)=moran;
   compute lagd=7 maxlag=10 autocorr(assum=random);
   coordinates xc=East yc=North;
   var Thick;
run;
```

For the autocorrelation analysis with binary weights and the Moran scatter plot, the LAGDISTANCE= option indicates that you consider as neighbors of an observation all other observations within the specified distance from it.

Figure 124.8 shows the output from the requested autocorrelation analysis. This includes the observed (computed) Moran's I and Geary's c coefficients, the expected value and standard deviation for each coefficient, the corresponding Z score, and the p-value in the Pr >| Z | column. The low p-values suggest strong autocorrelation for both statistics types. A two-sided p-value is reported, which is the probability that the observed coefficient lies farther away from | Z | on either side of the coefficient's expected value—that is, lower than $-Z$ or higher than Z. The sign of Z for both Moran's I and Geary's c coefficients indicates positive autocorrelation in the Thick data values; see the section "Interpretation" on page 10103 for more details.

Figure 124.8 Output Table for the Autocorrelation Statistics

Spatial Correlation Analysis with PROC VARIOGRAM

The VARIOGRAM Procedure

Dependent Variable: Thick

Autocorrelation Statistics

Assumption	Coefficient	Observed	Expected	Std Dev	Z	Pr > |Z|
Randomization	Moran's I	0.9240	-0.0244	0.145	6.53	<.0001
Randomization	Geary's c	0.0162	1.0000	0.175	-5.62	<.0001

The requested Moran scatter plot is shown in Figure 124.9. The plot includes all nonmissing observations that have neighbors within the specified LAGDISTANCE= distance. The horizontal axis displays the standardized Thick values, and the vertical axis displays the corresponding weighted average of their neighbors. The plot data points are concentrated in the upper right and lower left quadrants defined by the lines $x = 0$ and $y = 0$, and clearly around the axes' diagonal reference line $y = x$ of slope 1. This fact indicates strong positive spatial association in the thick data set observations. Therefore, for each observation its neighbors within the specified LAGDISTANCE= distance have overall similar Thick values to that observation. The plot also displays the linear regression slope, whose value is the Moran's I coefficient when the binary weights are row-averaged. See the section "The Moran Scatter Plot" on page 10103 for more details about the Moran scatter plot.

Figure 124.9 Moran Scatter Plot for Coal Seam Thickness Data

Theoretical Semivariogram Model Fitting

PROC VARIOGRAM features automated semivariogram fitting. In particular, the procedure selects a theoretical semivariogram model to fit the empirical semivariance and produces estimates of the model parameters in addition to a fit plot. You have the option to save these estimates in an item store, which is a binary file format that is defined by the SAS System and that you cannot modify. Then, you can retrieve this information at a later point from the item store for future analysis with PROC KRIGE2D or PROC SIM2D.

The coal seam thickness empirical semivariogram in Figure 124.7 shows first a slow, then rapid, rise from the origin. This behavior suggests that you can approximate the empirical semivariance with a Gaussian-type form

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

as shown in the section "Theoretical Semivariogram Models" on page 10072. Based on this remark, you choose to fit a Gaussian model to your classical semivariogram. Run PROC VARIOGRAM again and specify the MODEL statement with the FORM=GAU option. By default, PROC VARIOGRAM uses the weighted least squares (WLS) method to fit the specified model, although you can explicitly specify the METHOD= option to request the fitting method. You want additional information about the estimated parameters, so you specify the CL option in the MODEL statement to compute their 95% confidence limits and the COVB option of the MODEL statement to produce a table with their approximate covariances. You also specify the STORE statement to save the fitting outcome into an item store file with the name SemivStoreGau and a desired label. You run the following statements:

```
proc variogram data=sashelp.thick outv=outv;
   store out=SemivStoreGau / label='Thickness Gaussian WLS Fit';
   compute lagd=7 maxlag=10;
   coordinates xc=East yc=North;
   model form=gau cl / covb;
   var Thick;
run;

ods graphics off;
```

After you run the procedure you get a series of output objects from the fitting analysis. In particular, Figure 124.10 shows first a model fitting table with the name and a short label of the model that you requested to use for the fit. The table also displays the name and label of the specified item store.

Figure 124.10 Semivariogram Model Fitting General Information

Spatial Correlation Analysis with PROC VARIOGRAM

The VARIOGRAM Procedure

Dependent Variable: Thick
Angle: Omnidirectional
Current Model: Gaussian

Semivariogram Model Fitting	
Name	Gaussian
Label	Gau
Output Item Store	WORK.SEMIVSTOREGAU
Item Store Label	Thickness Gaussian WLS Fit

If you specify no parameters, as in the current example, then PROC VARIOGRAM initializes the model parameters for you with default values based on the empirical semivariance; for more details, see the section "Theoretical Semivariogram Model Fitting" on page 10092. The initial values provided by the VARIOGRAM procedure for the Gaussian model are displayed in the table in Figure 124.11.

Figure 124.11 Semivariogram Fitting Model Information

Model Information	
Parameter	**Initial Value**
Nugget	0
Scale	6.7992
Range	34.9635

Otherwise, in PROC VARIOGRAM you can specify initial values for parameters with the PARMS statement. Alternatively, you can specify fixed values for the model scale and range with the SCALE= and RANGE= options, respectively, in the MODEL statement. A nugget effect is always used in model fitting. Unless you explicitly specify a fixed nugget effect with the NUGGET= option in the MODEL statement or initialize the nugget parameter in the PARMS statement, the nugget effect is automatically initialized to zero. See the section "Syntax: VARIOGRAM Procedure" on page 10041 for more details about how the MODEL statement and the PARMS statement handle model parameters.

The output in Figure 124.12 comes from the optimization process that takes place during the model parameter estimation. The optimizer produces an optimization information table, information about the optimization technique that is used, optimization-related results, and notification about the optimization convergence.

Figure 124.12 Fitting Optimization Information

Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	3
Lower Boundaries	3
Upper Boundaries	0
Starting Values From	PROC

Spatial Correlation Analysis with PROC VARIOGRAM

The VARIOGRAM Procedure

Dependent Variable: Thick
Angle: Omnidirectional
Current Model: Gaussian

Dual Quasi-Newton Optimization

Dual Broyden - Fletcher - Goldfarb - Shanno Update (DBFGS)

Hessian Computed by Finite Differences (Using Analytic Gradient)

Optimization Results			
Iterations	12	**Function Calls**	45
Gradient Calls	0	**Active Constraints**	1
Objective Function	11.433894152	**Max Abs Gradient Element**	3.0128744E-8
Slope of Search Direction	-3.986332E-8		

Convergence criterion (GCONV=1E-8) satisfied.

The fitting process is successful, and the parameters converge to the estimated values shown in Figure 124.13. For each parameter, the same table also displays the approximate standard error, the degrees of freedom, the t value, the approximate p-value, and the requested 95% confidence limits.

Figure 124.13 Semivariogram Fitting Parameter Estimates

Parameter Estimates							
			Approximate 95% Confidence Limits				
Parameter	**Estimate**	**Approx Std Error**	**Lower**	**Upper**	**DF**	**t Value**	**Approx Pr > |t|**
Nugget	0	0	0	0	8	.	.
Scale	7.4599	0.2621	6.8555	8.0643	8	28.46	<.0001
Range	30.1111	1.1443	27.4724	32.7498	8	26.31	<.0001

The approximate covariance matrix of the estimated parameters is displayed in Figure 124.14.

Figure 124.14 Approximate Covariance Matrix of Parameter Estimates

Approximate Covariance Matrix			
Parameter	**Nugget**	**Scale**	**Range**
Nugget	0.0000	0.0000	0.0000
Scale	0.0000	0.0687	0.2326
Range	0.0000	0.2326	1.3094

The fitting summary table in Figure 124.15 displays statistics about the quality of the fitting process. In particular, the table shows the weighted error sum of squares in the Weighted SSE column and the Akaike information criterion in the AIC column. See more information about the fitting criteria in section "Quality of Fit" on page 10096.

Figure 124.15 Semivariogram Model Fitting Summary

Fit Summary		
Model	**Weighted SSE**	**AIC**
Gau	11.43389	6.42556

Figure 124.16 demonstrates the fitted theoretical semivariogram against the empirical semivariance estimates with the weighted least squares method. The fit seems to be more accurate closer to the origin $\boldsymbol{h} = 0$, and this is explained as follows: A smaller $\boldsymbol{h}$ corresponds to smaller semivariance; in turn, this corresponds to smaller semivariance variance, as shown in the section "Theoretical and Computational Details of the Semivariogram" on page 10077. By definition, the WLS optimization weights increase with decreasing variance, which leads to a more accurate fit for smaller distances $\boldsymbol{h}$ in the WLS fitting results.

Figure 124.16 Fitted Theoretical and Empirical Semivariogram for Coal Seam Thickness

Syntax: VARIOGRAM Procedure

The following statements are available in the VARIOGRAM procedure:

PROC VARIOGRAM *options* ;
  BY *variables* ;
  COMPUTE *computation-options* ;
  COORDINATES *coordinate-variables* ;
  DIRECTIONS *directions-list* ;
  ID *variable* ;
  MODEL *model-options* ;
  PARMS *parameters-list* < / *parameters-options* > ;
  NLOPTIONS < *options* > ;
  STORE *store-options* ;
  VAR *analysis-variables-list* ;

The COMPUTE and COORDINATES statements are required. The MODEL and PARMS statements are hierarchical. If you specify a PARMS statement, it must follow a MODEL statement.

PROC VARIOGRAM Statement

PROC VARIOGRAM *options* ;

The PROC VARIOGRAM statement invokes the VARIOGRAM procedure. Table 124.1 summarizes the *options* available in the PROC VARIOGRAM statement.

Table 124.1 PROC VARIOGRAM Statement Options

Option	Description
DATA=	Specifies the input data set
IDGLOBAL	Labels observations across BY groups using ascending observation numbers
IDNUM	Labels observations using the observation number
NOPRINT	Suppresses normal display of results
OUTACWEIGHTS=	Specifies a data set to store autocorrelation weights information
OUTDISTANCE=	Specifies a data set to store summary distance information
OUTMORAN=	Specifies a data set to store Moran scatter plot information
OUTPAIR=	Specifies a data set to store pairwise point information
OUTVAR=	Specifies a data set to store spatial continuity measures
PLOTS	Specifies the plot display and options

You can specify the following *options* in the PROC VARIOGRAM statement.

DATA=*SAS-data-set*
  specifies a SAS data set that contains the x and y coordinate variables and the VAR statement variables.

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 VARIOGRAM 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.

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 10111 for more information.

OUTACWEIGHTS=*SAS-data-set*

OUTACW=*SAS-data-set*

OUTA=*SAS-data-set*

specifies a SAS data set in which to store the autocorrelation weights information for each pair of points in the DATA= data set. Use this option with caution when the DATA= data set is large. If n denotes the number of observations in the DATA= data set, then the OUTACWEIGHTS= data set contains $[n(n-1)]/2$ observations.

See the section "OUTACWEIGHTS=*SAS-data-set*" on page 10105 for details.

OUTDISTANCE=*SAS-data-set*

OUTDIST=*SAS-data-set*

OUTD=*SAS-data-set*

specifies a SAS data set in which to store summary distance information. This data set contains a count of all pairs of data points within a given distance interval. The number of distance intervals is controlled by the NHCLASSES= option in the COMPUTE statement. The OUTDISTANCE= data set is useful for plotting modified histograms of the count data for determining appropriate lag distances. See the section "OUTDIST=*SAS-data-set*" on page 10106 for details.

OUTMORAN=*SAS-data-set*

OUTM=*SAS-data-set*

specifies a SAS data set in which to store information that is illustrated in the Moran plot, namely the standardized value of each observation in the DATA= data set and the weighted average of its local neighbors. You must also specify the LAGDISTANCE= and AUTOCORRELATION options in the COMPUTE statement; otherwise, the OUTMORAN= data set request is ignored.

The OUTMORAN= data set is useful when you want to save the information that is illustrated in the Moran scatter plot. The data set can also contain entries of missing observations with neighbors, although these observations are not displayed in the Moran plot. However, if the only observations with neighbors in your input data set are observations with missing values, then the OUTMORAN= output data set is empty.

See the section "OUTMORAN=*SAS-data-set*" on page 10106 for details.

OUTPAIR=*SAS-data-set*

OUTP=*SAS-data-set*

specifies a SAS data set in which to store distance and angle information for each pair of points in the DATA= data set.

Use this option with caution when your DATA= data set is large. Assume that your DATA= data set has n observations. When you specify the NOVARIOGRAM option in the COMPUTE statement, the OUTPAIR= data set is populated with all $[n(n-1)]/2$ pairs that can be formed with the n observations.

If the NOVARIOGRAM option is not specified, then the OUTPAIR= data set contains only pairs of data that are located within a certain distance away from each other. Specifically, it contains pairs whose distance between observations belongs to a lag class up to the specified MAXLAGS= option in the COMPUTE statement. Then, depending on your specification of the LAGDISTANCE= and MAXLAGS= options, the OUTPAIR= data set might contain $[n(n-1)]/2$ or fewer pairs.

Finally, you can restrict the number of pairs in the OUTPAIR= data set with the OUTPDISTANCE= option in the COMPUTE statement. The OUTPDISTANCE= option in the COMPUTE statement excludes pairs of points when the distance between the pairs exceeds the OUTPDISTANCE= value.

See the section "OUTPAIR=*SAS-data-set*" on page 10107 for details.

OUTVAR=*SAS-data-set*

OUTVR=*SAS-data-set*

specifies a SAS data set in which to store the continuity measures.

See the section "OUTVAR=*SAS-data-set*" on page 10108 for details.

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

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

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=observ
plots=(observ semivar)
plots(unpack)=semivar
plots=(semivar(cla unpack) semivar semivar(rob))
```

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

```
ods graphics on;

proc variogram data=sashelp.thick;
   compute novariogram;
   coordinates xc=East yc=North;
   var Thick;
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."

If ODS Graphics is enabled but you omit the PLOTS option or have specified PLOTS=ALL, then PROC VARIOGRAM produces a default set of plots, which might be different for different COMPUTE statement options, as discussed in the following.

- If you specify NOVARIOGRAM in the COMPUTE statement, the VARIOGRAM procedure produces a scatter plot of your observations spatial distribution, in addition to the histogram of the pairwise distances of your data. For an example of the observations plot, see Figure 124.2. For an example of the pairwise distances plot, see Figure 124.4.
- If you omit NOVARIOGRAM in the COMPUTE statement, the VARIOGRAM procedure computes the empirical semivariogram for the specified LAGDISTANCE= and MAXLAGS= options. The observations plot appears by default in this case too. The VARIOGRAM procedure also produces a plot of the classical empirical semivariogram. If you also specify ROBUST in the COMPUTE statement, then the VARIOGRAM procedure instead produces a plot of both the classical and robust empirical semivariograms, in addition to the observations plot. For an example of the empirical semivariogram plot, see Output 124.7. Moreover, if you specify the MODEL statement and perform model fitting, then PROC VARIOGRAM also produces a fit plot of the fitted semivariogram. An example of the fit plot is shown in Figure 124.16.

The following *global-plot-options* are available:

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

UNPACKPANEL
UNPACK
suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack the default plots. You can also specify UNPACKPANEL as a suboption with the SEMIVAR option.

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 default plots and an additional classical empirical semivariogram, specify PLOTS=(ALL SEMIVAR(CLA)).

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

FITPLOT < (*fitplot-options*) >
FIT < (*fitplot-options*) >
requests a plot that shows the model fitting results against the empirical semivariogram. By default, FITPLOT displays one plot of the fitted model (or a panel of plots for different angles in the anisotropic case).

If you specify the FORM=AUTO option in the MODEL statement, then each class of equivalent fitted models is displayed with a different curve on the plot. The best fitting model class is chosen based on the criteria that you specify in the CHOOSE option of the MODEL statement, and a thicker line on top of any other curve is shown for it. The plot legend shows the ranked classes by displaying the label of the representative model of each class in the plot. If appropriate, the number of additional models in the same equivalence class also shows within parentheses.

You can specify the following *fitplot-options*:

NCLASSES=*number*

NCLASSES=ALL

specifies the maximum number of classes to display on the fit plot, where *number* is a positive integer. The default is NCLASSES=5 for nonpaneled plots and NCLASSES=3 for paneled plots. The option takes effect when you specify the FORM=AUTO option in the MODEL statement, and it is ignored when you fit one single model. If you specify NCLASSES=ALL or a larger number than the available classes, then all available classes are shown on the fit plot. If you specify multiple instances of the NCLASSES= option, then only the last specified instance is honored.

UNPACK

suppresses paneling in paneled fit plots. By default, fit plots appear in a panel, when appropriate.

MORAN < (*moran-options*) >

MOR < (*moran-options*) >

produces a Moran scatter plot of the observations with nonmissing values. For more details about this plot, see the section "The Moran Scatter Plot" on page 10103. In addition to the Moran scatter plot points, the plot also displays the fit line for the linear regression of the weighted average on the standardized observation values, the regression fit line slope, and a reference line with slope equal to 1. The MORAN plot has the following *moran-options*:

LABEL < (*label-options*) >

labels the observations. The label is the ID variable if the ID statement is specified; otherwise, it is the observation number. The *label-options* can be one or more of the following:

HH

specifies that labels show for observations in the upper right (high-high) plot quadrant of positive spatial association.

HL

specifies that labels show for observations in the lower right (high-low) plot quadrant of negative spatial association.

LH

specifies that labels show for observations in the upper left (low-high) plot quadrant of negative spatial association.

LL
specifies that labels show for observations in the lower left (low-low) plot quadrant of positive spatial association.

If you specify multiple instances of the MORAN option and you specify the LABEL suboption in any of those, then the resulting Moran scatter plot displays the observations labels. By default, when you specify none of the *label-options*, the PLOTS=MORAN(LABEL) request puts labels in all observations.

ROWAVG=*rowavg-option*
specifies the flag value for row-averaging of weights in the computation of the weighted average. The *rowavg-option* can be either of the following:

OFF
specifies that autocorrelation weights not be row-averaged.

ON
specifies that row-averaged autocorrelation weights be used.

The default behavior is ROWAVG=ON. If you specify the ROWAVG= option more than once in the same MORAN plot request, then the behavior is set to ROWAVG=ON unless any of the instances is ROWAVG=OFF.

When you specify the PLOTS=MORAN option, you must specify both the AUTOCORRELATION and the LAGDISTANCE= options in the COMPUTE statement to produce the Moran scatter plot. For more information about the plot, see the section "The Moran Scatter Plot" on page 10103.

NONE
suppresses all plots.

OBSERVATIONS < (*observations-plot-options***) >**
OBSERV < (*observations-plot-options***) >**
OBS < (*observations-plot-options***) >**
produces the observed data plot. Only one observations plot 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.

PAIRS < (*pairs-plot-options***) >**
specifies that the pairwise distances histogram be produced. By default, the horizontal axis displays the lag class number. The vertical axis shows the frequency (count) of pairs in the lag classes. Notice that the zero lag class width is half the width of the other classes.

The PAIRS option has the following *suboptions*:

MIDPOINT
MID
specifies that the plot that is created with the PAIRS option display the lag class midpoint value on the horizontal axis, rather than the default lag class number. The midpoint value is the actual distance of a lag class center from the assumed origin point at distance zero. See also the illustration in Figure 124.22.

NOINSET

NOI

specifies that the plot created with the PAIRS option be produced without the default inset that provides additional information about the pairs distribution.

THRESHOLD=*minimum pairs*

THR=*minimum pairs*

specifies that a reference line appear in the plot that is created with the PAIRS option to indicate the *minimum pairs* frequency of data pairs. You can use this line as an exploratory tool when you want to select lag classes that contain at least THRESHOLD point pairs. The option helps you to identify visually any portion of the PAIRS distribution that lies below the specified THRESHOLD value.

Only one pairwise distances histogram is created if you specify the PAIRS option within a PLOTS option. If you specify multiple instances of the PAIRS option, the resulting plot has the following features:

- If the MIDPOINT or NOINSET suboption has been specified in any of the instances, it is activated in the resulting plot.
- If you have specified the THRESHOLD= suboption more than once, then the THRESHOLD= value specified last prevails.

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

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

specifies that the empirical semivariogram plot be produced. You can specify the SEMIVAR option multiple times in the same PLOTS option to request instances of plots with the following *semivar-plot-options*:

ALL | CLASSICAL | ROBUST

ALL | CLA | ROB

specifies a single type of empirical semivariogram (classical or robust) to plot, or specifies that all the available types be included in the same plot. The default is ALL.

UNPACKPANEL

UNPACK

specifies that paneled semivariogram plots be displayed separately. By default, plots appear in a panel, when appropriate.

BY Statement

BY *variables* **;**

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

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

COMPUTE Statement

COMPUTE *computation-options* **;**

The COMPUTE statement provides a number of options that control the computation of the semivariance, the robust semivariance, and the covariance.

Table 124.2 summarizes the *options* available in the COMPUTE statement.

Table 124.2 COMPUTE Statement Options

Option	Description
ALPHA=	Specifies the confidence level
ANGLETOLERANCE=	Specifies the tolerance
AUTOCORRELATION	Calculates autocorrelation statistics
BANDWIDTH=	Specifies the bandwidth
CL	Requests confidence limits
DEPSILON=	Specifies the distance value for declaring that two distinct points are zero distance apart
LAGDISTANCE=	Specifies the basic distance unit that defines the lags
LAGTOLERANCE=	Specifies the tolerance around the LAGDISTANCE= value
MAXLAGS=	Specifies the maximum number of lag classes to be used
NDIRECTIONS=	Specifies the number of angle classes to be used
NHCLASSES=	Specifies the number of distance classes to be used
NOVARIOGRAM	Prevents the computation of the continuity measures
OUTPDISTANCE=	Specifies the cutoff distance for writing observations to the OUTPAIR= data set
ROBUST	Calculates a robust version of the semivariance

ALPHA=*number*

specifies a parameter to obtain the confidence level for constructing confidence limits in the classical empirical semivariance estimation. The value of *number* must be in $(0, 1)$, and the confidence level is $1-$*number*. The default is ALPHA=0.05, which corresponds to the default confidence level of 95%. If the CL option is not specified, ALPHA= is ignored.

ANGLETOLERANCE=*angle-tolerance*

ANGLETOL=*angle-tolerance*

ATOL=*angle-tolerance*

specifies the tolerance, in degrees, around the angles determined by the NDIRECTIONS= specification. The default is $180°/(2n_d)$, where n_d is the NDIRECTIONS= specification. If you do not specify the NDIRECTIONS= option or the DIRECTIONS statement, ANGLETOLERANCE= is ignored.

See the section "Theoretical and Computational Details of the Semivariogram" on page 10077 for further information.

AUTOCORRELATION < (*autocorrelation-options***) >**

AUTOCORR < (*autocorrelation-options***) >**

AUTOC < (*autocorrelation-options***) >**

specifies that autocorrelation statistics be calculated. You can further specify the following *autocorrelation-options* in parentheses following the AUTOCORRELATION option.

ASSUMPTION < = *assumption-options* >

ASSUM < = *assumption-options* >

specifies the type of autocorrelation assumption to use. The *assumption-options* can be one of the following:

NORMALITY | NORMAL | NOR

specifies use of the normality assumption.

RANDOMIZATION | RANDOM | RAN

specifies use of the randomization assumption.

The default is ASSUMPTION=NORMALITY.

STATISTICS < = (*stats-options***) >**

STATS < = (*stats-options***) >**

specifies the autocorrelation statistics in detail. The *stats-options* can be one or more of the following:

ALL

applies all available types of autoregression statistics.

GEARY | GEA

specifies use of the Geary's c statistics.

MORAN | MOR

specifies use of the Moran's I statistics.

The default is STATISTICS=ALL.

WEIGHTS < = *weights-options* >

WEI < = *weights-options* >

specifies the scheme used for the computation of the autocorrelation weights. You can choose one of the following *weights-options*:

BINARY < (*binary-option*) >
specifies that binary weights be used. You also have the following *binary-option*:

ROWAVERAGING | ROWAVG | ROW
specifies that asymmetric autocorrelation weights be assigned to data pairs. For each observation, if there are nonzero weights, the ROWAVG option standardizes those weights so that they sum to 1. No row averaging is performed by default.

DISTANCE < (*distance-options*) >
specifies that autocorrelation weights be assigned based on the point pair distances. You also have the following *distance-options*:

NORMALIZE | NORMAL | NOR
specifies that normalized pair distances be used in the distance-based weights expression. The distances are normalized with respect to the maximum pairwise distance h_b, as it is defined in the section "Computation of the Distribution Distance Classes" on page 10086. By default, nonnormalized values are used in the computations.

POWER=*number*
POW=*number*
specifies the power to which the pair distance is raised in the distance-based weights expression. POWER is a nonnegative number, and its default value is POWER=1.

ROWAVERAGING | ROWAVG | ROW
specifies that asymmetric autocorrelation weights be assigned to data pairs. For each observation, if there are nonzero weights, the ROWAVG option standardizes those weights so that they sum to 1. No row averaging is performed by default.

SCALE=*number*
SCA=*number*
specifies the scaling factor in the distance-based weights expression. SCALE is a nonnegative number, and its default value is SCALE=1.

The default is WEIGHTS=BINARY. See the section "Autocorrelation Statistics" on page 10100 for further details about the autocorrelation weights.

When you specify the AUTOCORRELATION option with no *autocorrelation-options*, PROC VARIOGRAM computes by default both the Moran's I and Geary's c statistics with p-values computed under the normality assumption with binary weights.

If you specify more than one ASSUMPTION in the *autocorrelation-options*, all but the last specified ASSUMPTION are ignored. The same holds if you specify more than one POWER= or SCALE= parameter in the WEIGHT=DISTANCE *distance-options*.

If you specify the WEIGHT=BINARY option in the AUTOCORRELATION option and the NOVARIOGRAM option at the same time, then you must also specify the LAGDISTANCE= option in the COMPUTE statement. See the section "Autocorrelation Weights" on page 10100 for more information.

BANDWIDTH=*bandwidth-distance*

BANDW=*bandwidth-distance*

specifies the bandwidth, or perpendicular distance cutoff for determining the angle class for a given pair of points. The distance classes define a series of cylindrically shaped areas, while the angle classes radially cut these cylindrically shaped areas. For a given angle class $(\theta_1 - \delta\theta_1, \theta_1 + \delta\theta_1)$, as you proceed out radially, the area encompassed by this angle class becomes larger. The BANDWIDTH= option restricts this area by excluding all points with a perpendicular distance from the line $\theta = \theta_1$ that is greater than the BANDWIDTH= value. See Figure 124.23 for a visual representation of the bandwidth.

If you omit the BANDWIDTH= option, no restriction occurs. If you omit the NDIRECTIONS= option or the DIRECTIONS statement, BANDWIDTH= is ignored.

CL

requests confidence limits for the classical semivariance estimate. The lower bound of the confidence limits is always nonnegative, adhering to the behavior of the theoretical semivariance. You can control the confidence level with the ALPHA= option.

DEPSILON=*distance-value*

DEPS=*distance-value*

specifies the distance value for declaring that two distinct points are zero distance apart. Such pairs, if they occur, cause numeric problems. If you specify DEPSILON=$\Delta\varepsilon$, then pairs of points P_1 and P_2 for which the distance between them $\mid P_1 P_2 \mid < \Delta\varepsilon$ are excluded from the continuity measure calculations. The default value of the DEPSILON= option is 100 times the machine precision; this product is approximately 1E–10 on most computers.

LAGDISTANCE=*distance-unit*

LAGDIST=*distance-unit*

LAGD=*distance-unit*

specifies the basic distance unit that defines the lags. For example, a specification of LAGDISTANCE=x results in lag distance classes that are multiples of x. For a given pair of points P_1 and P_2, the distance between them, denoted $\mid P_1 P_2 \mid$, is calculated. If $\mid P_1 P_2 \mid = x$, then this pair is in the first lag class. If $\mid P_1 P_2 \mid = 2x$, then this pair is in the second lag class, and so on.

For irregularly spaced data, the pairwise distances are unlikely to fall exactly on multiples of the LAGDISTANCE= value. In this case, a distance tolerance of δx accommodates a spread of distances around multiples of x (the LAGTOLERANCE= option specifies the distance tolerance). For example, if $\mid P_1 P_2 \mid$ is within $x \pm \delta x$, you would place this pair in the first lag class; if $\mid P_1 P_2 \mid$ is within $2x \pm \delta x$, you would place this pair in the second lag class; and so on.

You can experiment and determine the candidate values for the LAGDISTANCE= option by plotting the pairwise distance histogram for different numbers of histogram classes, using the NHCLASSES= option.

A LAGDISTANCE= value is required for the semivariance and the autocorrelation computations. However, when you specify the NOVARIOGRAM option without the AUTOCORRELATION option, you need not specify the LAGDISTANCE= option.

See the section "Theoretical and Computational Details of the Semivariogram" on page 10077 for more information.

LAGTOLERANCE=*tolerance-number*

LAGTOL=*tolerance-number*

LAGT=*tolerance-number*

specifies the tolerance around the LAGDISTANCE= value for grouping distance pairs into lag classes. See the description of the LAGDISTANCE= option for information about the use of the LAGTOLERANCE= option, and the section "Theoretical and Computational Details of the Semivariogram" on page 10077 for more details.

If you omit the LAGTOLERANCE= option, a default value of $\frac{1}{2}$ times the LAGDISTANCE= value is used.

MAXLAGS=*number-of-lags*

MAXLAG=*number-of-lags*

MAXL=*number-of-lags*

specifies the maximum number of lag classes to be used in constructing the continuity measures in addition to a zero lag class; see also the section "Distance Classification" on page 10083. This option excludes any pair of points P_1 and P_2 for which the distance between them, $\mid P_1 P_2 \mid$, exceeds the MAXLAGS= value times the LAGDISTANCE= value.

You can determine candidate values for the MAXLAGS= option by plotting or displaying the OUTDISTANCE= data set.

A MAXLAGS= value is required unless you specify the NOVARIOGRAM option.

NDIRECTIONS=*number-of-directions*

NDIR=*number-of-directions*

ND=*number-of-directions*

specifies the number of angle classes to use in computing the continuity measures. This option is useful when there is potential anisotropy in the spatial continuity measures. Anisotropy is a field property in which the characterization of spatial continuity depends on the data pair orientation (or angle between the N–S direction and the axis defined by the data pair). Isotropy is the absence of this effect; that is, the description of spatial continuity depends only on the distance between the points, not the angle.

The angle classes formed from the NDIRECTIONS= option start from N–S and proceed clockwise. For example, NDIRECTIONS=3 produces three angle classes. In terms of compass points, these classes are centered at 0° (or its reciprocal, 180°), 60° (or its reciprocal, 240°), and 120° (or its reciprocal, 300°). For irregularly spaced data, the angles between pairs are unlikely to fall exactly in these directions, so an angle tolerance of $\delta\theta$ is used (the ANGLETOLERANCE= option specifies the angle tolerance). If NDIRECTIONS=n_d, the base angle is $\theta = 180°/n_d$, and the angle classes are

$$(k\theta - \delta\theta, k\theta + \delta\theta) \quad k = 0, \ldots, n_d - 1$$

If you omit the NDIRECTIONS= option, no angles are formed. This is the omnidirectional case where the spatial continuity measures are assumed to be isotropic.

The NDIRECTIONS= option is useful for exploring possible anisotropy. The DIRECTIONS statement, described in the section "DIRECTIONS Statement" on page 10055, provides greater control over the angle classes.

See the section "Theoretical and Computational Details of the Semivariogram" on page 10077 for more information.

NHCLASSES=*number-of-histogram-classes*
NHCLASS=*number-of-histogram-classes*
NHC=*number-of-histogram-classes*

specifies the number of distance classes to consider in the spatial domain in the exploratory stage of the empirical semivariogram computation. The actual number of classes is one more than the NHCLASSES= value, since a special lag zero class is also computed. The NHCLASSES= option is used to produce the distance intervals table, the histogram of pairwise distances, and the OUTDISTANCE= data set. See the OUTDISTANCE= option, the section "OUTDIST=*SAS-data-set*" on page 10106, and the section "Theoretical and Computational Details of the Semivariogram" on page 10077 for more information.

The default value is NHCLASSES=10.

NOVARIOGRAM

prevents the computation of the continuity measures. This option is useful for preliminary analysis, or when you require only the OUTDISTANCE= or OUTPAIR= data sets.

OUTPDISTANCE=*distance-limit*
OUTPDIST=*distance-limit*
OUTPD=*distance-limit*

specifies the cutoff distance for writing observations to the OUTPAIR= data set. If you specify OUTPDISTANCE=d_{max}, the distance $\mid P_1 P_2 \mid$ between each pair of points P_1 and P_2 is checked against d_{max}. If $\mid P_1 P_2 \mid > d_{max}$, the observation for this pair is not written to the OUTPAIR= data set. If you omit the OUTPDISTANCE= option, all distinct pairs are written. This option is ignored if you omit the OUTPAIR= data set.

ROBUST

requests that a robust version of the semivariance be calculated in addition to the classical semivariance.

COORDINATES Statement

COORDINATES *coordinate-variables* **;**

The following two options give the names of the variables in the DATA= data set that contains the values of the *x* and *y* coordinates of the data.

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

XCOORD=(*variable-name***)**
XC=(*variable-name***)**
X=(*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***)**
Y=(*variable-name***)**

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

DIRECTIONS Statement

DIRECTIONS *directions-list* **;**

You use the DIRECTIONS statement to define angle classes. You can specify angle classes as a list of angles, separated by commas, with optional angle tolerances and bandwidths within parentheses following the angle. You must specify at least one angle.

If you do not specify the optional angle tolerance, the default value of 45° is used. If you do not specify the optional bandwidth, no bandwidth is checked. If you specify a bandwidth, you must also specify an angle tolerance.

For example, suppose you want to compute three separate semivariograms at angles $\theta_1 = 0°$, $\theta_2 = 60°$, and $\theta_3 = 120°$, with corresponding angle tolerances $\delta\theta_1 = 22.5°$, $\delta\theta_2 = 12.5°$, and $\delta\theta_3 = 22.5°$, with bandwidths 50 and 40 distance units on the first two angle classes and no bandwidth check on the last angle class.

The appropriate DIRECTIONS statement is as follows:

```
directions 0.0(22.5,50), 60.0(12.5,40),120(22.5);
```

ID Statement

ID *variable* **;**

The ID statement specifies which variable to include for identification of the observations in the OUTPAIR= and the OUTACWEIGHTS= output data sets. The ID statement variable is also used for the labels and tool tips in the OBSERVATIONS plot.

In the VARIOGRAM procedure you can specify only one ID variable in the ID statement. If no ID statement is given, then PROC VARIOGRAM uses the observation number in the data sets and the OBSERVATIONS plot.

MODEL Statement

MODEL *fitting-options* < / *model-options* > **;**

You specify the MODEL statement if you want to fit a theoretical semivariogram model to the empirical semivariogram data that are produced in the COMPUTE statement. You must have nonmissing empirical semivariogram estimates at a minimum of three lags to perform model fitting.

Table 124.3 summarizes the *options* available in the MODEL statement.

Table 124.3 MODEL Statement Options

Option	Description
Fitting Options	
ALPHA=	Specifies confidence level
CHOOSE=	Ranks the fitted models and chooses the optimally fit model
CL	Constructs a *t*-type confidence interval
EQUIVTOL=	Specifies a positive upper value tolerance
FIT=	Specifies which type of empirical semivariogram to fit
FORM=	Specifies the functional form (type) of the semivariogram model
MDATA=	Specifies the input data set
METHOD=	Fits a theoretical model to the empirical semivariance
NEPSILON=	Adds a minimal nugget effect
NUGGET=	Specifies the nugget effect
RANGE=	Specifies the range parameter
RANGELAG=	Uses consecutive nonmissing empirical semivariance lags to fit model
RANKEPS=	Specifies the minimum threshold to compare fit quality
SCALE=	Specifies the scale parameter in semivariogram models
SMOOTH=	Specifies the positive smoothness parameter ν
Model Options	
COVB	Requests the covariance matrix
CORRB	Requests the approximate correlation matrix
DETAILS	Produces different levels of output
GRADIENT	Displays the gradient of the objective function
MTOGTOL=	Specifies a threshold value for the smoothness parameter
NOFIT	Suppresses the model fitting process
NOITPRINT	Suppresses the display of the iteration history table

You can choose to perform a fully automated fitting or to fit one model with specific forms. In the first case you simply specify a list of forms or no forms at all. All suitable combinations are tested, and the result is the model that produces the best fit according to specified criteria. In the second case you specify one theoretical semivariogram model, and you have more control over its parameters for the fitting process.

Furthermore, you can specify a theoretical semivariogram model in two ways:

- You explicitly specify the FORM option and any of the options SCALE, RANGE, and NUGGET in the MODEL statement.
- You can specify an MDATA= data set. This data set contains variables that correspond to the FORM option and to any of the options SCALE, RANGE, NUGGET, and SMOOTH. You can also use an MDATA= data set to request a fully automated fitting.

The two methods are exclusive; either you specify all parameters explicitly, or they all are read from the MDATA= data set.

The MODEL statement has the following *fitting-options*:

ALPHA=*number*

requests that a t-type confidence interval be constructed for each of the fitting parameters with confidence level $1 - \mathit{number}$. The value of *number* must be in $(0, 1)$; the default is 0.05 which corresponds to the default confidence level of 95%. If the CL option of the MODEL statement is not specified, then ALPHA= is ignored.

CHOOSE=*criterion* | **(***criterion1 . . . criterionk***)**

specifies that if the fitting task has more than one model to fit, then PROC VARIOGRAM ranks the fitted models and chooses the optimally fit model according to one or more available criteria.

If you want to use multiple fitting criteria, then the order in which you specify them in the CHOOSE= option defines how they are applied. This feature is useful when fitting suggests that two or more models perform equally well according to a certain criterion. For example, if two models are equivalent according to *criterioni*, then they are further ranked in the list based on the next criterion, *criterionj*, where $j = i + 1$.

Each *criterion* can be one of the following:

AIC

specifies Akaike's information criterion.

SSE

specifies the weighted sum of squares error for each fitted model when METHOD=WLS, and the residual sum of squares error for each fitted model when METHOD=OLS.

STATUS

classifies models based on their fitting process convergence status. CHOOSE=STATUS places on top models for which the fitting process is successful.

By default, the models are ranked in the fit summary table with the best fitted model at the top of the list, based on the criteria that you specify in the CHOOSE= option. This model is the fit choice of PROC VARIOGRAM for the particular fitting task. If you omit the CHOOSE= option, then the default behavior is CHOOSE=(SSE AIC).

Regardless of the specified fitting criteria, models for which the fitting process is unsuccessful always appear at the bottom of the fit summary table. For more details about the fitting criteria, see the section "Fitting Criteria" on page 10097. After multiple models are ranked, they are further categorized in classes of equivalence depending on whether any two models calculate the same semivariance value at the same distance for a series of different distances. For more details, see the section "Classes of Equivalence" on page 10099.

If you specify the same criterion multiple times in the CHOOSE= option, then only the first instance is used for the ranking process and any additional ones are ignored. If you specify only one model to fit in the MODEL statement and you specify the CHOOSE= option, then the option is ignored.

CL

requests that *t*-type confidence limits be constructed for each of the fitting parameters estimates. The confidence level is 0.95 by default; this can be changed with the ALPHA= option of the MODEL statement.

EQUIVTOL=*etol-value*

ETOL=*etol-value*

specifies a positive upper value tolerance to use when categorizing multiple models in classes of equivalence. For this categorization, the VARIOGRAM procedure computes the sum of absolute differences of semivariances for pairs of consecutively ranked models. If the sum is lower than the EQUIVTOL= value for any such model pair, then these two models are deemed to be equivalent. As a result, the EQUIVTOL= option can affect the number and size of classes of equivalence in the fit summary table. Smaller values of the EQUIVTOL= parameter result in a more strict model comparison and can lead to a higher number of classes of equivalence. For more details, see the section "Classes of Equivalence" on page 10099.

The default value for the EQUIVTOL= parameter is 10^{-3}. The EQUIVTOL= option applies when you fit multiple models with the FORM=AUTO option of the MODEL statement; otherwise, it is ignored.

The EQUIVTOL= option is independent of the ranking results from the RANKEPS= option of the MODEL statement. This means that you could possibly have models listed but not ranked in the fit summary table, and still have equivalence classes assigned according to the order in which the models appear in the table.

FIT=*fit-type-options*

specifies which type of empirical semivariogram to fit. You can choose between the following *fit-type-options*:

CLASSICAL

CLA

fits a model for the classical empirical semivariance.

ROBUST

ROB

fits a model for the robust empirical semivariance. This option can be used only when the ROBUST option is specified in the COMPUTE statement.

The default value is FIT=CLASSICAL.

FORM=*form* | (*form1, . . . , formk*) | **AUTO** (*auto-options*)

specifies the functional form (type) of the semivariogram model. The supported structures are two-parameter models that use the sill and range as parameters. The Matérn model is an exception that makes use of a third smoothing parameter ν.

The FORM= option is required when you specify the MODEL statement. You can perform fitting of a theoretical semivariogram model either explicitly or in an automated manner. For the explicit specification you specify suitable model forms in the FORM= option. For an automated fit you specify the FORM=AUTO option which has the AUTO(MLIST=) and AUTO(NEST=) suboptions. You can read more details in the following two subsections.

Explicit Model Specification

You can explicitly specify a theoretical semivariogram model to fit by using any combination of one, two, or three forms. Use the syntax with the single *form* to specify a non-nested model. Use the syntax with k structures *formi*, $i = 1, \ldots, k$, to specify up to three nested structures ($k \leq 3$) in a semivariogram model. Each of the forms can be any of the following:

CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |
PENTASPHERICAL | POWER | SINEHOLEEFFECT | SPHERICAL
CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH
specify a form.

All of these forms are presented in more detail in the section "Theoretical Semivariogram Models" on page 10072. In addition, you can optionally specify a nugget effect for your model with the NUGGET option in the MODEL statement.

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.

When you explicitly specify the types of structures, you can fix parameter values or ask PROC VARIOGRAM to select default initial values for the forms parameters by using the SCALE, RANGE, NUGGET, and SMOOTH options. You can set your own, non-default initial parameter values by using the PARMS statement in combination with an explicitly specified semivariogram model in the MODEL statement.

Automated Model Selection

Use the FORM=AUTO option to request the highest level of automation in the best fit selection of the parameters. If you specify FORM=AUTO, any of the SCALE, RANGE, or SMOOTH options that are also specified are ignored. When you specify the FORM=AUTO option, you cannot specify the PARMS statement for the corresponding MODEL statement. As a result, when you use the FORM=AUTO option, you cannot fix any of the model parameters and PROC VARIOGRAM sets initial values for them.

The AUTO option has the following *auto-options*:

MLIST=*mform* **|** (*mform1, . . . , mformp*)
specifies one or more different model forms to use in combinations during the model fitting process. If you omit the MLIST= suboption, then combinations are made among all available model types. The *mform* can be any of the following eight forms:

CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |
PENTASPHERICAL | POWER | SINEHOLEEFFECT | SPHERICAL
CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH
specify a form.

If you use more than one *mform*, then each *mformi*, $i = 1, \ldots, p$ must be different from the others in the group of $p \leq 8$ forms that you specify.

NEST=*nest-list*
specifies the number of nested structures to use for the fitting. You can choose between the following to specify the *nest-list*:

n	a single value
m TO *n*	a sequence in which *m* equals the starting value and *n* equals the ending value

For example,

```
NEST=1
```

produces the best fit with one single model among all model types specified in the MLIST= suboption. Also,

```
NEST=2 TO 3
```

produces the best fit among all combinations of the model types specified in the MLIST= suboption that result in nested models with two or three structures. The combinations that are tested include repetitions. Hence, if you specify, for example,

```
MODEL FORM=AUTO(MLIST=(EXP,SPH) NEST=1 TO 2)
```

then the different models that are tested are equivalent to the specifications FORM=EXP, FORM=SPH, FORM=(EXP,EXP), FORM=(EXP,SPH), FORM=(SPH,SPH) and FORM=(SPH,EXP). **NOTE:** The models EXP-SPH and SPH-EXP are taken as two separate models. Although they are mathematically equivalent (see the section "Nested Models" on page 10077), PROC VARIOGRAM assigns different initial values to the model structures in each case, which can lead to different fitting results. (See the section "Example 124.1: Aspects of Semivariogram Model Fitting" on page 10112.)

If you omit the NEST suboption, then by default PROC VARIOGRAM searches for the best fit with up to three nested structures in a model. The default behavior is equivalent to

```
NEST=1 TO 3
```

In the VARIOGRAM procedure you can use a maximum of three nested structures to fit an empirical semivariogram; that is, $n \leq 3$.

You can use the AUTO value for the form in the MDATA= data set, and also in the FORM= option. However, in the former case the automation functionality is limited compared to the latter case and the *auto-options* of the FORM=AUTO option. In particular, when you specify the form to be AUTO in the MDATA= data set, then PROC VARIOGRAM follows only the default behavior and searches among all available forms for the best fit with up to three nested structures in a model.

MDATA=*SAS-data-set*

specifies the input data set that contains parameter values for the covariance or semivariogram model. The MDATA= data set must contain a variable named FORM, and it can optionally include any of the variables SCALE, RANGE, NUGGET, and SMOOTH.

The FORM variable must be a character variable. It accepts only the AUTO value or the *form* values that can be specified in the FORM= option in the MODEL statement. The RANGE, SCALE, NUGGET, and SMOOTH variables must be numeric or missing.

The number of observations present in the MDATA= data set corresponds to the level of nesting of the semivariogram model. Each observation line describes a structure of the model you submit for fitting.

If you specify the AUTO value for the FORM variable in an observation, then you cannot specify additional nested structures in the same data set, and any parameters you specify in the same structure are ignored. In that case, PROC VARIOGRAM performs a crude automated search among all available forms to obtain the best fit with up to three nested structures in a model. You can refine this type of search with additional suboptions when you perform it with the FORM=AUTO option instead of the MDATA= option in the MODEL statement.

When you have a nested model, you might want to specify parameter values for only some of the nested structures. In this case, you must specify the corresponding parameter values for the remaining model structures as missing values.

For example, you can use the following DATA step to specify a non-nested model that uses a spherical covariance within an MDATA= data set:

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

Then, you can use the md1 data in the MODEL statement of PROC VARIOGRAM as shown in the following statements:

```
proc variogram data=...;
   compute ...;
   model mdata=md1;
run;
```

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

```
proc variogram data=...;
   compute ...;
   model form=sph scale=25 range=10;
run;
```

The following data set md2 is an example of a nested model:

```
data md2;
   input form $ scale range nugget smooth;
   datalines;
SPH 20 8 5 .
MAT 12 3 5 0.7
GAU .  1 5 .
;
```

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

```
proc variogram data=...;
   compute ....;
   model form=(sph,mat,gau)
         scale=(20,12,.) range=(8,3,1) smooth=0.7 nugget=5;
run;
```

Use the SMOOTH variable column in the MDATA= data set to specify the smoothing parameter ν in the Matérn semivariogram models. The SMOOTH variable values must be positive and no greater than 1,000,000. PROC VARIOGRAM sets this upper limit for numerical and performance reasons. In any case, if the fitting process leads the smoothness value to exceed the default threshold value 10,000, then the VARIOGRAM procedure converts the Matérn form into a Gaussian form and repeats the model fitting. To adjust the switching threshold value, you can use the MTOGTOL= option in the MODEL statement.

If you specify a SMOOTH column in the MDATA= data set, then its elements are ignored except for the rows in which the corresponding FORM is Matérn.

The NUGGET variable value is the same for all nested structures. This is the way to specify a nugget effect in the MDATA= data set. If you specify more than one nugget value for different structures, then the last nugget value specified is used.

METHOD=*method-options*

must be specified in the MODEL statement to fit a theoretical model to the empirical semivariance. The METHOD option has the following *suboptions*:

OLS

specifies that ordinary least squares be used for the fitting.

WLS

specifies that weighted least squares be used for the fitting.

The default is METHOD=WLS.

NEPSILON=*min-nugget-factor*

NEPS=*min-nugget-factor*

specifies that a minimal nugget effect be added to the theoretical semivariance in the unlikely occasion that the theoretical semivariance becomes zero during fitting with weighted least squares. As explained in the section "Theoretical and Computational Details of the Semivariogram" on page 10077, the theoretical semivariance is always positive for any distance larger than zero. If a conflicting situation emerges as a result of numerical fitting issues, then the NEPSILON= option can help you alleviate the problem by adding a minimal variance at the distance lag where the issue is encountered. For more details, see the section "Parameter Initialization" on page 10094.

If you omit the NEPSILON= option, then PROC VARIOGRAM sets a default value of 10^{-6}. If a minimal nugget effect is used, its value is case-specific and is based on the *min-nugget-factor*. Specifically, its value is defined as *min-nugget-factor* times the sample variance of the input data set, or as *min-nugget-factor* when the sample variance is equal to zero.

NUGGET=*number*

specifies the nugget effect for the model. The nugget effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram; see "Theoretical Semivariogram Models" on page 10072 for more details. The NUGGET= parameter is a nonnegative number. If you specify a nonmissing value, then it is used as a fixed parameter in the fitting process.

PROC VARIOGRAM assigns a default initial value for the nugget effect in the following cases:

- if you specify a missing value.
- if you omit the NUGGET= option and you do not specify an associated PARMS statement with initial values for the nugget.

The NUGGET= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

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

specifies the range parameter in semivariogram models. The RANGE= option is optional. However, if you specify the RANGE= option, then you must provide range values for all structures that you have specified explicitly in the FORM= option. All nonmissing range values are considered as fixed parameters. PROC VARIOGRAM assigns a default initial value to any of the model structures for which you specify a missing range value. PROC VARIOGRAM assigns default initial values to all model structures if you omit the RANGE= option, unless you specify an associated PARMS statement and initial values for the range in it.

The range parameter is a positive number, has the units of distance, and is related to the correlation scale of the underlying spatial process.

NOTE: If you specify this parameter for a power model, then it does not correspond to a range. For power models, the parameter you specify in the RANGE option is a dimensionless power exponent whose value must range within [0,2) so that the power model is a valid semivariance function.

The RANGE= option is ignored when you specify the FORM=AUTO option. The RANGE= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

RANGELAG=*rlag-list*

RLAG=*rlag-list*

specifies that you prefer to use the range of consecutive nonmissing empirical semivariance lags in the *rlag-list* for the semivariogram fitting process, instead of using all MAXLAGS+1 lag classes by default. You can specify *rlag-list* in either of the following forms:

k — a single value that designates the width of the selected lag range by starting at lag zero. You must use at least three lags to perform model fitting, so you can specify *k* within [3, . . . , MAXLAGS+1].

m TO *n* — a sequence in which *m* equals the starting lag and *n* equals the ending lag. The parameters *m* and *n* must be nonnegative integer numbers to designate lag classes between zero and MAXLAGS. Use at least three lags for model fitting; hence it holds that $n - m \geq 2$.

The following two brief examples exhibit the use of the RANGELAG option. These examples assume that you have set the MAXLAGS= option to 9 or higher to indicate nonmissing empirical semivariance estimates at 10 lags or more.

In the first example,

```
RANGELAG=8
```

uses the empirical semivariance in the first eight lags to fit a theoretical model. Hence, RANGELAG=8 uses only the lag classes zero to seven. This approach enables you to account only for the correlation behavior described by the first *k* empirical semivariogram lag classes.

In the second example,

```
RANGELAG=2 TO 9
```

specifies that the empirical semivariance values at lag classes zero, one, and after lag class nine are excluded from the model fitting process.

RANKEPS=*reps-value*

REPS=*reps-value*

specifies the minimum threshold to compare fit quality of two models for a specific criterion. Beyond this threshold the criterion values become insensitive to comparison. In particular, when you fit multiple models, PROC VARIOGRAM computes for each one the value of the fitting criterion specified in the CHOOSE= option of the MODEL statement. These values are examined in pairs at the sorting stage. If the difference of a given pair exceeds the *reps-value*, then the sort order of the corresponding models is reversed; otherwise, the two models retain their relative order in the rankings. Hence, the RANKEPS= option can affect model ranking in the fit summary table.

The default value for the RANKEPS= parameter is 10^{-6} and accounts for the default optimization convergence tolerance at the fitting stage prior to model ranking. The convergence tolerance itself limits the accuracy that you can use to compare two models under a given criterion. As a result, smaller values of the RANKEPS= parameter might not lead to a sensible and more strict model comparison because for a smaller *reps-value*, ranking could depend on digits beyond the accuracy limit.

In the opposite end, if the specified *reps-value* turns out to be large compared to the criterion value differences, then it can make the sorting process insensitive to the specified sorting criterion. When this happens, the fit summary table ranking reflects only the order in which different models are examined in the procedure flow. You can tell whether the criterion is bypassed; if it is, then one or more values of the specified criterion might not appear to be sorted in the fit summary table.

The RANKEPS= parameter must be a positive number. The RANKEPS= option applies when you fit multiple models with the FORM=AUTO option of the MODEL statement; otherwise, it is ignored.

SCALE=*scale* | (*scale1, . . . , scalek*)

specifies the scale parameter in semivariogram models. The SCALE= option is optional. However, if you specify the SCALE= option, then you must provide sill values for all structures that you have specified explicitly in the FORM= option. All nonmissing scale values are considered as fixed parameters. PROC VARIOGRAM assigns a default initial value to any of the model structures for which you specify a missing scale value. PROC VARIOGRAM assigns default initial values to all model structures if you omit the SCALE= option, unless you specify an associated PARMS statement with initial values for scale.

The scale parameter is a positive number. It has the same units as the variance of the variable in the VAR statement. The scale of each structure in a semivariogram model represents the variance contribution of the structure to the total model variance.

In power models the SCALE= parameter does not correspond to a sill because the power model has no sill. Instead, PROC VARIOGRAM uses the SCALE= option to designate the slope (or scaling factor) in power model forms. The power model slope has the same variance units as the variable in the VAR statement.

The SCALE= option is ignored when you specify the FORM=AUTO option. The SCALE= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

SMOOTH=*smooth* | (*smooth1, . . . , smoothm*)

specifies the positive smoothness parameter ν in the Matérn type of semivariance structures. The special case $\nu = 0.5$ is equivalent to the exponential model, whereas the theoretical limit $\nu \to \infty$ gives the Gaussian model.

The SMOOTH= option is optional. When you specify an explicit model in the FORM= option with m Matérn structures, you can provide up to m smoothness values. You can specify a value for *smoothi*, $i = 1, \ldots, m$ that is positive and no greater than 1,000,000. PROC VARIOGRAM sets this upper limit for the SMOOTH= option values for numerical and performance reasons. In any case, if the fitting process leads the smoothness value to exceed the default threshold value 10,000, then the VARIOGRAM procedure converts the Matérn form into a Gaussian form and repeats the model fitting. To adjust the switching threshold value, you can use the MTOGTOL= option in the MODEL statement.

If you specify fewer than m values, then the remaining Matérn structures have their smoothness parameters initialized to missing values. If you specify more than m values, then values in excess are ignored.

All nonmissing smoothness values are considered as fixed parameters of the corresponding Matérn structures. PROC VARIOGRAM assigns a default initial value to any of the model Matérn structures, if any, for which you specify a missing smoothness value. PROC VARIOGRAM assigns default initial values to all model Matérn structures if you omit the SMOOTH= option, unless you specify an associated PARMS statement and initial values for smoothness in it.

The SMOOTH= option is ignored when you specify the FORM=AUTO option. The SMOOTH= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

In addition to the *fitting-options*, you can specify the following *model-options* after a slash (/) in the MODEL statement.

COVB

requests the approximate covariance matrix for the parameter estimates of the model fitting. The COVB option is ignored when you also specify the DETAILS=ALL option.

When you specify an explicit model with the FORM= option in the MODEL statement, the COVB option produces the requested approximate covariance matrix. When you specify the FORM=AUTO option in the MODEL statement, by default the COVB option produces output only for the selected model, where the choice is based on the criteria that you specify in the CHOOSE= option of the MODEL statement. If you specify the DETAILS option in addition to FORM=AUTO in the MODEL statement, then the COVB option produces output for each one of the fitted models.

CORRB

requests the approximate correlation matrix for the parameter estimates of the model fitting. The CORRB option is ignored when you also specify the DETAILS=ALL option.

When you specify an explicit model with the FORM= option in the MODEL statement, the CORRB option produces the requested approximate correlation matrix. When you specify the FORM=AUTO option in the MODEL statement, by default the CORRB option produces output only for the selected model, where the choice is based on the criteria that you specify in the CHOOSE= option of the MODEL statement. If you specify the DETAILS option in addition to FORM=AUTO in the MODEL statement, then the CORRB option produces output for each one of the fitted models.

DETAILS < = *detail-level* >

requests different levels of output to be produced during the fitting process. You can specify any of the following *detail-level* arguments:

MOD

specifies that the default output for all candidate models be produced when the FORM=AUTO option is specified in the MODEL statement. If you fit only one explicit model, then the DETAILS=MOD option has no effect and is ignored.

ITR

requests that a complete iteration history be produced in addition to the default output. The output for DETAILS=ITR includes the current values of the parameter estimates, their gradients, and additional optimization statistics.

ALL

requests the most detailed level of output when fitting a model. Specifically, except for the default output, the DETAILS=ALL option produces optimization statistics in addition to the combined output of the DETAILS=ITR, COVB, and CORRB options.

When you fit multiple models with the FORM=AUTO option in the MODEL statement, only the selected model default output is produced. The model selection is based on the criteria that you specify in the CHOOSE= option of the MODEL statement. With the DETAILS option you can produce ODS tables with information about the fitting process of all the models that you fit. Moreover, you can produce output at different levels of detail that you can specify with the *detail-level* argument.

Omitting the DETAILS option or specifying the DETAILS option without any argument is equivalent to specifying DETAILS=MOD.

GRADIENT
displays the gradient of the objective function with respect to the parameter estimates in the "Parameter Estimates" table.

MTOGTOL=*number*
MTOL=*number*
specifies a threshold value for the smoothness parameter of the Matérn form. Above this threshold, a Matérn form in a model switches to the Gaussian form. The *number* value must be positive and no greater than 1,000,000, which is the smoothness upper bound set by the VARIOGRAM procedure.

By default, if the fitting process progressively increases the Matérn smoothness parameter ν without converging to a smoothness estimate, then PROC VARIOGRAM converts the Matérn form into a Gaussian form when smoothness exceeds the default value 10,000. If you specify the *number* value to be greater than the 1,000,000 boundary value, then it is ignored and reset to the default threshold value. For more details about the Matérn-to-Gaussian form conversion, see the section "Fitting with Matérn Forms" on page 10099.

NOFIT
suppresses the model fitting process.

NOITPRINT
suppresses the display of the iteration history table when you have also specified the DETAILS=ITR or DETAILS=ALL option in the MODEL statement. Otherwise, the NOITPRINT option is ignored.

PARMS Statement

PARMS (*value-list***)**. . . *< / options >* **;**

The PARMS statement specifies initial values for the semivariance parameters of a single specified model in the MODEL statement. Alternatively, the PARMS statement can request a grid search over several values of these parameters. You must specify the values by starting with the nugget effect parameter. You continue in the order in which semivariogram forms are specified in the FORM= option of the MODEL statement by specifying for each structure the values for its scale, range, and any other parameters as applicable.

The PARMS statement is optional and must follow the associated MODEL statement.

The *value-list* specification can take any of several forms:

m	a single value
$m_1, m_2, \ldots, m_n$	several values
m to n	a sequence in which m equals the starting value, n equals the ending value, and the increment equals 1
m to n by i	a sequence in which m equals the starting value, n equals the ending value, and the increment equals i
m_1, m_2 to m_3	mixed values and sequences

You can use the PARMS statement to input fixed values for parameters and also initial values that you want to optimize.

Suppose that you want to fit a semivariogram model with a Matérn component of scale 3, range 20, smoothing parameter 4.5, and an exponential component of unspecified scale and range 15. Assume that you also want to fix all the specified parameter values for the optimization. Including the nugget effect, you have a model with six parameters.

In terms of the PARMS statement, your specifications mean that you have initial values for the second, third, fourth, and sixth parameter in the parameter list. Also, the same specifications imply that you provide no initial values for the first parameter (which corresponds to the nugget effect) and the fifth parameter (which corresponds to the exponential model scale). For these parameters you prefer that PROC VARIOGRAM selects initial values, instead. Since you must specify values for all model parameters in the PARMS statement, you simply specify missing values for the first and fifth parameter. This is the way to request that PROC VARIOGRAM assigns default initial values to parameters. The SAS statements to implement these specifications are as follows:

```
proc variogram data=FirstData;
   < other VARIOGRAM statements >
   model form=(mat,exp);
   parms (.) (3) (20) (4.5) (.) (15) / hold=(2 to 4,6);
run;
```

NOTE: The preceding statements are equivalent to the following ones in which the PARMS statement is omitted:

```
proc variogram data=FirstData;
   < other VARIOGRAM statements >
   model form=(mat,exp) scale=(3,.) range(20,15) smooth=4.5;
run;
```

This example might suggest that you can always use either the PARMS or the MODEL statement to specify the same fitting parameters in the VARIOGRAM procedure. However, the PARMS statement gives you more flexibility in two ways:

- You can set non-default initial parameter values by using the PARMS statement, whereas in the MODEL statement you can request default initial values only by setting parameters to missing values. For this reason the PARMS statement cannot be specified when the FORM=AUTO option is specified in the associated MODEL statement. As an example, the following statements do not have an equivalent without using the PARMS statement, because the first parameter in the PARMS statement list (which corresponds to the NUGGET parameter) is set to the specific initial value of 2.1 and the fifth parameter (which corresponds to the exponential structure scale) is set to the specific initial value of 0.3.

  ```
  proc variogram data=FirstData;
     < other VARIOGRAM statements >
     model form=(mat,exp);
     parms (2.1) (3) (20) (4.5) (0.3) (15) / hold=(2 to 4,6);
  run;
  ```

- In the MODEL statement all the nonmissing parameter values that you specify remain fixed. Instead, the PARMS statement considers all values in the specified parameter sets to be subjected to optimization

unless you force values to be fixed with the HOLD= option. In the previous example, you can specify that you want to optimize all of your parameters by skipping the HOLD= option as shown in the following modified statements:

```
proc variogram data=FirstData;
   < other VARIOGRAM statements >
   model form=(mat,exp);
   parms (2.1) (3) (20) (4.5) (1) (15);
run;
```

When you omit the PARMS statement list and the PDATA= data set in a PARMS statement, the specification is equivalent to a PARMS statement list where all the parameters have missing initial values. However, if you specify no other option in the PARMS statement, then the PARMS statement is ignored.

In order to avoid ambiguity, you cannot specify the PARMS statement if any of the scale, range, nugget, or smoothness parameters has been specified in the associated MODEL statement either explicitly or in the MDATA= data set. This condition is in effect even when you specify an empty PARMS statement.

If you specify more than one set of initial values, a grid of initial values sets is created. PROC VARIOGRAM seeks among the specified sets for the one that gives the lowest objective function value. Then, the procedure uses the initial values in the selected set for the fitting optimization.

The results from the PARMS statement are the values of the parameters on the specified grid. The ODS name of the "Parameter Search" table is ParmSearch.

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

HOLD=*value-list*

EQCONS=*value-list*

specifies which parameter values be constrained to equal the specified values. For example, the following statement constrains the first and third semivariance parameters to equal 0.5 and 12, respectively. The fourth parameter is fixed to the default initial value that is assigned to it by PROC VARIOGRAM.

```
parms (0.5) (3) (12) (.) / hold=1,3,4;
```

The HOLD= option accepts only nonmissing values in its list. If you specify more than the available parameters in the HOLD= option list, then the ones in excess are ignored. If the HOLD= option list has integer values that do not correspond to variables in the PARMS list, then they are also ignored. Noninteger values are rounded to the closest integer and evaluated accordingly.

When you specify more than one set of parameter initial values, the HOLD= option list applies to the set that gives the lowest objective function value before this set is sent to the optimizer for the fitting.

LOWERB=*value-list*

specifies lower boundary constraints on the semivariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC VARIOGRAM uses for the semivariance parameters, and each number corresponds to the lower boundary constraint. A missing value instructs PROC VARIOGRAM to use its default constraint.

If you do not specify lower bounds for all of the semivariance parameters, then PROC VARIOGRAM assumes that the remaining parameters are not bounded. If you specify more lower bounds in the

value-list than the available parameters, then the numbers in excess are ignored. If you specify lower bounds for parameters with missing initial values, then the VARIOGRAM procedure enforces the specified bounds in the fitting process. By default, the lower bound for all parameters is zero.

When you specify the HOLD= option together with the LOWERB= option, the lower bounds in the LOWERB= option *value-list* that correspond to fixed parameters are ignored. When you specify the NOBOUND option together with the LOWERB= option, the LOWERB= option is ignored.

MAXSCALE=*maxscale*

specifies a positive upper threshold for the fitted semivariogram sill. This option imposes a linear constraint on the optimization of the nonfixed semivariogram scale and nugget parameters so that the sum of all scale and nugget parameters does not exceed the specified MAXSCALE= value. The MAXSCALE= constraint is ignored if all the semivariogram scale and nugget parameters are fixed.

NOBOUND

requests the removal of boundary constraints on semivariance parameters. For example, semivariance parameters have a default zero lower boundary constraint since they have a physical meaning only for positive values. The NOBOUND option enables the fitting process to derive negative estimates; hence, you need to be cautious with the outcome when you specify this option.

The NOBOUND option has no effect on the power model exponent parameter. The exponent must range within [0,2) so that the model is a valid semivariance function. Also, the NOBOUND option has no effect on the Matérn smoothness parameter. The options LOWERB= and UPPERB= are ignored if either of them is specified together with the NOBOUND option in the PARMS statement.

PARMSDATA=*SAS-data-set*

PDATA=*SAS-data-set*

specifies that semivariance parameters values be read from a SAS data set. The data set should contain the values in the sequence required by the PARMS statement in either of the following two ways:

- Specify one single column under the variable Estimate (or Est) that contains all the parameter values.
- Use one column for each parameter, and place the *n* columns under the Parm1–Parm*n* variables.

For example, the following two data sets are valid and equivalent ways to specify initial values for the nugget effect and the parameters of the Matérn and exponential structures that have been used in the previous examples in the PARMS statement section:

```
data parData1;
   input Estimate @@;
   datalines;
. 3 20 4.5 . 15
;


data parData2;
   input Parm1 Parm2 Parm3 Parm4 Parm5 Parm6;
   datalines;
. 3 20 4.5 . 15
;
```

If you have the parData1 data set, then you can import this information into the PARMS statement as follows:

```
proc variogram data=FirstData;
   < other VARIOGRAM statements >
   model form=(mat,exp);
   parms / pdata=parData1 hold=(2 to 4,6);
run;
```

You can specify more than one set of initial values in the PDATA= data set by following the preceding guidelines. PROC VARIOGRAM seeks among the specified sets for the one that gives the lowest objective function value. Then, the procedure uses the initial values in the selected set for the fitting optimization.

You can explicitly specify initial parameter values in the PARMS statement or use the PDATA= option, but you cannot use both at the same time.

UPPERB=*value-list*

specifies upper boundary constraints on the semivariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC VARIOGRAM uses for the semivariance parameters, and each number corresponds to the upper boundary constraint. A missing value instructs PROC VARIOGRAM to use its default constraint.

If you do not specify upper bounds for all of the semivariance parameters, then PROC VARIOGRAM assumes that the remaining parameters are not bounded. If you specify more upper bounds in the *value-list* than the available parameters, then the numbers in excess are ignored. If you specify upper bounds for parameters with missing initial values, then the VARIOGRAM procedure enforces the specified bounds in the fitting process. By default, the scale, range, nugget, and Matérn smoothness parameters have no upper bounds, whereas the power model exponent parameter is lower than two.

When you specify the HOLD= option together with the UPPERB= option, the upper bounds in the UPPERB= option *value-list* that correspond to fixed parameters are ignored. When you specify the NOBOUND option together with the UPPERB= option, the UPPERB= option is ignored.

NLOPTIONS Statement

NLOPTIONS < *options* > **;**

By default, PROC VARIOGRAM uses the technique TECH=NRRIDG, which corresponds to Newton-Raphson optimization with ridging. For more information about the NLOPTIONS, see the section "NLOPTIONS Statement" on page 489 in Chapter 19, "Shared Concepts and Topics."

STORE Statement

STORE OUT=*store-name* < / *option* > **;**

The STORE statement requests that the procedure save the context and results of the semivariogram model fitting analysis in an item store. An item store is a binary file defined by the SAS System. You cannot modify

the contents of an item store. The contents of item stores produced by PROC VARIOGRAM can be processed only with the KRIGE2D or the SIM2D procedure. After you save results in an item store, you can use them at a later time without having to fit the model again.

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*. If an item store by the same name as specified in the STORE statement already exists, the existing store is replaced.

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

LABEL=*store-label*
specifies a custom label for the item store that is produced by PROC VARIOGRAM. When another procedure processes an item store, the label appears in the procedure's output along with other identifying information.

VAR Statement

VAR *analysis-variables-list* **;**

Use the VAR statement to specify the analysis variables. You can specify only numeric variables. If you omit the VAR statement, all numeric variables in the DATA= data set that are not in the COORDINATES statement are used.

Details: VARIOGRAM Procedure

Theoretical Semivariogram Models

The VARIOGRAM procedure computes the empirical (also known as *sample* or *experimental*) semivariogram from a set of point measurements. Semivariograms are used in the first steps of spatial prediction as tools that provide insight into the spatial continuity and structure of a random process. Naturally occurring randomness is accounted for by describing a process in terms of the *spatial random field* (SRF) concept (Christakos 1992). An SRF is a collection of random variables throughout your spatial domain of prediction. For some of them you already have measurements, and your data set constitutes part of a single realization of this SRF. Based on your sample, spatial prediction aims to provide you with values of the SRF at locations where no measurements are available.

Prediction of the SRF values at unsampled locations by techniques such as ordinary kriging requires the use of a theoretical semivariogram or covariance model. Due to the randomness involved in stochastic processes, the theoretical semivariance cannot be computed. Instead, it is possible that the empirical semivariance can provide an estimate of the theoretical semivariance, which then characterizes the spatial structure of the process.

The VARIOGRAM procedure follows a general flow of investigation that leads you from a set of spatial observations to an expression of theoretical semivariance to characterize the SRF continuity. Specifically,

the empirical semivariogram is computed after a suitable choice is made for the LAGDISTANCE= and MAXLAGS= options. For computations in more than one direction you can further use the NDIRECTIONS= option or the DIRECTIONS statement. Potential theoretical models (which can also incorporate nesting, anisotropy, and the nugget effect) can be fitted to the empirical semivariance by using the MODEL statement, and then plotted against the empirical semivariogram. The flow of this analytical process is illustrated in Figure 124.17. After a suitable theoretical model is determined, it is used in PROC KRIGE2D for the prediction stage. The prediction analysis is presented in detail in the section "Details of Ordinary Kriging" on page 5047 in Chapter 68, "The KRIGE2D Procedure."

Figure 124.17 Flowchart for Semivariogram Selection

It is critical to note that the empirical semivariance provides an estimate of its theoretical counterpart only when the SRF satisfies stationarity conditions. These conditions imply that the SRF has a constant (or zero) expected value. Consequently, your data need to be sampled from a trend-free random field and need to have a constant mean, as assumed in "Getting Started: VARIOGRAM Procedure" on page 10027. Equivalently, your data could be residuals of an initial sample that has had a surface trend removed, as portrayed in "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122. For a closer look at stationarity, see the section "Stationarity" on page 10079. For details about different stationarity types and conditions see, for example, Chilès and Delfiner (1999, section 1.1.4).

Characteristics of Semivariogram Models

When you obtain a valid empirical estimate of the theoretical semivariance, it is then necessary to choose a type of theoretical semivariogram model based on that estimate. Commonly used theoretical semivariogram

shapes rise monotonically as a function of distance. The shape is typically characterized in terms of particular parameters; these are the *range* a_0, the *sill* (or *scale*) c_0, and the *nugget effect* c_n. Figure 124.18 displays a theoretical semivariogram of a spherical semivariance model and points out the semivariogram characteristics.

Figure 124.18 A Theoretical Semivariogram of Spherical Type and Its Characteristics

Specifically, the sill is the semivariogram upper bound. The range a_0 denotes the distance at which the semivariogram reaches the sill. When the semivariogram increases asymptotically toward its sill value, as occurs in the exponential and Gaussian semivariogram models, the term *effective* (or *practical*) range is also used. The effective range r_ϵ is defined as the distance at which the semivariance value achieves 95% of the sill. In particular, for these models the relationship between the range and effective range is $r_\epsilon = 3a_0$ (exponential model) and $r_\epsilon = \sqrt{3}a_0$ (Gaussian model).

The nugget effect c_n represents a discontinuity of the semivariogram that can be present at the origin. It is typically attributed to microscale effects or measurement errors. The semivariance is always 0 at distance $\boldsymbol{h} = 0$; hence, the nugget effect demonstrates itself as a jump in the semivariance as soon as $\boldsymbol{h} > 0$ (note in Figure 124.18 the discontinuity of the function at $\boldsymbol{h} = 0$ in the presence of a nugget effect).

The sill c_0 consists of the nugget effect, if present, and the *partial sill* ${\sigma_0}^2$; that is, $c_0 = c_n + {\sigma_0}^2$. If the SRF $Z(\boldsymbol{s})$ is second-order stationary (see the section "Stationarity" on page 10079), the estimate of the sill is an estimate of the constant variance $\mathrm{Var}[Z(\boldsymbol{s})]$ of the field. Nonstationary processes have variances that depend on the location $\boldsymbol{s}$. Their semivariance increases with distance; hence their semivariograms have no sill.

Not every function is a suitable candidate for a theoretical semivariogram model. The semivariance function $\gamma_z(\boldsymbol{h})$, as defined in the following section, is a so-called *conditionally negative-definite* function that satisfies (Cressie 1993, p. 60)

$$\sum_{i=1}^{m}\sum_{j=i}^{m} q_i q_j \gamma_z(\boldsymbol{s}_i - \boldsymbol{s}_j) \le 0$$

for any number m of locations $\boldsymbol{s}_i, \boldsymbol{s}_j$ in $\mathcal{R}^2$ with $\boldsymbol{h} = \boldsymbol{s}_i - \boldsymbol{s}_j$, and any real numbers q_i such that $\sum_{i=1}^{m} q_i = 0$. PROC VARIOGRAM can use a variety of permissible theoretical semivariogram models. Specifically, Table 124.4 shows a list of such models that you can use for fitting in the MODEL statement of the VARIOGRAM procedure.

Table 124.4 Permissible Theoretical Semivariogram Models ($a_0 > 0$, unless noted otherwise)

Model Type	Semivariance
Exponential	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[1 - \exp\left(-\frac{\lvert \boldsymbol{h} \rvert}{a_0}\right)\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Gaussian	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[1 - \exp\left(-\frac{\lvert \boldsymbol{h} \rvert^2}{a_0^2}\right)\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Power	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \boldsymbol{h}^{a_0} & \text{if } 0 < \lvert \boldsymbol{h} \rvert, 0 \le a_0 < 2 \end{cases}$
Spherical	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[\frac{3}{2}\frac{\lvert \boldsymbol{h} \rvert}{a_0} - \frac{1}{2}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^3\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \le a_0 \\ c_0 & \text{if } a_0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Cubic	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[7(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^2 - \frac{35}{4}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^3 + \frac{7}{2}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^5 - \frac{3}{4}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^7\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \le a_0 \\ c_0 & \text{if } a_0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Pentaspherical	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[\frac{15}{8}\frac{\lvert \boldsymbol{h} \rvert}{a_0} - \frac{5}{4}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^3 + \frac{3}{8}(\frac{\lvert \boldsymbol{h} \rvert}{a_0})^5\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \le a_0 \\ c_0 & \text{if } a_0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Sine hole effect	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[1 - \frac{\sin(\pi \lvert \boldsymbol{h} \rvert / a_0)}{\pi \lvert \boldsymbol{h} \rvert / a_0}\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert \end{cases}$
Matérn class	$\gamma_z(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \lvert \boldsymbol{h} \rvert = 0 \\ c_n + {\sigma_0}^2 \left[1 - \frac{2}{\Gamma(\nu)} \left(\frac{\lvert \boldsymbol{h} \rvert \sqrt{\nu}}{a_0}\right)^{\nu} K_{\nu}\left(2\frac{\lvert \boldsymbol{h} \rvert \sqrt{\nu}}{a_0}\right)\right] & \text{if } 0 < \lvert \boldsymbol{h} \rvert, \nu > 0 \end{cases}$

All of these models, except for the power model, are transitive. A transitive model characterizes a random process whose variation reaches the sill value c_0 within a specific range from any location in the field.

The power model is nontransitive and applies to processes whose variance increases with distance. It has no scale and range; instead, it quantifies the process variation by using a positive slope parameter and a dimensionless power exponent α that indicate how fast the variance increases. The expression for the power model is a valid semivariogram only when the exponent parameter ranges within $0 \le \alpha < 2$. For convenience, PROC VARIOGRAM registers the power model slope parameter under the SCALE= option parameters in the MODEL statement. For the same reason, the scale and power slope parameters are represented with the common symbol ${\sigma_0}^2$ in Table 124.4. Also for convenience, PROC VARIOGRAM registers the power model

exponent parameter under the RANGE= option parameters. The range and the power exponent parameters are represented with the common symbol a_0 in Table 124.4.

The power model is a generalized case of the linear model, which is not included explicitly in the model set of PROC VARIOGRAM. The linear model is derived from the power model when you specify the exponent $\alpha = 1$.

Among the models displayed in Table 124.4, the Matérn (or K-Bessel) class is a class of semivariance models that distinguish from each other by means of the positive smoothing parameter ν. Different values of ν correspond to different correlation models. Most notably, for $\nu = 0.5$ the Matérn semivariance is equivalent to the exponential model, whereas $\nu \to \infty$ gives the Gaussian model. Also, Table 124.4 shows that the Matérn semivariance computations use the gamma function $\Gamma(\nu)$ and the second kind Bessel function K_ν.

In PROC VARIOGRAM, you can input the model parameter values either explicitly as arguments of options, or as lists of values. In the latter case, you are expected to provide the values in the order the models are specified in the SAS statements, and furthermore in the sequential order of the scale, range, and smoothing parameter for each model as appropriate, and always starting with the nugget effect. If the parameter values are specified through an input file, then the total of n parameters should be provided either as one variable named Estimate or as many variables with the respective names Parm1–Parm$n$.

You can review in further detail the models shown in Table 124.4 in the section "Theoretical Semivariogram Models" on page 5031 in Chapter 68, "The KRIGE2D Procedure."

The theoretical semivariogram models are used to describe the spatial structure of random processes. Based on their shape and characteristics, the semivariograms of these models can provide a plethora of information (Christakos 1992, section 7.3):

- Examination of the semivariogram variation in different directions provides information about the isotropy of the random process. (See also the discussion about isotropy in the following section.)
- The semivariogram range determines the zone of influence that extends from any given location. Values at surrounding locations within this zone are correlated with the value at the specific location by means of the particular semivariogram.
- The semivariogram behavior at large distances indicates the degree of stationarity of the process. In particular, an asymptotic behavior suggests a stationary process, whereas either a linear increase and slow convergence to the sill or a fast increase is an indicator of nonstationarity.
- The semivariogram behavior close to the origin indicates the degree of regularity of the process variation. Specifically, a parabolic behavior at the origin implies a very regular spatial variation, whereas a linear behavior characterizes a nonsmooth process. The presence of a nugget effect is additional evidence of irregularity in the process.
- The semivariogram behavior within the range provides description of potential periodicities or anomalies in the spatial process.

A brief note on terminology: In some fields (for example, geostatistics) the term homogeneity is sometimes used instead of stationarity in spatial analysis; however, in statistics homogeneity is defined differently (Banerjee, Carlin, and Gelfand 2004, section 2.1.3). In particular, the alternative terminology characterizes as homogeneous the stationary SRF in $\mathcal{R}^n, n > 1$, whereas it retains the term stationary for such SRF in $\mathcal{R}^1$ (SRF in $\mathcal{R}^1$ are also known as *random processes*). Often, studies in a single dimension refer to

temporal processes; hence, you might see time-stationary random processes called "temporally stationary" or simply stationary, and stationary SRF in $\mathcal{R}^n, n > 1$, characterized as "spatially homogeneous" or simply homogeneous. This distinction made by the alternative nomenclature is more evident in spatiotemporal random fields (S/TRF), where the different terms clarify whether stationarity applies in the spatial or the temporal part of the S/TRF.

Nested Models

When you try to represent an empirical semivariogram by fitting a theoretical model, you might find that using a combination of theoretical models results in a more accurate fit onto the empirical semivariance than using a single model. This is known as model nesting. The semivariance models that result as the sum of two or more semivariance structures are called *nested* models.

In general, a linear combination of permissible semivariance models produces a new permissible semivariance model. Nested models are based on this premise. You can include in a sum any combination of the models presented in Table 124.4. For example, a nested semivariance $\gamma_z(\boldsymbol{h})$ that contains two structures, one exponential $\gamma_{z,\mathrm{EXP}}(\boldsymbol{h})$ and one spherical $\gamma_{z,\mathrm{SPH}}(\boldsymbol{h})$, can be expressed as

$$\gamma_z(\boldsymbol{h}) = \gamma_{z,\mathrm{EXP}}(\boldsymbol{h}) + \gamma_{z,\mathrm{SPH}}(\boldsymbol{h})$$

If you have a nested model and a nugget effect, then the nugget effect c_n is a single parameter that is considered jointly for all the nested structures.

Nested models, anisotropic models, and the nugget effect increase the scope of theoretical models available. You can find additional discussion about these concepts in the section "Theoretical Semivariogram Models" on page 5031 in Chapter 68, "The KRIGE2D Procedure."

Theoretical and Computational Details of the Semivariogram

Let $\{Z(\boldsymbol{s}), \boldsymbol{s} \in D \subset \mathcal{R}^2\}$ be a spatial random field (SRF) with n measured values $z_i = Z(\boldsymbol{s}_i)$ at respective locations $\boldsymbol{s}_i, i = 1, \ldots, n$. You use the VARIOGRAM procedure because you want to gain insight into the spatial continuity and structure of $Z(\boldsymbol{s})$. A good measure of the spatial continuity of $Z(\boldsymbol{s})$ is defined by means of the variance of the difference $Z(\boldsymbol{s}_i) - Z(\boldsymbol{s}_j)$, where $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ are locations in D. Specifically, if you consider $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ to be spatial increments such that $\boldsymbol{h} = \boldsymbol{s}_j - \boldsymbol{s}_i$, then the variance function based on the increments $\boldsymbol{h}$ is independent of the actual locations $\boldsymbol{s}_i, \boldsymbol{s}_j$. Most commonly, the continuity measure used in practice is one half of this variance, better known as the *semivariance* function,

$$\gamma_z(\boldsymbol{h}) = \frac{1}{2}\mathrm{Var}[Z(\boldsymbol{s} + \boldsymbol{h}) - Z(\boldsymbol{s})]$$

or, equivalently,

$$\gamma_z(\boldsymbol{h}) = \frac{1}{2}\left(\mathrm{E}\{[Z(\boldsymbol{s} + \boldsymbol{h}) - Z(\boldsymbol{s})]^2\} - \{\mathrm{E}[Z(\boldsymbol{s} + \boldsymbol{h})] - \mathrm{E}[Z(\boldsymbol{s})]\}^2\right)$$

The plot of semivariance as a function of $\boldsymbol{h}$ is the *semivariogram*. You might also commonly see the term *semivariogram* used instead of the term *semivariance*.

Assume that the SRF $Z(\boldsymbol{s})$ is free of nonrandom (or systematic) surface trends. Then, the expected value $\mathrm{E}[Z(\boldsymbol{s})]$ of $Z(\boldsymbol{s})$ is a constant for all $\boldsymbol{s} \in \mathcal{R}^2$, and the semivariance expression is simplified to the following:

$$\gamma_z(\boldsymbol{h}) = \frac{1}{2}\mathrm{E}\{[Z(\boldsymbol{s}+\boldsymbol{h}) - Z(\boldsymbol{s})]^2\}$$

Given the preceding assumption, you can compute an estimate $\hat{\gamma}_z(\boldsymbol{h})$ of the semivariance $\gamma_z(\boldsymbol{h})$ from a finite set of points in a practical way by using the formula

$$\hat{\gamma}_z(\boldsymbol{h}) = \frac{1}{2 \mid N(\boldsymbol{h}) \mid} \sum_{N(\boldsymbol{h})} [Z(\boldsymbol{s}_i) - Z(\boldsymbol{s}_j)]^2$$

where the sets $N(\boldsymbol{h})$ contain all the neighboring pairs at distance $\boldsymbol{h}$,

$$N(\boldsymbol{h}) = \{i, j : \boldsymbol{s}_i - \boldsymbol{s}_j = \boldsymbol{h}\}$$

and $\mid N(\boldsymbol{h}) \mid$ is the number of such pairs (i, j).

The expression for $\hat{\gamma}_z(\boldsymbol{h})$ is called the *empirical semivariance* (Matheron 1963). This is the quantity that PROC VARIOGRAM computes, and its corresponding plot is the *empirical semivariogram*.

The empirical semivariance $\hat{\gamma}_z(\boldsymbol{h})$ is also referred to as *classical*. This name is used so that it can be distinguished from the *robust semivariance* estimate $\bar{\gamma}_z(\boldsymbol{h})$ and the corresponding *robust semivariogram*. The robust semivariance was introduced by Cressie and Hawkins (1980) to weaken the effect that outliers in the observations might have on the semivariance. It is described by Cressie (1993, p. 75) as

$$\bar{\gamma}_z(\boldsymbol{h}) = \frac{\Psi^4(\boldsymbol{h})}{2[0.457 + 0.494/N(\boldsymbol{h})]}$$

In the preceding expression the parameter $\Psi(\boldsymbol{h})$ is defined as

$$\Psi(\boldsymbol{h}) = \frac{1}{N(\boldsymbol{h})} \sum_{P_i P_j \in N(\boldsymbol{h})} [Z(\boldsymbol{s}_i) - Z(\boldsymbol{s}_j)]^{\frac{1}{2}}$$

According to Cressie (1985), the estimate $\hat{\gamma}_z(\boldsymbol{h})$ has approximate variance

$$\mathrm{Var}[\hat{\gamma}_z(\boldsymbol{h})] \simeq \frac{2[\gamma_z(\boldsymbol{h})]^2}{N(\boldsymbol{h})}$$

This approximation is possible by assuming $Z(\boldsymbol{s})$ to be a Gaussian SRF, and by further assuming the squared differences in empirical semivariances to be uncorrelated for different distances $\boldsymbol{h}$. Typically, semivariance estimates are correlated because of the underlying spatial correlation among the observations, and also because the same observation pairs might be used for the estimation of more than one semivariogram point, as described in the following subsections. Despite these restrictive assumptions, the approximate variance provides an idea about the semivariance estimate variance and enables fitting of a theoretical model to the empirical semivariance; see the section "Theoretical Semivariogram Model Fitting" on page 10092 for more details about the fitting process.

NOTE: If your data include a surface trend, then the empirical semivariance $\hat{\gamma}_z(\boldsymbol{h})$ is not an estimate of the theoretical semivariance function $\gamma_z(\boldsymbol{h})$. Instead, rather than the spatial increments variance, it represents a

different quantity known as *pseudo-semivariance*, and its corresponding plot is a *pseudo-semivariogram*. In principle, pseudo-semivariograms do not provide measures of the spatial continuity. They can thus lead to misinterpretations of the $Z(\boldsymbol{s})$ spatial structure, and are consequently unsuitable for the purpose of spatial prediction. For further information, see the detailed discussion in the section "Empirical Semivariograms and Surface Trends" on page 10091. Under certain conditions you might be able to gain some insight about the spatial continuity with a pseudo-semivariogram. This case is presented in "Example 124.3: Analysis without Surface Trend Removal" on page 10136.

Stationarity

In the combined presence of the previous two assumptions—that is, when $\mathrm{E}[Z(\boldsymbol{s})]$ is constant and spatial increments define $\gamma_z(\boldsymbol{h})$—the SRF $Z(\boldsymbol{s})$ is characterized as *intrinsically stationary* (Cressie 1993, p. 40).

The expected value $\mathrm{E}[Z(\boldsymbol{s})]$ is the first statistical moment of the SRF $Z(\boldsymbol{s})$. The second statistical moment of the SRF $Z(\boldsymbol{s})$ is the *covariance* function between two points $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ in $Z(\boldsymbol{s})$, and it is defined as

$$C_z(\boldsymbol{s}_i, \boldsymbol{s}_j) = \mathrm{E}\left([Z(\boldsymbol{s}_i) - \mathrm{E}[Z(\boldsymbol{s}_i)]]\left[Z(\boldsymbol{s}_j) - \mathrm{E}[Z(\boldsymbol{s}_j)]\right]\right)$$

When $\boldsymbol{s}_i = \boldsymbol{s}_j = \boldsymbol{s}$, the covariance expression provides the variance at $\boldsymbol{s}$.

The assumption of a constant $\mathrm{E}[Z(\boldsymbol{s})] = m$ means that the expected value is invariant with respect to translations of the spatial location $\boldsymbol{s}$. The covariance is considered invariant to such translations when it depends only on the distance $\boldsymbol{h} = \boldsymbol{s}_i - \boldsymbol{s}_j$ between any two points $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$. If both of these conditions are true, then the preceding expression becomes

$$C_z(\boldsymbol{s}_i, \boldsymbol{s}_j) = C_z(\boldsymbol{s}_i - \boldsymbol{s}_j) = C_z(\boldsymbol{h}) = \mathrm{E}\left([Z(\boldsymbol{s}) - m][Z(\boldsymbol{s} + \boldsymbol{h}) - m]\right)$$

When both $\mathrm{E}[Z(\boldsymbol{s})]$ and $C(\boldsymbol{s}_i, \boldsymbol{s}_j)$ are invariant to spatial translations, the SRF $Z(\boldsymbol{s})$ is characterized as *second-order stationary* (Cressie 1993, p. 53).

In a second-order stationary SRF the quantity $C(\boldsymbol{h})$ is the same for any two points that are separated by distance $\boldsymbol{h}$. Based on the preceding formula, for $\boldsymbol{h} = 0$ you can see that the variance is constant throughout a second-order stationary SRF. Hence, second-order stationarity is a stricter condition than intrinsic stationarity.

Under the assumption of second-order stationarity, the semivariance definition at the beginning of this section leads to the conclusion that

$$\gamma_z(\boldsymbol{h}) = C(\boldsymbol{0}) - C(\boldsymbol{h})$$

which relates the theoretical semivariance and covariance. Keep in mind that the empirical estimates of these quantities are not related in exactly the same way, as indicated in Schabenberger and Gotway (2005, section 4.2.1).

Ergodicity

In addition to the constant $\mathrm{E}[Z(\boldsymbol{s})]$ and the assumption of intrinsic stationarity, *ergodicity* is a necessary third hypothesis to estimate the empirical semivariance. Assume that for the SRF $Z(\boldsymbol{s})$ you have measurements z_i whose sample mean is estimated by $\bar{Z}$. The hypothesis of ergodicity dictates that $\bar{Z} = \mathrm{E}[Z(\boldsymbol{s})]$.

In general, an SRF $Z(\boldsymbol{s})$ is characterized as ergodic if the statistical moments of its realizations coincide with the corresponding ones of the SRF. In spatial analysis you are often interested in the first two statistical

moments, and consequently a more relaxed ergodicity assumption is made only for them. See Christakos (1992, section 2.12) for the use of the ergodicity hypothesis in SRF, and Cressie (1993, p. 57) for a more detailed discussion of ergodicity.

The semivariogram analysis makes implicit use of the ergodicity hypothesis. The VARIOGRAM procedure works with the residual centered values $V(\boldsymbol{s}_i) = v_i = z_i - \bar{Z}$, $i = 1, \ldots, n$, where it is assumed that the sample mean $\bar{Z}$ is the constant expected value $\mathrm{E}[Z(\boldsymbol{s})]$ of $Z(\boldsymbol{s})$. This is equivalent to using the original values, since $V(\boldsymbol{s}_i) - V(\boldsymbol{s}_j) = Z(\boldsymbol{s}_i) - Z(\boldsymbol{s}_j)$, which shows the property of the semivariance to filter out the mean. See the section "Semivariance Computation" on page 10090 for the exact expressions PROC VARIOGRAM uses to compute the empirical classical $\hat{\gamma}_z(\boldsymbol{h})$ and robust $\bar{\gamma}_z(\boldsymbol{h})$ semivariances.

Anisotropy

Semivariance is defined on the basis of the spatial increment vector $\boldsymbol{h}$. If the variance characteristics of $Z(\boldsymbol{s})$ are independent of the spatial direction, then $Z(\boldsymbol{s})$ is called *isotropic*; if not, then $Z(\boldsymbol{s})$ is called *anisotropic*. In the case of isotropy, the semivariogram depends only on the length h of $\boldsymbol{h}$ and $\gamma_z(\boldsymbol{h}) = \gamma_z(h)$. Anisotropy is characterized as *geometric*, when the range a_0 of the semivariogram varies in different directions, and *zonal*, when the semivariogram sill c_0 depends on the spatial direction. Either type or both types of anisotropy can be present.

In the more general case, an SRF can be anisotropic. For an accurate characterization of the spatial structure it is necessary to perform individual analyses in multiple directions. Goovaerts (1997, p. 98) suggests an initial investigation in at least one direction more than the working spatial dimensions—for example, at least three different directions in $\mathcal{R}^2$. Olea (2006) supports exploring as many directions as possible when the data set allows.

You might not know in advance whether you have anisotropy or not. If the semivariogram characteristics remain unchanged in different directions, then you assume the SRF is isotropic. If your directional analysis reveals anisotropic behavior in particular directions, then you proceed to focus your analysis on these directions. For example, in an anisotropic SRF in $\mathcal{R}^2$ you should expect to find two distinct directions where you observe the *major axis* and the *minor axis* of anisotropy. Typically, these two directions are perpendicular, although they might be at other than right angles when zonal anisotropy is present.

If you can distinguish a maximum and a minimum sill in different directions, then you have a case of zonal anisotropy. The SRF exhibits strongest continuity in the direction of the lowest sill, which is the direction of the major anisotropy axis. If the sill does not change across directions, then the major axis direction of strongest continuity is the one in which the semivariogram has maximum range. See "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122 for a detailed demonstration of a case with anisotropy when you use PROC VARIOGRAM.

You can find additional information about anisotropy analysis in the section "Anisotropic Models" on page 5040 in Chapter 68, "The KRIGE2D Procedure."

Pair Formation

The basic starting point in computing the empirical semivariance is the enumeration of pairs of points for the spatial data. Figure 124.19 shows the spatial domain D and the set of n measurements z_i, $i = 1, \ldots, n$, that have been sampled at the indicated locations in D. Two data points P_1 and P_2, with coordinates $\boldsymbol{s}_1 = (x_1, y_1)$ and $\boldsymbol{s}_2 = (x_2, y_2)$, respectively, are selected for illustration.

A vector, or directed line segment, is drawn between these points. If the length

$$| P_i P_j | = | \boldsymbol{s}_2 - \boldsymbol{s}_1 | = (x_2 - x_1)^2 + (y_2 - y_1)^2$$

of this vector is smaller than the specified DEPSILON= value, then the pair is excluded from the continuity measure calculations because the two points P_1 and P_2 are considered to be at zero distance apart (or *collocated*). Spatial collocation might appear due to different scales in sampling, observations made at the same spatial location at different time instances, and errors in the data sets. PROC VARIOGRAM excludes such pairs from the pairwise distance and semivariance computations because they can cause numeric problems in spatial analysis.

If this pair is not discarded on the basis of collocation, it is then classified—first by orientation of the directed line segment $\boldsymbol{s}_2 - \boldsymbol{s}_1$, and then by its length $| P_i P_j |$. For example, it is unlikely for actual data that the distance $| P_i P_j |$ between any pair of data points P_i and P_j located at $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$, respectively, would exactly satisfy $| P_i P_j | = | \boldsymbol{h} | = h$ in the preceding computation of $\hat{\gamma}_z(\boldsymbol{h})$. A similar argument can be made for the orientation of the segment $\boldsymbol{s}_2 - \boldsymbol{s}_1$. Consequently, the pair $P_1 P_2$ is placed into an angle and distance class.

The following subsections give more details about the nature of these classifications. You can also find extensive discussions about the size and the number of classes to consider for the computation of the empirical semivariogram.

Figure 124.19 Selection of Points P_1 and P_2 in Spatial Domain D

Angle Classification

Suppose you specify NDIRECTIONS=3 in the COMPUTE statement in PROC VARIOGRAM. This results in three angle classes defined by midpoint angles between 0° and 180°: $0° \pm \delta\theta$, $60° \pm \delta\theta$, and $120° \pm \delta\theta$, where $\delta\theta$ is the angle tolerance. If you do not specify an angle tolerance by using the ANGLETOLERANCE= option in the COMPUTE statement, the following default value is used:

$$\delta\theta = \frac{180°}{2 \times \mathrm{NDIR}}$$

For example, if NDIRECTIONS=3, the default angle tolerance is $\delta\theta = 30°$. When the directed line segment $P_1 P_2$ in Figure 124.19 is superimposed on the coordinate system that shows the angle classes, its angle is approximately 45°, measured clockwise from north. In particular, it falls within $[60° - \delta\theta, 60° + \delta\theta) = [30°, 90°)$, the second angle class (Figure 124.20).

NOTE: If the designated points P_1 and P_2 are labeled in the opposite order, the orientation is in the opposite direction—that is, approximately 225° instead of approximately 45°. This does not affect angle class selection; the angle classes $[60° - \delta\theta, 60° + \delta\theta)$ and $[240° - \delta\theta, 240° + \delta\theta)$ are the same.

Figure 124.20 Selected Pair $P_1 P_2$ Falls within the Second Angle Class

If you specify an angle tolerance less than the default, such as ATOL=15°, some point pairs might be excluded. For example, the selected point pair $P_1 P_2$ in Figure 124.20, while closest to the 60° axis, might lie outside $[60 - \delta\theta, 60 + \delta\theta) = [45°, 75°)$. In this case, the point pair $P_1 P_2$ would be excluded from the semivariance computation. This setting can be desirable if you want to reduce interference between neighboring angles. An angle tolerance that is too small might result in too few point pairs in some distance classes for the empirical semivariance estimation (see also the discussion in the section "Choosing the Size of Classes" on page 10087).

On the other hand, you can specify an angle tolerance *greater* than the default. This can result in a point pair being counted in more than one angle classes. This has a smoothing effect on the variogram and is useful when only a small amount of data is present or the available data are sparsely located. However, in cases of anisotropy the smoothing effect might have the side effect of amplifying weaker anisotropy in some direction and weakening stronger anisotropy in another (Deutsch and Journel 1992, p. 59).

Changes in the values of the BANDWIDTH= option have a similar effect. See the section "Bandwidth Restriction" on page 10085 for an explanation of how BANDWIDTH= functions.

An alternative way to specify angle classes and angle tolerances is with the DIRECTIONS statement. The DIRECTIONS statement is useful when angle classes are not equally spaced. When you use the DIRECTIONS statement, consider specifying the angle tolerance too. The default value of the angle tolerance is 45° when a DIRECTIONS statement is used instead of the NDIRECTIONS= option in the COMPUTE statement. This might not be appropriate for a particular set of angle classes. See the section "DIRECTIONS Statement" on page 10055 for more details.

Distance Classification

The distance class for a point pair $P_1 P_2$ is determined as follows. The directed line segment $P_1 P_2$ is superimposed on the coordinate system that shows the distance or lag classes. These classes are determined by the LAGDISTANCE= option in the COMPUTE statement. Denoting the length of the line segment by $| P_1 P_2 |$ and the LAGDISTANCE= value by Δ, the lag class L is determined by

$$L(P_1 P_2) = \left\lfloor \frac{| P_1 P_2 |}{\Delta} + 0.5 \right\rfloor$$

where $\lfloor x \rfloor$ denotes the largest integer $\leq x$.

When the directed line segment $P_1 P_2$ is superimposed on the coordinate system that shows the distance classes, it is seen to fall in the first lag class; see Figure 124.21 for an illustration for $\Delta = 1$.

Figure 124.21 Selected Pair $P_1 P_2$ Falls within the First Lag Class

Pairwise distances are positive. Therefore, the line segment $| P_1 P_2 |$ might belong to one of the MAXLAG lag classes or it could be shorter than half the length of the LAGDISTANCE= value. In the last case the segment is said to belong to the lag class zero. Hence, lag class zero is smaller than lag classes $1, \ldots,$ MAXLAGS. The definition of lag classes in this manner means that when you specify the MAXLAGS= parameter, PROC VARIOGRAM produces a semivariogram with a total of MAXLAGS+1 lag classes including the zero lag class. For example, if you specify LAGDISTANCE=1 and MAXLAGS=10 and you do not specify a LAGTOLERANCE= value in the COMPUTE statement in PROC VARIOGRAM, the 11 lag classes generated by the preceding equation are

$$[0, 0.5), [0.5, 1.5), [1.5, 2.5), \ldots, [9.5, 10.5)$$

The preceding lag classes description is correct under the assumption of the default lag tolerance, which is half the LAGDISTANCE= value. Using the default lag tolerance results in no gaps between the distance class intervals, as shown in Figure 124.22.

Figure 124.22 Lag Distance Axis Showing Lag Classes

On the other hand, if you do specify a distance tolerance with the LAGTOLERANCE= option in the COMPUTE statement, a further check is performed to see whether the point pair falls within this tolerance of the nearest lag. In the preceding example, if you specify LAGDISTANCE=1 and MAXLAGS=10 (as before)

and also specify LAGTOLERANCE=0.25, the intervals become

$$[0, 0.25), [0.75, 1.25), [1.75, 2.25), \ldots, [9.75, 10.25)$$

You might want to avoid this specification because it results in gaps in the lag classes. For example, if a point pair $P_1 P_2$ falls in an interval such as

$$| P_1 P_2 | \in [1.25, 1.75)$$

then it is excluded from the semivariance calculation. The maximum LAGTOLERANCE= value allowed is half the LAGDISTANCE= value; no overlap of the distance classes is allowed.

See the section "Computation of the Distribution Distance Classes" on page 10086 for a more extensive discussion of practical aspects in the specification of the LAGDISTANCE= and MAXLAGS= options.

Bandwidth Restriction

Because the areal segments that are generated from the angle and distance classes increase in area as the lag distance increases, it is sometimes desirable to restrict this area (Deutsch and Journel 1992, p. 45). If you specify the BANDWIDTH= option in the COMPUTE statement, the lateral, or perpendicular, distance from the axis that defines the angle classes is fixed.

For example, suppose two points P_3, P_4 are picked from the domain in Figure 124.19 and are superimposed on the grid that defines distance and angle classes, as shown in Figure 124.23.

The endpoint of vector $P_3 P_4$ falls within the angle class around 60° and the fifth lag class; however, it falls outside the restricted area that is defined by the bandwidth. Hence, it is excluded from the semivariance calculation.

Figure 124.23 Selected Pair $P_3 P_4$ Falls outside Bandwidth Limit

Finally, a pair $P_i P_j$ that falls in a lag class larger than the value of the MAXLAGS= option is excluded from the semivariance calculation.

The BANDWIDTH= option complements the angle and lag tolerances in determining how point pairs are included in distance classes. Clearly, the number of pairs within each angle/distance class is strongly affected by the angle and lag tolerances and whether BANDWIDTH= has been specified. See also the section "Angle Classification" on page 10082 for more details about the effects these rules can have, since BANDWIDTH= operates in a manner similar to the ANGLETOLERANCE= option.

Computation of the Distribution Distance Classes

This section deals with theoretical considerations and practical aspects when you specify the LAGDISTANCE= and MAXLAGS= options. In principle, these values depend on the amount and spatial distribution of your experimental data.

The value of the LAGDISTANCE= option regulates how many pairs of data are contained within each distance class. In effect, this information defines the pairwise distance distribution (see the following subsection). Your choice of MAXLAGS= specifies how many of these lags you want to include in the empirical semivariogram computation. Adjusting the values of these parameters is a crucial part of your analysis. Based on your observations sample, they determine whether you have sufficient points for a descriptive empirical semivariogram, and they can affect the accuracy of the estimated semivariance, too.

The simplest way of determining the distribution of pairwise distances is to determine the maximum distance h_{max} between any pair of points in your data, and then to divide this distance by some number N of intervals to produce distance classes of length $\delta = h_{max}/N$. The distance $\mid P_1 P_2 \mid$ between each pair of points P_1, P_2 is computed, and the pair $P_1 P_2$ is counted in the kth distance class if $\mid P_1 P_2 \mid \in [(k-1)\delta, k\delta)$ for $k = 1, \ldots, N$.

The actual computation is a slight variation of this. A bound, rather than the actual maximum distance, is computed. This bound is the length of the diagonal of a bounding rectangle for the data points. This bounding rectangle is found by using the maximum and minimum x and y coordinates, $x_{max}, x_{min}, y_{max}, y_{min}$, and forming the rectangle determined by the following points:

(x_{min}, y_{max})	(x_{max}, y_{max})
(x_{min}, y_{min})	(x_{max}, y_{min})

See Figure 124.24 for an illustration of the bounding rectangle applied to the data of the domain D in Figure 124.19. PROC VARIOGRAM provides you with the sizes of $x_{max} - x_{min}$, $y_{max} - y_{min}$, and h_b. For example, in Figure 124.4 in the preliminary analysis, the specified parameters named "Max Data Distance in East," "Max Data Distance in North," and "Max Data Distance" correspond to the lengths $x_{max} - x_{min}$, $y_{max} - y_{min}$, and h_b, respectively.

Figure 124.24 Bounding Rectangle to Determine Maximum Pairwise Distance in Domain D

The pairwise distance bound, denoted by h_b, is given by

$$h_b = \sqrt{(x_{max} - x_{min})^2 + (y_{max} - y_{min})^2}$$

Using h_b, the interval $(0, h_b]$ is divided into $N + 1$ subintervals, where N is the value of the NHCLASSES= option specified in the COMPUTE statement, or $N = 10$ (default) if the NHCLASSES= option is not specified. The basic distance unit is $h_0 = \frac{h_b}{N}$; the distance intervals are centered on $h_0, 2h_0, \ldots, Nh_0$, with a distance tolerance of $\pm\frac{h_0}{2}$. The extra subinterval is $(0, h_0/2)$ and corresponds to lag class zero. It is half the length of the remaining subintervals, and it often contains the smallest number of pairs. Figure 124.22 shows an example where the lag classes correspond to $h_0 = 1$. This method of partitioning the interval $(0, h_b]$ is used in the empirical semivariogram computation.

Choosing the Size of Classes

When you start with a data sample, the VARIOGRAM procedure computes all the distinct point pairs in the sample. The OUTPAIR= output data set, described in the section "OUTPAIR=*SAS-data-set*" on page 10107, contains information about these pairs. The point pairs are then categorized in classes. The size of each class depends on the common distance that separates consecutive classes. In PROC VARIOGRAM you need to provide this distance value with the LAGDISTANCE= option. Practically, you can define the distance between classes to be about the size of the average sampling distance (Olea 2006).

Under a more scrutinized approach, before you specify a value for the LAGDISTANCE= option, it is helpful to be aware of two issues. First, estimate how many classes of data pairs you might need. Each class contributes one point to the empirical semivariogram. Therefore, you need enough classes for an adequate

number of points, so that your empirical semivariogram can suggest a suitable theoretical model shape for the description of the spatial continuity. Second, keep in mind that a larger number of data pairs in a class can contribute to a more accurate estimate of the corresponding semivariogram point.

The first consideration is a more general issue, and both this and the following subsection address it in detail. Based on the second consideration, the class size problem translates into having a sufficient number of data pairs in each class to produce an accurate semivariance estimate. However, only empirical rules of thumb exist to guide you with this choice. Examples of minimum-pairs empirical rules include the suggestion by Journel and Huijbregts (1978, p. 194) to use at least 30 point pairs for each lag class. Also, in a different approach, Chilès and Delfiner (1999, p. 38) increase this number to 50 point pairs.

Obviously, smaller data samples provide fewer data pairs in the sample. According to Olea (2006), it is difficult to properly estimate a semivariogram with fewer than 50 measurements. The preceding minimum-pairs practical rules are useful in cases where small samples are involved. When you work with a relatively small sample, the key is to specify the value of LAGDISTANCE= such that you can strike a balance between the number of the classes you can form and their pairs count. In the coal seam thickness example of the section "Preliminary Spatial Data Analysis" on page 10028, it is not possible to create a desirable large number of classes and maintain an adequate size for each one. On the other hand, there is no practical need to invoke these rules in the case of the much larger sample of ozone concentrations in "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122.

The spatial distribution of the sample might also affect the grouping of pairs into classes. For example, data that are sampled in clusters might prove difficult to classify according to the preceding practical rules. One strategy to address this problem is to accept fewer than 30 pairs for the underpopulated distance classes. Then, at the stage when you determine what theoretical semivariogram model to use, either disregard the corresponding empirical semivariogram points or use them and accept the increased uncertainty.

The VARIOGRAM procedure can help you decide on a suitable class size before you proceed with the empirical semivariogram computation. First, provide a number for the class count by specifying the NHCLASSES= value. Run the procedure with the option NOVARIOGRAM in the COMPUTE statement and examine the distribution data pairs. Use different values of NHCLASSES= to investigate how this parameter affects the data pairs distribution in each distance class. The pairwise distance intervals table (for example, Figure 124.3) shows the number of pairs in each distance class in the "Number of Pairs" column, and you can use the preceding rule of thumb to adjust the NHCLASSES= value accordingly.

PROC VARIOGRAM displays a rounded value of the distance between the lag bounds as the "Lag Distance" parameter in the pairs information table (see Figure 124.5) or the pairwise distances histogram (see Figure 124.4), which you can use for the LAGDISTANCE= specification. However, this is only one tool. For the semivariogram computation you can specify your own LAGDISTANCE= value based on your experience. Smaller LAGDISTANCE= values result in fewer data pairs in the classes. In that sense, you might find smaller values useful when you work with large samples so that you obtain more semivariogram points. Also, if the LAGDISTANCE= value is too large, you might end up "wasting" too many point pairs in fewer classes at the expense of computing fewer semivariogram points and no significant accuracy gains in the estimation.

As explained earlier, depending on the sample size and its spatial distribution you might have classes with fewer points than what the practical rules advise. Most commonly, the deficient distance classes are the limiting ones close to the origin $\boldsymbol{h} = 0$ and the most remote ones at large $\boldsymbol{h}$. The classes near the origin correspond to lags 0 and 1. These lags are crucial because the empirical semivariogram in small distances $\boldsymbol{h}$ characterizes the process smoothness and can help you detect the presence of a nugget effect. However, as discussed in the section "Distance Classification" on page 10083, lag zero is half the size of the rest of the classes by definition, so it can be expected to violate the rule of thumb for the number of pairs in a class.

The classes located at higher and extreme distances within a spatial domain are often not accounted for in the empirical semivariogram. The fewer pairs that can be formed in these distances do not allow for an accurate assessment of the spatial correlation, as is explained in the following section.

Spatial Extent of the Empirical Semivariogram

Given your choice for the LAGDISTANCE= value in your spatial domain, the following paragraphs provide guidelines on how many classes to consider when you compute the empirical semivariogram.

Obviously, you want to include no more classes beyond the limit where the pairs count falls below the minimum-pairs empirical rule threshold, as discussed in the preceding subsection. PROC VARIOGRAM provides you with a visual way to inspect this upper limit, if you decide to make use of the minimum-pairs empirical rule. In particular, specify your threshold choice for the minimum pairs per class by using the THRESHOLD= parameter for the PLOTS=PAIRS option.

Then, the procedure produces in the pairwise distances histogram a reference line at the specified THRESHOLD= value, which leaves below the line all lags whose pairs count is lower than the threshold value; see, for example, Figure 124.4. The last lag class whose pair population is above the THRESHOLD= value is reported in the pairs information table as "Highest Lag With Pairs > Threshold." This value is not a recommendation for the MAXLAGS= option, but rather is an upper limit for your choice. Detailed information about the pairs count in each class is displayed in the corresponding pairwise distance intervals table, as Figure 124.3 demonstrates.

The preceding suggests that you have an upper limit indication, but you still need some criterion to decide how many lags to include in the semivariogram estimation. The criterion is the extent of spatial dependence in your domain.

Spatial dependence can exist beyond your domain limits. However, you have no data past your domain scale to define a range for larger-scale spatial dependencies. As you look for pairs of data that are gradually farther apart, the number of pairs naturally decreases with distance. The pairs at the more distant classes might be so few that they are likely to be independent with respect to the spatial dependence scale that you can detect. If you include the largest distances in your empirical semivariogram plot, then these pairs only contribute added noise. In the same sense, you cannot explore in detail spatial dependencies in scales smaller than an average minimum distance between your data. The nugget effect represents then microscale correlations whose effect is evident in your working scale.

You specify the spatial dependence extent with commonly used measures such as the *correlation range* (or *correlation length*) ϵ and the *correlation radius* h_c. Both are defined in a similar manner. The correlation range ϵ is the distance at which the covariance is 5% of its value at $\boldsymbol{h} = 0$, and shows that beyond ϵ the covariance is considered to be negligible. The correlation radius h_c is the distance at which the covariance is about half the variance at $\boldsymbol{h} = 0$, and indicates the distance over which significant correlations prevail (Christakos 1992, p. 76). The physical meanings of these measures are similar to that of the semivariogram range. Also, the effective range r_ϵ used in asymptotically increasing semivariance models has essentially the same definition as the correlation range ϵ (see the section "Theoretical Semivariogram Models" on page 10072).

A rough estimate of the correlation extent measures might be available from previous studies of a similar site, or from prior information about related measurements. In such an event, you typically want to consider a maximum pairwise distance that does not exceed the length of two or three correlation radii, or one and a half correlation ranges. You can then specify the MAXLAGS= value on the basis of the lags that fit in that distance.

When you have no estimates of correlation extent measures, you can use first use a crude measure to get started with your analysis: you can typically expect MAXLAGS= to be about half of the lag classes shown in the pairwise distances histogram.

Then, if necessary, you can refine your MAXLAGS= choice by using the following maximum lags rule of thumb: Journel and Huijbregts (1978, p. 194) advise considering lags up to about half of the extreme distance between data in the direction of interest. The VARIOGRAM procedure assists you in this task by providing the overall extreme data distance h_b, in addition to the extreme data distances in the vertical and horizontal axes directions. For example, h_b is reported in the pairs information table as "Maximum Data Distance" (see Figure 124.5), and in the pairwise distances histogram as "Max Data Distance" (see Figure 124.4).

Overall, avoid significant deviations from the maximum lags rule of thumb. As was stated earlier, a MAXLAGS= value that takes you well beyond the half-extreme distance between data in a given direction might give you limited accuracy in the empirical semivariance estimates at higher distances. At the other end, a value of MAXLAGS= that is too small might lead you to omit important information about the spatial structure that potentially lies within the range of distances you skipped.

Semivariance Computation

With the classification of a point pair $P_i P_j$ into an angle/distance class, as shown earlier in this section, the semivariance computation proceeds as follows.

Denote all pairs that $P_i P_j$ belong to angle class $[\theta_k - \delta\theta_k, \theta_k + \delta\theta_k)$ and distance class $L = L(P_i P_j)$ as $N(\theta_k, L)$. For example, based on Figure 124.20 and Figure 124.21, $P_1 P_2$ belongs to $N(60°, 1)$.

Let $\mid N(\theta_k, L) \mid$ denote the *number* of such pairs. The component of the standard (or method of moments) semivariance that correspond to angle/distance class $N(\theta_k, L)$ is given by

$$\hat{\gamma}(h_k) = \frac{1}{2 \mid N(\theta_k, L) \mid} \sum_{P_i P_j \in N(\theta_k, L)} [V(\boldsymbol{s}_i) - V(\boldsymbol{s}_j)]^2$$

where h_k is the average distance in class $N(\theta_k, L)$; that is,

$$h_k = \frac{1}{\mid N(\theta_k, L) \mid} \sum_{P_i P_j \in N(\theta_k, L)} \mid P_i P_j \mid$$

The robust version of the semivariance is given by

$$\bar{\gamma}(h_k) = \frac{\Psi^4(h_k)}{2[0.457 + 0.494/N(\theta_k, L)]}$$

where

$$\Psi(h_k) = \frac{1}{N(\theta_k, L)} \sum_{P_i P_j \in N(\theta_k, L)} [V(\boldsymbol{s}_i) - V(\boldsymbol{s}_j)]^{\frac{1}{2}}$$

This robust version of the semivariance is computed when you specify the ROBUST option in the COMPUTE statement in PROC VARIOGRAM.

PROC VARIOGRAM computes and writes to the OUTVAR= data set the quantities $h_k, \theta_k, L, N(\theta_k, L), \hat{\gamma}(h)$, and $\bar{\gamma}(h)$.

Empirical Semivariograms and Surface Trends

It was stressed in the beginning of the section "Theoretical and Computational Details of the Semivariogram" on page 10077 that if your data are not free of nonrandom surface trends, then the empirical semivariance $\hat{\gamma}_z(\boldsymbol{h})$ you obtain from PROC VARIOGRAM represents a pseudo-semivariance rather than an estimate of the theoretical semivariance $\gamma_z(\boldsymbol{h})$.

In practice, two major difficulties appear. First, you might have no knowledge of underlying surface trends in your SRF $Z(\boldsymbol{s})$. It can be possible to have this information when you deal with a repetitive phenomenon (Chilès and Delfiner 1999, p. 123), or if you work within a subdomain of a broader region with known characteristics; often, though, this is not the case. Second, even if you suspect the existence of an underlying nonrandom trend, its precise nature might be unknown (Cressie 1993, p. 114, 162).

Based on the last remark, the criteria to define the exact form of a surface trend can be subjective. However, statistical methods can identify the presence and remove an estimate of such a trend. Different trend forms can be estimated in your SRF depending on the trend estimation model that you choose. This choice can lead to different degrees of smoothing in the residual random fluctuations. It might also have an effect on the residuals spatial structure characterization, because trend removals with different models are essentially different operations acting upon the values of your original observations. Following the comment by Chilès and Delfiner (1999, section 2.7.3), there are as many semivariograms of residuals as there are ways of estimating the trend. The same source also examines the introduction of bias in the semivariance of the residuals as a side effect of trend removal processes. This bias is small when you examine distances close to the origin $\boldsymbol{h} = 0$, and it can increase with distance.

Keeping in mind the preceding remarks, an approach you can take is to use one of the many predictive modeling tools in SAS/STAT software to estimate the unknown trend. Then you use PROC VARIOGRAM to analyze the residuals after you remove the trend. If the resulting model does not require too many degrees of freedom (such as if you use a low-order polynomial), then this approach might be sufficient. The section "Analysis with Surface Trend Removal" on page 10126 demonstrates how to use PROC GLM (see Chapter 47, "The GLM Procedure") for that purpose.

Apart from the standard semivariogram analysis, you can attempt to fit a theoretical semivariogram model to your empirical semivariogram if (a) either the analysis itself or your knowledge of the SRF does not clearly suggest the presence of any surface trend, or (b) the analysis can indicate a potentially trend-free direction, along which your data have a constant mean.

For example, you might observe overall similar values in your data. This can be an indication that your data are free of nonrandom trends, or that a very mild trend is present. The case falls under the preceding option (a). A very mild trend still allows a good determination of the semivariance at short distances according to Chilès and Delfiner (1999, p. 125), and this can be sufficient for your spatial prediction goal. An analysis of this type is assumed in the section "Preliminary Spatial Data Analysis" on page 10028.

If you observe similar values locally across a particular direction, this an instance of option (b). Olea (2006) suggests recognizing a trend-free direction as being perpendicular to the axis of the maximum dip in the values of $Z(\boldsymbol{s})$. If you suspect that at least one such direction exists for your data, then run PROC VARIOGRAM for a series of directions in the angular vicinity. The trend-free direction, if it exists, coincides with the one whose pseudo-semivariogram exhibits minimal increase with distance; see "Example 124.3: Analysis without Surface Trend Removal" on page 10136 for a demonstration of this approach. However, you cannot test $Z(\boldsymbol{s})$ for anisotropy in this case, because you can investigate the semivariogram only in the single trend-free direction (Olea 1999, p. 76). Chilès and Delfiner (1999, section 2.7.4) suggest fitting a theoretical model in a trend-free direction only if the hypothesis of an isotropic semivariogram appears reasonable in your analysis.

As a result, you need to be very cautious when you choose to perform semivariogram analysis on data you have not previously examined for surface trends. In this event, both of the options (a) and (b) that were reviewed in the preceding paragraphs rely mostly on empirical and subjective criteria. As noted in this section, a degree of subjectivity exists in the selection of the surface trend itself. This fact suggests that a significant part of the semivariogram analysis is based on metastatistical decisions and on your understanding of your data and the physical considerations that govern your study. In any case, as shown in the section "Theoretical and Computational Details of the Semivariogram" on page 10077, your semivariogram analysis relies fundamentally on the use of trend-free data.

Theoretical Semivariogram Model Fitting

You can choose between two approaches to select a theoretical semivariogram model and fit the empirical semivariance. The first one is manual fitting, in which a theoretical semivariogram model is selected based on visual inspection of the empirical semivariogram. For example, see Hohn (1988, p. 25) and comments from defendants of this approach in Olea (1999, p. 82). The second approach is to perform model fitting in an automated manner. For this task you can use methods such as least squares, maximum likelihood, and robust methods (Cressie 1993, section 2.6).

The VARIOGRAM procedure features automated semivariogram model fitting that uses the weighted least squares (WLS) or the ordinary least squares (OLS) method. Use the MODEL statement to request that specific model forms or an array of candidate models be tested for optimal fitting to the empirical semivariance.

Assume that you compute first the empirical semivariance $\gamma_z^*(\boldsymbol{h})$ at MAXLAGS=k distance classes, where $\gamma_z^*(\boldsymbol{h})$ can be either the classical estimate $\hat{\gamma}_z(\boldsymbol{h})$ or the robust estimate $\bar{\gamma}_z(\boldsymbol{h})$, as shown in the section "Theoretical and Computational Details of the Semivariogram" on page 10077. In fitting based on least squares, you want to estimate the parameters vector $\boldsymbol{\theta}$ of the theoretical semivariance $\gamma_z(\boldsymbol{h})$ that minimizes the sum of square differences $R(\boldsymbol{\theta})$ given by the expression

$$R(\boldsymbol{\theta}) = \sum_{i=1}^{k} {w_i}^2 \left[\gamma_z^*(\boldsymbol{h}_i) - \gamma_z(\boldsymbol{h}_i; \boldsymbol{\theta})\right]^2$$

For $i = 1, \ldots, k$, the weights are ${w_i}^2 = 1/\mathrm{Var}[\gamma_z^*(\boldsymbol{h}_i)]$ in the case of WLS and ${w_i}^2 = 1$ in the case of OLS. Therefore, the parameters $\boldsymbol{\theta}$ are estimated in OLS by minimizing

$$R(\boldsymbol{\theta})_{OLS} = \sum_{i=1}^{k} \left[\gamma_z^*(\boldsymbol{h}_i) - \gamma_z(\boldsymbol{h}_i; \boldsymbol{\theta})\right]^2$$

For WLS, Cressie (1985) investigated approximations for the variance of both the classical and robust empirical semivariances. Then, under the assumptions of normally distributed observations and uncorrelated squared differences in the empirical semivariance, the approximate weighted least squares estimate of the parameters $\boldsymbol{\theta}$ can be obtained by minimizing

$$R(\boldsymbol{\theta})_{WLS} = \frac{1}{2}\sum_{i=1}^{k} N(\boldsymbol{h}_i)\left[\frac{\gamma_z^*(\boldsymbol{h}_i)}{\gamma_z(\boldsymbol{h}_i;\boldsymbol{\theta})} - 1\right]^2$$

where $N(\boldsymbol{h}_i)$ is the number of pairs of points in the ith distance lag.

PROC VARIOGRAM relies on nonlinear optimization to minimize the least squares objective function $R(\boldsymbol{\theta})$. The outcome is the model that best fits the empirical semivariogram according to your criteria. The fitting process flow is displayed in Figure 124.25. Goovaerts (1997, section 4.2.4) suggests that fitting a theoretical model should aim to capture the major spatial features. An accurate fit is desirable, but overfitting does not offer advantages, because you might find yourself trying to model possibly spurious details of the empirical semivariogram. At the same time, it is important to describe the correlation behavior accurately near the semivariogram origin. As pointed out by Chilès and Delfiner (1999, pp. 104–105), a poor description of spatial continuity at small lags can lead to loss of optimality in kriging predictions and erroneous reproduction of the variability in conditional simulations.

The significance of achieving better accuracy near the semivariogram origin is an advantage of the WLS method compared to OLS. In particular, the semivariance variance decreases when you get closer the origin $\boldsymbol{h} = 0$, as suggested in the section "Theoretical and Computational Details of the Semivariogram" on page 10077. The WLS weights are expressed as the inverse of this variance; as a result, WLS fitting is more accurate for distances $\boldsymbol{h}$ near the semivariogram origin. In contrast, the OLS approach performs a least squares overall best fit because it assumes constant variance at all distances $\boldsymbol{h}$. Another advantage of WLS over OLS is that OLS falsely assumes that the differences in the optimization process are normally distributed and independent. However, WLS has the disadvantage that the weights depend on the fitting parameters.

Depending on your application, you can use WLS or OLS with PROC VARIOGRAM to fit classical semivariance. Other fitting methods include maximum likelihood approaches that rely crucially on the normality assumption for the data distribution, and the generalized least squares method that offers better accuracy but is computationally more demanding. You can find extensive discussions about these issues in Cressie (1993, section 2.3), Jian, Olea, and Yu (1996), Stein (1988), and Schabenberger and Gotway (2005).

The sections "Parameter Initialization" on page 10094 and "Quality of Fit" on page 10096 provide details and insight about semivariogram fitting, in addition to ways to cope with poor fits or no fit at all. These strategies can help you reach a meaningful description of spatial correlation in your problem.

Figure 124.25 Semivariogram Fitting Process Flowchart

Parameter Initialization

An important stage when you prepare for the model fitting process is initialization of the model parameters. As stated earlier, nonlinear optimization techniques are used in the fitting process. These techniques assist in the estimation of the model parameters, and being nonlinear means they can be very sensitive to selection of the initial values.

You can specify initial values close to the expected estimates when you have a relatively simple problem, such as in the example of the section "Getting Started: VARIOGRAM Procedure" on page 10027. In the case of nested models the selection of initial values can be more challenging because you have to assess the level of contribution for each one of the nested components.

The VARIOGRAM procedure features automatic selection of initial values based on the recommendations in Jian, Olea, and Yu (1996). Specifically, if you compute the estimated empirical semivariogram $\hat{\gamma}_z(\boldsymbol{h})$ at k lags, then:

- The default initial nugget effect $c_{n,0}$ is

$$c_{n,0} = \text{Max}\left[0, \hat{\gamma}_z(\boldsymbol{h}_1) - \frac{\boldsymbol{h}_1}{\boldsymbol{h}_2 - \boldsymbol{h}_1}\left[\hat{\gamma}_z(\boldsymbol{h}_2) - \hat{\gamma}_z(\boldsymbol{h}_1)\right]\right]$$

- The default initial slope ${\sigma_{0,0}}^2$ and initial exponent $a_{0,0}$ for the power model are

$${\sigma_{0,0}}^2 = \frac{\left[\hat{\gamma}_z(\boldsymbol{h}_{k-2}) + \hat{\gamma}_z(\boldsymbol{h}_{k-1}) + \hat{\gamma}_z(\boldsymbol{h}_k)\right]/3 - c_{n,0}}{\boldsymbol{h}_k - \boldsymbol{h}_1}$$

$$a_{0,0} = 1$$

- The default initial scale ${\sigma_{0,0}}^2$ and initial range $a_{0,0}$ for all other models are

$${\sigma_{0,0}}^2 = \frac{\left[\hat{\gamma}_z(\boldsymbol{h}_{k-2}) + \hat{\gamma}_z(\boldsymbol{h}_{k-1}) + \hat{\gamma}_z(\boldsymbol{h}_k)\right]}{3} - c_{n,0}$$

$$a_{0,0} = 0.5\boldsymbol{h}_k$$

When you use the Matérn form, PROC VARIOGRAM sets the default initial value for the Matérn smoothness to $\nu_0 = 1$.

These rules are observed in the case of single, non-nested model fitting, and they are slightly modified to apply for nested model fitting as follows: Assume that you want to fit a nested model composed of m structures. As stated in the section "Nested Models" on page 10077, the nugget effect is a single parameter and is independent of the number of nested structures in a model. Also, the sum of the nested structure scales and the nugget effect, if any, must be equal to the total variance. For this reason, PROC VARIOGRAM simply divides the initial scale value it would assign to a non-nested model into m components ${\sigma_{0,0,1}}^2, \ldots, {\sigma_{0,0,m}}^2$. For the range parameter, the VARIOGRAM procedure sets the initial range $a_{0,0,1}$ of the first nested structure equal to the value it would assign to a non-nested model initial range. Then, the initial range $a_{0,0,m}$ of the m-component is set recursively to half the value of the initial range $a_{0,0,m-1}$ of the $(m-1)$-component.

Your empirical semivariogram must have nonmissing estimates at least at three lags so that you can use the automated fitting feature in PROC VARIOGRAM. Overall, if you specify a model form with q parameters to fit to an empirical semivariogram with nonmissing estimates at k lags, then the fitting problem is well-defined only when the degrees of freedom are $\text{DF} = k - q \geq 0$.

A potential numerical issue is that fitting could momentarily lead the fitting parameters to near-zero semivariance values at lags away from zero distance. The theoretical semivariance is always positive for any distance larger than zero, and this is also a requirement for the numerical computation of $R(\boldsymbol{\theta})_{WLS}$ in weighted least squares fitting. Such numerical issues are unlikely but possible, depending on the data set you use and the parameter initial values. If an event of nonpositive semivariance at a given lag occurs during an iteration, then PROC VARIOGRAM transparently adds a minimal amount of variance at that lag for the specific iteration. You can control this amount of variance with the NEPSILON= option of the MODEL statement. It is recommended that you leave this parameter at its default value.

The section concludes with a reminder of the fitting process sensitivity to the initial parameter values selection. The VARIOGRAM procedure facilitates this selection for you by using the simple rules shown

earlier. However, the suggested initial values might not always be the best choice. In simple cases, such as the introductory example in the section "Getting Started: VARIOGRAM Procedure" on page 10027, this approach is very convenient and effective.

In principle, you are strongly encouraged to experiment with initial values. You want to make sure that the fitting process leads the model parameters to converge to estimates that make sense for your problem. When a parameter estimate seems unreasonable on the basis of your problem specification (for example, a model scale might be estimated to be 10 times the size of your sample variance, or the estimate of a range might be zero), PROC VARIOGRAM produces a note to let you know about a potentially ambiguous fit. These issues are examined in more detail in the section "Quality of Fit" on page 10096.

Parameter Estimates

When the fit process is complete, the VARIOGRAM procedure produces the "Parameter Estimates" table with information about the fitted model parameters. The table includes estimates of the parameters, their approximate standard error, the statistical degrees of freedom DF, the corresponding t statistic, and its approximate p-value. For a model with q parameters that fits an empirical semivariogram of k nonmissing lags, $\mathrm{DF} = k - q$.

NOTE: Parameter estimates might have nonzero standard errors even in the rather extreme case where $\mathrm{DF} = 0$. This can typically occur when there are active optimization constraints in the fitting process.

You can request the confidence intervals for the parameter estimates of a fitted model by specifying the CL option of the MODEL statement. These confidence intervals are computed using the Wald-based formula

$$\widehat{\beta}_i \pm \mathrm{stderr}_i \times t(k-q, 1-\alpha/2)$$

where $\widehat{\beta}_i$ is the ith parameter estimate, stderr_i is its estimated approximate standard error, $t(k-q, 1-\alpha/2)$ is the t statistic with $\mathrm{DF} = k - q$ degrees of freedom. The confidence intervals are only asymptotically valid. The significance level α used in the construction of these confidence limits can be set with the ALPHA= option of the MODEL statement; the default value is $\alpha = 0.05$.

Specify the COVB and the CORRB options in the MODEL statement to request the approximate covariance and approximate correlation matrices of the fitted parameters, respectively. These matrices are based on the optimization process results. In agreement with reporting similar optimization output in SAS/STAT software, parameters with active restraints have zeros in the corresponding rows and columns in the covariance and correlation matrices, and display 1 in the correlation matrix diagonal.

Quality of Fit

The VARIOGRAM procedure produces a fit summary table to report about the goodness of fit. When you specify multiple models to fit with the FORM=AUTO option in the MODEL statement, the VARIOGRAM procedure uses two processes to rank the fitted models: The first one depends on your choice among available fitting criteria. The second one is based on an operational classification of equivalent models in classes. The two processes are described in more detail in the following subsections.

Overall, no absolutely correct way exists to rank and classify multiple models. Your choice of ranking criteria could depend on your study specifications, physical considerations, or even your personal assessment of fitting performance. The VARIOGRAM procedure provides you with fitting and comparison features to facilitate and help you better understand the fitting process.

Fitting Criteria

The fit summary table ranks multiple models on the basis of one or more fitting criteria that you can specify with the CHOOSE= option of the MODEL statement, as explained in the section "Syntax: VARIOGRAM Procedure" on page 10041. Currently, the VARIOGRAM procedure offers two numerical criteria (for which a smaller value indicates a better fit) and a qualitative criterion:

- The residual sum of squares error (SSE) is based on the objective function of the fitting process. When the specified method is weighted least squares, the sum of squares of the weighted differences (WSSE) is computed according to the expression

  $$\mathrm{WSSE} = \sum_{i=1}^{k} {w_i}^2 \left[\gamma_z^*(\boldsymbol{h}_i) - \gamma_z(\boldsymbol{h}_i;\boldsymbol{\theta})\right]^2$$

  where $\gamma_z^*(\boldsymbol{h}_i)$ can be either the classical or robust semivariance estimate of the theoretical semivariance $\gamma_z(\boldsymbol{h}_i;\boldsymbol{\theta})$ at the ith lag and the weights ${w_i}^2$ are taken at lags $i = 1,\ldots,k$. When you specify the METHOD=OLS option in the MODEL, the weights ${w_i}^2 = 1$ for $i = 1,\ldots,k$, and the SSE is expressed as

  $$\mathrm{SSE} = \sum_{i=1}^{k} \left[\gamma_z^*(\boldsymbol{h}_i) - \gamma_z(\boldsymbol{h}_i;\boldsymbol{\theta})\right]^2$$

- Akaike's information criterion (AIC) is included in the fit summary table when there is at least one nonfixed parameter. In its strict definition, AIC assumes that the model errors are normally and independently distributed. This assumption is not correct in the semivariance fitting analysis. However, the AIC can be also defined in an operational manner on the basis of the weighted squared error sum WSSE as

  $$\mathrm{AIC} = k \ln\left(\frac{\mathrm{WSSE}}{k}\right) + 2q$$

  for k lags and q model parameters; see, for example, Olea (1999, p. 84). The operational definition of the AIC is provided as an additional criterion for the comparison of fitted models in PROC VARIOGRAM.

  The AIC expression suggests that when you specify multiple models with the FORM=AUTO option in the MODEL statement, all models with the same number of parameters are ranked in the same way by the AIC and the WSSE criteria. Among models with the same WSSE value, AIC ranks higher the ones with fewer parameters.

- The third qualitative criterion enables you to classify multiple models based on their convergence status. A model is sent to the bottom of the ranking table if the parameter estimation optimization fails to converge or fitting is unsuccessful due to any other issue. These two cases are distinguished by the different notes they produce in the fit summary ODS table. If you specify the STORE statement to save the fitting output in an item store, then models that have failed to fit are not passed to the item store.

With respect to convergence status, PROC VARIOGRAM ranks higher those models that have successfully completed the fitting process. It might occur that the selection of parameter initial values, physical considerations about the forms that are used for the fit, or numerical aspects of the nonlinear optimization could result in ambiguous fits. For example, you might see that model parameters converge at or near their boundary

values, or that parameters have unreasonably high estimates when compared to the empirical semivariogram characteristics. Then, the fit summary table designates such fits as questionable.

You might not need to take any action if you are satisfied with the fitting results and the selected model. You can investigate questionable fits in one or more of the following ways:

- If a form in a nested model makes no contribution to the model due to a parameter at or near its boundary value, then you could have a case of a degenerate fit. When you fit multiple models, a model with degenerate fit can collapse to the more simple model that does not include the noncontributing form. The VARIOGRAM procedure includes in its fit summary all models that are successfully fit. In such cases you can ignore degenerate fits. You can also try subsequent fits of individual models and exclude noncontributing forms or use different initial values.
- Unreasonably low or high parameter estimates might be an indication that the current initial values are not a good guess for the nonlinear optimizer. In most cases, fitting an empirical semivariogram gives you the advantage of a fair understanding about the value range of your parameters. Then, you can use the PARMS statement to specify a different set of initial values and try the fit again.
- Try replacing the problematic form with another one. A clear example is that you can expect a very poor fit if you specify an exponential model to fit an empirical semivariogram that suggests linear behavior.

Eventually, if none of the aforementioned issues exist, then a model is ranked in the highest positions of the fit summary table. You can combine two or more of the fitting criteria to manage classification of multiple fitted models in a more detailed manner.

In some cases you might still experience a poor quality of fit or no fit at all. If none of the earlier suggestions results in a satisfactory fit, then you could decide to re-estimate the empirical semivariogram for your same input data. The following actions can produce different empirical semivariograms to fit a theoretical model to:

- If you compute the semivariogram for different angles and you experience optimization failures, try specifying explicitly the same direction angles with different tolerance or bandwidth value in the DIRECTIONS statement.
- Modify slightly the LAGDISTANCE= option in the COMPUTE statement to obtain a different empirical semivariogram.

Finally, it is possible to have models in the fitting summary table ranked in a way that seemingly contradicts the specification in the CHOOSE= option of the MODEL statement. Consider an example with the default behavior CHOOSE=(SSE AIC), where you might observe that models have the same SSE values but are not ranked further as expected by the AIC criterion. A closer examination of such cases typically reduces this issue to a matter of the accuracy shown in the table. That is, the displayed accuracy of the SSE values might hide additional decimal digits that justify the given ranking.

In such scenarios, discrimination of models at the limits of numerical accuracy might suggest that you choose a model of questionable fit or a nested structure over a more simple one. You can then review the candidate models and exercise your judgment to select the model that works best for you. If all values of a criterion are equal, then the ranking order is simply the order in which models are examined unless more criteria follow that can affect the ranking.

Classes of Equivalence

The fit summary that is produced after fitting multiple models further categorizes the ranked models in classes of equivalence. Equivalence classification is an additional investigation that is unrelated to the ranking criteria presented in the previous subsection; it is an operational criterion that provides you with a qualitative overview of multiple model fit performance under given fitting conditions.

To examine model equivalence, the VARIOGRAM procedure computes the semivariances for each one of the fitted models at a set of distances. For any pair of consecutively ranked models, if the sum of their semivariance absolute differences at all designated distances is smaller than the tolerance specified by the EQUIVTOL= parameter, then the two models are deemed equivalent and placed in the same class; otherwise, they are placed in different classes. Equivalence classification depends on the existing ranking; hence the resulting classes can differ when you specify different ranking criteria in the CHOOSE= option of the MODEL statement.

The equivalence class numbers start at 1 for the top-ranked model in the fit summary table. You can consider the top model of each equivalence class to be a representative of the class behavior. When you specify that fit plots be produced and there are equivalence classes, the plot displays the equivalence classes and the legend designates each one by its representative model.

Consequently, if an equivalence class contains multiple members after a fit, then all of its members produce in general the exact same semivariogram. A typical reason could be that the fitting process estimates of scale parameters are at or close to their zero boundaries in one or more nested forms in a model. In such cases, the behavior of this model reduces to the behavior of its nested components with nonzero parameters. When one or more models share this situation or have the same contributing nested forms, they could end up as members of the same equivalence class depending on the ranking criteria.

It is not necessary for all models in the same equivalence class to produce the exact same semivariogram. If a fit of two obviously different forms involves semivariance values that are small enough for the equivalence criterion to be satisfied by the default value of the EQUIVTOL= option, then you might need to specify an even smaller value in the EQUIVTOL= option to rank these two models in separate equivalence classes.

Fitting with Matérn Forms

When you use a Matérn form in the fitting process, it is possible that the fitting optimizer might encounter numerical difficulties if it tries to push the smoothing parameter ν towards increasingly high values. The VARIOGRAM procedure addresses this issue by imposing an amply elevated upper bound of 1,000,000 on the smoothness values it processes. The section "Characteristics of Semivariogram Models" on page 10073 mentions that $\nu \to \infty$ gives the Gaussian model. In the scenario of progressively increasing smoothness values, PROC VARIOGRAM acknowledges that the Matérn form behavior tends asymptotically to become Gaussian and replaces automatically the Matérn with a Gaussian form in the model. Subsequently, fitting resumes with the resulting model.

If you explore fitting of multiple models, then any duplicate models that might occur due to Matérn-to-Gaussian form conversions are fitted only once. Also, if a nested model has more than one Matérn form, then the fitting process checks one of them at a time about whether they need to be replaced by a Gaussian form. Consequently, following the switch of one Matérn form, the fitting process starts anew with the resulting model before any decisions for additional form conversions are made.

Replacement of the Matérn form with the Gaussian form occurs by default when $\nu > 10,000$. However, you can control this threshold value with the MTOGTOL= parameter of the MODEL statement. Practically, the Matérn form starts to resemble the Gaussian behavior for ν values that are about $\nu > 10$. If you encounter

such conversions of the Matérn form into Gaussian and you prefer to set a lower ν threshold for the conversion than the default, you might experience improved code performance because computation of the Matérn semivariance can be numerically demanding.

Autocorrelation Statistics

Spatial autocorrelation measures offer you additional insight into the interdependence of spatial data. These measures quantify the correlation of an SRF $Z(\boldsymbol{s})$ with itself at different locations, and they can be very useful whether you have information at exact locations (point-referenced data) or measurements that characterize an area type such as counties, census tracts, zip codes, and so on (areal data).

As in the semivariogram computation, a key issue for the autocorrelation statistics is that you work with a set z_i of measurements, $i = 1, \ldots, n$, that are free of nonrandom surface trends and have a constant mean.

Autocorrelation Weights

In general, the choice of a weighting scheme is subjective. You can obtain different results by using different schemes, options, and parameters. PROC VARIOGRAM offers you considerable flexibility in choosing weights that are appropriate for prior considerations such as different hypotheses about neighboring areas, definition of the neighborhood structure, and accounting for natural barriers or other spatial characteristics; see the discussion in Cliff and Ord (1981, p. 17). As stressed for all types of spatial analysis, it is important to have good knowledge of your data. In the autocorrelation statistics, this knowledge can help you avoid spurious correlations when you choose the weights.

The starting point is to assign individual weights to each one of the n data values z_i, $i = 1, \ldots, n$, with respect to the rest. An $n \times n$ matrix of weights is thus defined, such that for any two locations $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$, the weight w_{ij} denotes the effect of the value z_i at location $\boldsymbol{s}_i$ on the value z_j at location $\boldsymbol{s}_j$. Depending on the nature of your study, the weights w_{ij} need not be symmetric; that is, it can be true that $w_{ij} \neq w_{ji}$.

Binary and Nonbinary Weights

The weights w_{ij} can be either binary or nonbinary values. Binary values of 1 or 0 are assigned if the SRF $Z(\boldsymbol{s}_i)$ at one location $\boldsymbol{s}_i$ is deemed to be connected or not, respectively, to its value $Z(\boldsymbol{s}_j)$ at another location $\boldsymbol{s}_j$. Nonbinary values can be used in the presence of more refined measures of connectivity between any two data points P_i and P_j. PROC VARIOGRAM offers a choice between a binary and a distance-based nonbinary weighting scheme.

In the binary weighting scheme the weight $w_{ij} = 1$ if the data pair at $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ is closer than the user-defined distance that is defined by the LAGDISTANCE= option, and $w_{ij} = 0$ if $i = j$ or in any other case. For that reason, in the COMPUTE statement, if you specify the WEIGHTS=BINARY suboption of the AUTOCORRELATION option when the NOVARIOGRAM option is also specified, then you must also specify the LAGDISTANCE= option.

The nonbinary weighting scheme is based on the pair distances and is invoked with the WEIGHTS=DISTANCE suboption of the AUTOCORRELATION option. PROC VARIOGRAM uses a variation of the Pareto form functional to set the weights. Namely, the autocorrelation weight for every point pair P_i and P_j located at $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$, respectively, is defined as

$$w_{ij} = s\frac{1}{1+ \mid \boldsymbol{h} \mid^p}$$

where $\boldsymbol{h} = \boldsymbol{s}_i - \boldsymbol{s}_j$ and $p \geq 0$ and $s \geq 0$ are user-defined parameters for the adjustment of the weights.

In particular, the power parameter p is specified in the POWER= option of the DISTANCE suboption within the AUTOCORRELATION option. The default value for this parameter is $p = 1$. Also, the scaling parameter s is specified by the SCALE= option in the DISTANCE suboption of the AUTOCORRELATION option. The default value for the scaling parameter is $s = 1$. You can use the p and s parameters to adjust the actual values of the weights according to your needs. Variations in the scaling parameter s do not affect the computed values of the Moran's I and Geary's c autocorrelation coefficients that are introduced in the section "Autocorrelation Statistics Types" on page 10101.

Nonbinary Weights with Normalized Distances

PROC VARIOGRAM offers additional flexibility in the DISTANCE weighting scheme through an option to use normalized pair distances. You can invoke this feature by specifying the NORMALIZE option in the DISTANCE suboption of the AUTOCORRELATION option. In this case, the distances used in the definition of the weights are normalized by the maximum pairwise distance h_b (see the section "Computation of the Distribution Distance Classes" on page 10086 and Figure 124.24); the weights are then defined as $w_{ij} = s/[1 + (|\boldsymbol{h}| / h_b)^p]$.

Most likely, h_b has a different value for different data sets. Hence, it is suggested that you avoid using the weights you obtain from the preceding equation and one data set for comparisons with the weights you derive from different data sets.

Symmetric and Asymmetric Weights

The weighting schemes presented in the preceding paragraphs are symmetric; that is, $w_{ij} = w_{ji}$ for every data pair at locations $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$. However, you can also define asymmetric weights w'_{ij} such that

$$\sum_{j \in J} w'_{ij} = 1$$

for $i = 1, 2, \ldots, n$, where $w'_{ij} = w_{ij} / \sum_{j \in J} w_{ij}$, $i = 1, 2, \ldots, n$. In the distance-based scheme, J is the set of all locations that form point pairs with the point at $\boldsymbol{s}_i$. In the binary scheme, J is the set of the locations that are connected to $\boldsymbol{s}_i$ based on your selection of the LAGDISTANCE= option; see Cliff and Ord (1981, p. 18). The weights w'_{ij} are *row-averaged* (or *standardized* by the count of their connected neighbors). You can apply row averaging in weights when you specify the ROWAVG option within either the BINARY or DISTANCE suboptions in the AUTOCORRELATION option.

Autocorrelation Statistics Types

One measure of spatial autocorrelation provided by PROC VARIOGRAM is Moran's I statistic, which was introduced by Moran (1950) and is defined as

$$I = \frac{n}{(n-1)S^2 W} \sum_i \sum_j w_{ij} v_i v_j$$

where $S^2 = (n-1)^{-1} \sum_i v_i^2$, and $W = \sum_i \sum_{j \neq i} w_{ij}$.

Another measure of spatial autocorrelation in PROC VARIOGRAM is Geary's c statistic (Geary 1954), defined as

$$c = \frac{1}{2S^2 W} \sum_i \sum_j w_{ij} (z_i - z_j)^2$$

These expressions indicate that Moran's I coefficient makes use of the centered variable, whereas the Geary's c expression uses the noncentered values in the summation.

Inference on these two statistic types comes from approximate tests based on the asymptotic distribution of I and c, which both tend to a normal distribution as n increases. To this end, PROC VARIOGRAM calculates the means and variances of I and c. The outcome depends on the assumption made regarding the distribution $Z(\boldsymbol{s})$. In particular, you can choose to investigate any of the statistics under the *normality* (also known as *Gaussianity*) or the *randomization* assumption. Cliff and Ord (1981) provided the equations for the means and variances of the I and c distributions, as described in the following.

The normality assumption asserts that the random field $Z(\boldsymbol{s})$ follows a normal distribution of constant mean ($\bar{Z}$) and variance, from which the z_i values are drawn. In this case, the I statistics yield

$$\mathrm{E}_g[I] = -\frac{1}{n-1}$$

and

$$\mathrm{E}_g[I^2] = \frac{1}{(n+1)(n-1)W^2}(n^2 S_1 - nS_2 + 3W^2)$$

where $S_1 = 0.5\sum_i \sum_{j \neq i}(w_{ij} + w_{ji})^2$ and $S_2 = \sum_i(\sum_j w_{ij} + \sum_j w_{ji})^2$. The corresponding moments for the c statistics are

$$\mathrm{E}_g[c] = 1$$

and

$$\mathrm{Var}_g[c] = \frac{(2S_1 + S_2)(n-1) - 4W^2}{2(n+1)W^2}$$

According to the randomization assumption, the I and c observations are considered in relation to all the different values that I and c could take, respectively, if the n z_i values were repeatedly randomly permuted around the domain D. The moments for the I statistics are now

$$\mathrm{E}_r[I] = -\frac{1}{n-1}$$

and

$$\mathrm{E}_r[I^2] = \frac{A_1 + A_2}{(n-1)(n-2)(n-3)W^2}$$

where $A_1 = n[(n^2 - 3n + 3)S_1 - nS_2 + 3W^2]$, $A_2 = -b_2[n(n-1)S_1 - 2nS_2 + 6W^2]$. The factor $b_2 = m_4/(m_2{}^2)$ is the coefficient of kurtosis that uses the sample moments $m_k = \frac{1}{n}\sum_i v_i^k$ for $k = 2, 4$. Finally, the c statistics under the randomization assumption are given by

$$\mathrm{E}_r[c] = 1$$

and

$$\mathrm{Var}_r[c] = \frac{B_1 + B_2 + B_3}{n(n-2)(n-3)W^2}$$

with $B_1 = (n-1)S_1[n^2 - 3n + 3 - (n-1)b_2]$, $B_2 = -\frac{1}{4}(n-1)S_2[n^2 + 3n - 6 - (n^2 - n + 2)b_2]$, and $B_3 = W^2[n^2 - 3 - b_2(n-1)^2]$.

If you specify LAGDISTANCE= to be larger than the maximum data distance in your domain, the binary weighting scheme used by the VARIOGRAM procedure leads to all weights $w_{ij} = 1, i \neq j$. In this extreme case the preceding definitions can show that the variances of the I and c statistics become zero under either the normality or the randomization assumption.

A similar effect might occur when you have collocated observations (see the section "Pair Formation" on page 10080). The Moran's I and Geary's c statistics allow for the inclusion of such pairs in the computations. Hence, contrary to the semivariance analysis, PROC VARIOGRAM does not exclude pairs of collocated data from the autocorrelation statistics.

Interpretation

For Moran's I coefficient, $I > \mathrm{E}[I]$ indicates positive autocorrelation. Positive autocorrelation suggests that neighboring values $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ tend to have similar feature values z_i and z_j, respectively. When $I < \mathrm{E}[I]$, this is a sign of negative autocorrelation, or dissimilar values at neighboring locations. A measure of strength of the autocorrelation is the size of the absolute difference $\mid I - \mathrm{E}[I] \mid$.

Geary's c coefficient interpretation is analogous to that of Moran's I. The only difference is that $c > \mathrm{E}[c]$ indicates negative autocorrelation and dissimilarity, whereas $c < \mathrm{E}[c]$ signifies positive autocorrelation and similarity of values.

The VARIOGRAM procedure uses the mathematical definitions in the preceding section to provide the observed and expected values, and the standard deviation of the autocorrelation coefficients in the autocorrelation statistics table. The Z scores for each type of statistics are computed as

$$Z_I = \frac{I - \mathrm{E}[I]}{\sqrt{\mathrm{Var}[I]}}$$

for Moran's I coefficient, and

$$Z_c = \frac{c - \mathrm{E}[c]}{\sqrt{\mathrm{Var}[c]}}$$

for Geary's c coefficient. PROC VARIOGRAM also reports the two-sided p-value for each coefficient under the null hypothesis that the sample values are not autocorrelated. Smaller p-values correspond to stronger autocorrelation for both the I and c statistics. However, the p-value does not tell you whether the autocorrelation is positive or negative. Based on the preceding remarks, you have positive autocorrelation when $Z_I > 0$ or $Z_c < 0$, and you have negative autocorrelation when $Z_I < 0$ or $Z_c > 0$.

The Moran Scatter Plot

The Moran scatter plot (Anselin 1996) is a useful visual tool for exploratory analysis, because it enables you to assess how similar an observed value is to its neighboring observations. Its horizontal axis is based on the values of the observations and is also known as the response axis. The vertical Y axis is based on the weighted average or spatial lag of the corresponding observation on the horizontal X axis. **NOTE:** The term *spatial lag* in the current context is unrelated to the concept of the semivariogram lag presented in the section "Distance Classification" on page 10083.

The Moran scatter plot provides a visual representation of spatial associations in the neighborhood around each observation. You specify a neighborhood size with the LAGDISTANCE= option in the COMPUTE statement. The observations are represented by their standardized values; therefore only nonmissing observations are shown in the plot. For each one of those, the VARIOGRAM procedure computes the weighted average, which is the weighted mean value of its neighbors. Then, the centered weighted average is plotted against the standardized observations. As a result, the scatter plot is centered on the coordinates $(0, 0)$, and distances in the plot are expressed in deviations from the origin $(0, 0)$.

Depending on their position on the plot, the Moran plot data points express the level of spatial association of each observation with its neighboring ones. Conceptually, these characteristics differentiate the Moran plot from the semivariogram. The latter is typically used in geostatistics to depict spatial associations across the whole domain as a continuous function of a distance metric.

You can find the data points on the Moran scatter plot in any of the four quadrants defined by the horizontal line $y = 0$ and the vertical line $x = 0$. Points in the upper right (or high-high) and lower left (or low-low) quadrants indicate positive spatial association of values that are higher and lower than the sample mean, respectively. The lower right (or high-low) and upper left (or low-high) quadrants include observations that exhibit negative spatial association; that is, these observed values carry little similarity to their neighboring ones.

When you use binary, row-averaged weights for the creation of the Moran scatter plot and in autocorrelation statistics, Moran's I coefficient is equivalent to the regression slope of the Moran scatter plot. That is, when you specify

```
PLOTS=MORAN(ROWAVG=ON)
```

in the PROC VARIOGRAM statement and

```
AUTOCORR(WEIGHTS=BINARY(ROWAVERAGING))
```

in the COMPUTE statement, then the regression line slope of the Moran scatter plot is the Moran's I coefficient shown in the section "Autocorrelation Statistics Types" on page 10101. In this sense, the Moran's I coefficient has a global character, whereas the Moran scatter plot provides you with a more detailed exploratory view of the autocorrelation behavior of the individual observations.

This detailed view can reveal outliers with respect to the regression line slope of the Moran scatter plot. Outliers, if present, can function as leverage points that affect the value of Moran's I coefficient. As noted by Anselin (1996), such extremes indicate local instability in spatial association. This instability can be caused either by problems with the autocorrelation weights matrix or by fine-scale characteristics of the spatial structure, which are beneath the current observation structure.

Computational Resources

The fundamental computation of the VARIOGRAM procedure is binning: for each pair of observations in the input data set, a distance class and an angle class are determined and recorded. Let N_d denote the number of distance classes, N_a denote the number of angle classes, and N_v denote the number of VAR variables. The memory requirements for these operations are proportional to $N_d \times N_a \times N_v$. This is typically small.

The CPU time required for the computations is proportional to the number of pairs of observations, or to $N^2 \times N_v$, where N is the number of observations in the input data set.

Output Data Sets

The VARIOGRAM procedure produces four data sets: the OUTACWEIGHTS=*SAS-data-set*, the OUTDIST=*SAS-data-set*, the OUTPAIR=*SAS-data-set*, and the OUTVAR=*SAS-data-set*. These data sets are described in the following sections.

OUTACWEIGHTS=*SAS-data-set*

The OUTACWEIGHTS= data set contains one observation for each pair of points P_1, P_2 in the original data set, where P_1 is different from P_2, with information about the data distance and autocorrelation weight of each point pair.

The OUTACWEIGHTS= data set can be very large, even for a moderately sized DATA= data set. For example, if the DATA= data set has NOBS=500, then the OUTACWEIGHTS= data set has NOBS(NOBS $-$ 1)/2=124,750 observations.

When you perform autocorrelation computations, the OUTACWEIGHTS= data set is a practical way to save the autocorrelation weights for further use.

The OUTACWEIGHTS= data set contains the following variables:

- ACWGHT12, the autocorrelation weight for the pair P_1, P_2
- ACWGHT21, the autocorrelation weight for the pair P_2, P_1
- DISTANCE, the distance between the data in the pair
- ID1, the ID variable value or observation number for the first point in the pair
- ID2, the ID variable value or observation number for the second point in the pair
- V1, the variable value for the first point in the pair
- V2, the variable value for the second point in the pair
- VARNAME, the variable name for the current VAR variable
- X1, the x coordinate of the first point in the pair
- X2, the x coordinate of the second point in the pair
- Y1, the y coordinate of the first point in the pair
- Y2, the y coordinate of the second point in the pair

When the autocorrelation weights are symmetric, the pair P_1, P_2 has the same weight as the pair P_2, P_1. For this reason, in the case of symmetric weights the OUTACWEIGHTS= data set contains only the autocorrelation weights ACWGHT12.

If no ID statement is specified, then the corresponding observation number is assigned to each one of the variables ID1 and ID2, instead.

OUTDIST=*SAS-data-set*

The OUTDIST= data set contains counts for a modified histogram that shows the distribution of pairwise distances. This data set provides you with information related to the choice of values for the LAGDISTANCE= option in the COMPUTE statement.

To request an OUTDIST= data set, specify the OUTDIST= data set in the PROC VARIOGRAM statement and the NOVARIOGRAM option in the COMPUTE statement. The NOVARIOGRAM option prevents any semivariogram or covariance computation from being performed.

The following variables are written to the OUTDIST= data set:

- COUNT, the number of pairs that fall into this lag class
- LAG, the lag class value
- LB, the lower bound of the lag class interval
- UB, the upper bound of the lag class interval
- PER, the percent of all pairs that fall in this lag class
- VARNAME, the name of the current VAR variable

OUTMORAN=*SAS-data-set*

The OUTMORAN= data set contains the standardized value (or response) of each observation and the weighted average of its N neighbors, based on a neighborhood within a LAGDISTANCE= distance from the observation. To request this data set, specify the OUTMORAN= data set in the PROC VARIOGRAM statement, in addition to the AUTOCORRELATION and LAGDISTANCE= options in the COMPUTE statement.

The following variables are written to the OUTMORAN= data set:

- DISTANCE, the value of the neighborhood radius, which is specified with the LAGDISTANCE= option
- ID, the ID variable value or observation number for the current observation
- N, the number of neighbors within the specified DISTANCE from the current observation
- RESPONSE, the standardized value of the current observation
- STDWAVG, the standardized weighted average of the neighbors for the current observation
- V, the variable value of the current observation
- VARNAME, the variable name for the current VAR variable
- X, the x coordinate of the current observation
- Y, the y coordinate of the current observation
- WAVG, the weighted average of the neighbors for the current observation

For zero neighbors in the neighborhood of a nonmissing observation, the corresponding value of the variable N=0 and the variables STDWAVG and WAVG are assigned missing values. Observations with missing values are included in the OUTMORAN= data set if they have neighbors and only if nonmissing observations with neighbors also exist in the same data set.

OUTPAIR=*SAS-data-set*

When you specify the NOVARIOGRAM option in the COMPUTE statement, the OUTPAIR= data set contains one observation for each distinct pair of points P_1, P_2 in the original data set. Otherwise, the OUTPAIR= data set might have fewer observations, depending on the values you specify in the LAGDISTANCE= and MAXLAGS= options and whether you specify the OUTPDISTANCE= option in the COMPUTE statement.

If the NOVARIOGRAM option is not specified in the COMPUTE statement, then the OUTPAIR= data set contains one observation for each distinct pair of points that are up to a distance within MAXLAGS= away from each other. If you also specify the OUTPDISTANCE=D_{max} option in the COMPUTE statement, then all pairs P_1, P_2 in the original data set that satisfy the relation $\mid P_1 P_2 \mid \leq D_{max}$ are written to the OUTPAIR= data set.

Given the aforementioned specifications, note that the OUTPAIR= data set can be very large even for a moderately sized DATA= data set. For example, if the DATA= data set has NOBS=500, then the OUTPAIR= data could have up to NOBS(NOBS $-$ 1)/2=124,750 observations if no OUTPDISTANCE= restriction is given in the COMPUTE statement.

The OUTPAIR= data set contains information about the distance and orientation of each point pair, and you can use it for specialized continuity measure calculations.

The OUTPAIR= data set contains the following variables:

- AC, the angle class value
- COS, the cosine of the angle between pairs
- DC, the distance (lag) class
- DISTANCE, the distance between the data in pairs
- ID1, the ID variable value or observation number for the first point in the pair
- ID2, the ID variable value or observation number for the second point in the pair
- V1, the variable value for the first point in the pair
- V2, the variable value for the second point in the pair
- VARNAME, the variable name for the current VAR variable
- X1, the *x* coordinate of the first point in the pair
- X2, the *x* coordinate of the second point in the pair
- Y1, the *y* coordinate of the first point in the pair
- Y2, the *y* coordinate of the second point in the pair

If no ID statement is specified, then the corresponding observation number is assigned to each one of the variables ID1 and ID2, instead.

OUTVAR=*SAS-data-set*

The OUTVAR= data set contains the standard and robust versions of the sample semivariance, the covariance, and other information in each lag class.

The OUTVAR= data set contains the following variables:

- ANGLE, the angle class value (clockwise from N to S)
- ATOL, the angle tolerance for the lag or angle class
- AVERAGE, the average variable value for the lag or angle class
- BANDW, the bandwidth for the lag or angle class
- COUNT, the number of pairs in the lag or angle class
- COVAR, the covariance value for the lag or angle class
- DISTANCE, the average lag distance for the lag or angle class
- LAG, the lag class value (in LAGDISTANCE= units)
- RVARIO, the sample robust semivariance value for the lag or angle class
- STDERR, the approximate standard error of the sample semivariance estimate
- VARIOG, the sample semivariance value for the lag or angle class
- VARNAME, the name of the current VAR variable

The robust semivariance estimate, RVARIO, is not included in the data set if you omit the option ROBUST in the COMPUTE statement.

The bandwidth variable, BANDW, is not included in the data set if no bandwidth specification is given in the COMPUTE statement or in a DIRECTIONS statement.

The OUTVAR= data set contains a line where the LAG variable is –1. The AVERAGE variable in this line displays the sample mean value $\bar{Z}$ of the SRF $Z(\boldsymbol{s})$, and the COVAR variable shows the sample variance $\mathrm{Var}[Z(\boldsymbol{s})]$.

Displayed Output

In addition to the output data sets, the VARIOGRAM procedure produces a variety of output objects. Most of these are produced depending on whether you specify either NOVARIOGRAM or LAGDISTANCE= and MAXLAGS= in the COMPUTE statement. The VARIOGRAM 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 default map that shows the spatial distribution of the observations of the current variable in the VAR statement. The observations are displayed by default with circled markers whose color indicates the VAR value at the corresponding location.
- a table with basic information about the lags and the extreme distance between data pairs, when NOVARIOGRAM is specified
- a table that describes the distribution of data pairs in distance intervals, when NOVARIOGRAM is specified
- a histogram plot of the pairwise distance distribution, when NOVARIOGRAM is specified). The plot also displays a reference line at a user-specified pairs frequency threshold when you specify the THRESHOLD= parameter in the PLOTS=PAIRS option. The option PLOTS=PAIRS(NOINSET) forces the informational inset that appears in the plot to hide.
- empirical semivariogram details, when NOVARIOGRAM is not specified and LAGDISTANCE= and MAXLAGS= are specified. This table also includes the semivariance estimate variance and confidence limits when CL is specified, and estimates of the robust semivariance when ROBUST is specified.
- plots of the appropriate empirical semivariograms, when NOVARIOGRAM is not specified and LAGDISTANCE= and MAXLAGS= are specified. If you perform the analysis in more than one direction simultaneously, the output is a panel that contains the empirical semivariogram plots for the specified angles. If the semivariograms are nonpaneled, then each plot includes in the lower part a needle plot of the contributing pairs distribution.
- a table that provides autocorrelation statistics, when the options AUTOCORRELATION and LAGDISTANCE= are specified
- the Moran scatter plot of the standardized observation values against the weighted averages of their neighbors, when the options PLOTS=MORAN, AUTOCORRELATION, and LAGDISTANCE= are specified

When you specify the MODEL statement and request a fit of a theoretical model to the empirical semivariogram, the VARIOGRAM procedure also produces the following default output:

- a table with some general fitting information, in addition to the output item store if you have specified one with the STORE statement
- a table with more specific information about the selected model's parameters and their initial values
- a table with general information about the optimization that provides the fitting parameters of the selected model
- a table with the optimization process output and a table with the convergence status of the optimization process, if you have specified a single model to fit
- a "Parameter Estimates" table with information about the fitted parameters estimates
- a "Fit Summary" table that reports the fit quality of all models you requested to fit

- plots of fitted theoretical semivariogram models. If you perform model fitting in more than one direction angle or for more than one variable in your DATA= data set, then the output is a panel that contains all fitted models for the respective directions or variables.

Additional output can be produced in model fitting if you specify a higher level of output detail with the DETAILS option in the MODEL statement. This output can be information tables for each separate model when you specify multiple models to fit, tables with more details about the optimization process, and the covariance and correlation matrices of the model parameter estimates. The complete listing of the PROC VARIOGRAM output follows in the section "ODS Table Names" on page 10110 and the section "ODS Graph Names" on page 10111.

ODS Table Names

Each table created by PROC VARIOGRAM has a name associated with it, and you must use this name to refer to the table when using ODS Graphics. These names are listed in Table 124.6.

Table 124.6 ODS Tables Produced by PROC VARIOGRAM

ODS Table Name	Description	Required Statement	Option
AutoCorrStats	Autocorrelation statistics information	COMPUTE	AUTOCORRELATION
ConvergenceStatus	Status of optimization at conclusion	MODEL	Default output
CorrB	Approximate correlation matrix of model parameter estimates	MODEL	CORRB
CovB	Approximate covariance matrix of model parameter estimates	MODEL	COVB
DistanceIntervals	Pairwise distances matrix	COMPUTE	NOVARIOGRAM
FitGenInfo	General fitting information	MODEL	Default output
FitSummary	Fitting process summary	MODEL	Default output
InputOptions	Optimization input options	MODEL	DETAILS=ALL
IterHist	Iteration history	MODEL	DETAILS=ITR
IterStop	Optimization-related results	MODEL	Default output
Lagrange	Information about Lagrange multipliers	MODEL	DETAILS=ALL
ModelInfo	Model information	MODEL	Default output
NObs	Number of observations read and used	PROC	Default output
OptInfo	Optimization information	MODEL	Default output
PairsInformation	General information about the pairs distribution in classes and data maximum distances in selected directions	COMPUTE	NOVARIOGRAM

Table 124.6 *continued*

ODS Table Name	Description	Required Statement	Option
ParameterEstimates	Model fitting solution and statistics	MODEL	Default output
ParameterEstimatesResults	Parameter estimates and gradient information	MODEL	DETAILS=ALL
ParameterEstimatesStart	More detailed model information	MODEL	DETAILS=ITR
ParmSearch	Parameter search values	MODEL	Default output
ProblemDescription	Information at the optimization start	MODEL	DETAILS=ITR
ProjGrad	Projected gradient information	MODEL	DETAILS=ALL
SemivariogramTable	Empirical semivariance classes, parameters, and estimates	COMPUTE	LAGD=, MAXLAGS=

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 VARIOGRAM Statement" on page 10041.

ODS Graph Names

PROC VARIOGRAM assigns a name to each graph it creates by using ODS Graphics. You can use this name to refer to the graph when using ODS Graphics. You must also specify the PLOTS= option indicated in Table 124.7.

Table 124.7 Graphs Produced by PROC VARIOGRAM

ODS Graph Name	Plot Description	Statement	Option
FitPanel	Panel of one or more classes of fitted semivariograms in different angles	PROC	PLOTS=FIT
FitPlot	Plot of one or more classes of fitted semivariograms	PROC	PLOTS=FIT

Table 124.7 *continued*

ODS Graph Name	Plot Description	Statement	Option
MoranPlot	Scatter plot of standardized observed values against weighted averages	PROC	PLOTS=MORAN
ObservationsPlot	Scatter plot of observed data and colored markers that indicates observed values	PROC	PLOTS=OBSERV
PairDistPlot	Histogram of the pairwise distance distribution	PROC	PLOTS=PAIRS
Semivariogram	Plots of empirical classical and robust (optional) semivariograms	PROC	PLOTS=SEMIVAR
SemivariogramPanel	Panel of empirical classical and robust (optional) semivariogram plots	PROC	PLOTS=SEMIVAR

Examples: VARIOGRAM Procedure

Example 124.1: Aspects of Semivariogram Model Fitting

This example helps you explore aspects of automated semivariogram fitting with PROC VARIOGRAM. The test case is a spatial study of arsenic (As) concentration in drinking water.

Arsenic is a toxic pollutant that can occur in drinking water because of human activity or, typically, due to natural release from the sediments in water aquifers. The World Health Organization has a standard that allows As concentration up to a maximum of 10 μg/lt (micrograms per liter) in drinking water.

In general, natural release of arsenic into groundwater is very slow. Arsenic concentration in water might exhibit no significant temporal fluctuations over a period of a few months. For this reason, it is acceptable to perform a spatial study of arsenic with input from time-aggregated pollutant concentrations. This example makes use of this assumption for its data set logAsData. The data set consists of 138 simulated observations from wells across a square area of 500 km $\times$ 500 km. The variable logAs in the logAsData data set is the natural logarithm of arsenic concentration. Often, the natural logarithm of arsenic concentration (logAs) is used as the random variable to facilitate the analysis because its distribution tends to resemble the normal distribution.

The goal is to explore spatial continuity in the logAs observations. The following statements read the logAs values from the logAsData data set:

```
title 'Semivariogram Model Fitting of Log-Arsenic Concentration';

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
;
```

First you want to inspect the logAs data for surface trends and the pairwise distribution. You run the VARIOGRAM procedure with the NOVARIOGRAM option in the COMPUTE statement. You also request the PLOTS=PAIRS(MID) option, which prompts the pair distance plot to display the actual distance between pairs, rather than the lag number itself, in the midpoint of the lags. You use the following statements:

```
ods graphics on;

proc variogram data=logAsData plots=pairs(mid);
   compute novariogram nhc=50;
   coord xc=East yc=North;
   var logAs;
run;
```

The observations scatter plot in Output 124.1.1 shows a rather uniform distribution of the locations in the study domain. Reasonably, neighboring values of logAs seem to exhibit some correlation. There seems to be no definite sign of an overall surface trend in the logAs values. You can consider that the observations are trend-free, and proceed with estimation of the empirical semivariance.

Output 124.1.1 logAs Observation Data Scatter Plot

The observed logAs values go as high as 3.28091, which corresponds to a concentration of 26.6 μg/lt. In fact, only three observations exceed the health standard of 10 μg/lt (or about 2.3 in the log scale), and they are situated in relatively neighboring locations to the east of the domain center.

Based on the discussion in section "Preliminary Spatial Data Analysis" on page 10028, the pair distance plot in Output 124.1.2 suggests that you could consider pairs that are anywhere around up to half the maximum pairwise distance of about 700 km.

Output 124.1.2 Distribution of Pairwise Distances for logAs Data

After some experimentation with values for the LAGDISTANCE= and MAXLAGS= options, you actually find that a lag distance of 5 km over 40 lags can provide a clear representation of the logAs semivariance. With respect to Output 124.1.2, this finding indicates that in the current example it is sufficient to consider pairs separated by a distance of up to 200 km. You run the following statements to obtain the empirical semivariogram:

```
proc variogram data=logAsData plots(only)=semivar;
   compute lagd=5 maxlag=40;
   coord xc=East yc=North;
   var logAs;
run;
```

The first few lag classes of the logAs empirical semivariance table are shown in Output 124.1.3.

Output 124.1.3 Partial Output of the Empirical Semivariogram Table for logAs Data

Semivariogram Model Fitting of Log-Arsenic Concentration

The VARIOGRAM Procedure
Dependent Variable: logAs

Empirical Semivariogram

Lag Class	Pair Count	Average Distance	Semivariance
0	1	1.9	0.111
1	5	4.9	0.145
2	6	9.7	0.286
3	11	14.6	0.545
4	27	20.0	0.900

Output 124.1.3 and Output 124.1.4 indicate that the logarithm of arsenic spatial correlation starts with a small nugget effect around 0.11 and rises to a sill value that is most likely between 1.4 and 1.8. The rise could be of exponential type, although the smooth increase of semivariance close to the origin could also suggest Gaussian behavior. You suspect that a Matérn form might also work, since its smoothness parameter ν can regulate the form to exhibit an intermediate behavior between the exponential and Gaussian forms.

Output 124.1.4 Empirical Semivariogram for logAs Data

You can investigate all of the preceding clues with the model fitting features of PROC VARIOGRAM. The simplest way to fit a model is to specify its form in the MODEL statement. In this case, you have the added complexity of having more than one possible candidate. For this reason, you use the FORM=AUTO option that picks the best fit out of a list of candidates. Within this option you specify the MLIST= suboption to use the exponential, Gaussian, and Matérn forms. You also specify the NEST= suboption to request fitting of a model with up to two nested structures. Eventually, you specify the PLOTS=FIT option to produce a plot of the fitted models. The STORE statement saves the fitting output into an item store you name SemivAsStore for future use. You apply these specifications with the following statements:

```
proc variogram data=logAsData plots(only)=fit;
   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;

ods graphics off;
```

The table of general information about fitting is shown in Output 124.1.5. The table lets you know that 12 model combinations are to be tested for weighted least squares fitting, based on the three forms that you specified.

Output 124.1.5 Semivariogram Model Fitting General Information

Semivariogram Model Fitting of Log-Arsenic Concentration

The VARIOGRAM Procedure

Dependent Variable: logAs
Angle: Omnidirectional

Semivariogram Model Fitting	
Model	Selection from 12 form combinations
Output Item Store	WORK.SEMIVASSTORE
Item Store Label	LogAs Concentration Models

The combinations include repetitions. For example, you specified the GAU form; hence the GAU-GAU form is tested, too. The model combinations also include permutations. For example, you specified the GAU and the EXP forms; hence the GAU-EXP and EXP-GAU models are fitted separately. According to the section "Nested Models" on page 10077, it might seem that the same model is fitted twice. However, in each of these two cases, each structure starts the fitting process with different parameter initial values. This can lead GAU-EXP to a different fit than EXP-GAU leads to, as seen in the fitting summary table in Output 124.1.6. The table shows all the model combinations that were tested and fitted. By default, the ordering is based on the weighted sum of squares error criterion, and you can see that the lowest values in the Weighted SSE column are in top slots of the list.

Output 124.1.6 Semivariogram Model Fitting Summary

Fit Summary			
Class	**Model**	**Weighted SSE**	**AIC**
1	Gau-Gau	25.42435	-9.59246
	Gau-Mat	25.42482	-7.59169
2	Exp-Gau	25.97835	-8.70865
3	Exp-Mat	26.36846	-6.09754
4	Mat	26.37519	-10.08708
5	Gau	26.78629	-11.45296
6	Exp	28.01200	-9.61851
	Exp-Exp	28.01200	-5.61850
	Mat-Exp	28.01200	-3.61850
	Gau-Exp	28.01200	-5.61850

Note the leftmost Class column in Output 124.1.6. As explained in detail in section "Classes of Equivalence" on page 10099, when you fit more than one model, all fitted models that compute the same semivariance are placed in the same class of equivalence. For example, in this fitting example the top ranked GAU-GAU and GAU-MAT nested models produce indistinguishable semivariograms; for that reason they are both placed in the same class 1 of equivalence. The same occurs with the EXP, GAU-EXP, EXP-EXP, and MAT-EXP models in the bottom of the table. By default, PROC VARIOGRAM uses the AIC as a secondary classification criterion; hence models in each equivalence class are already ordered based on their AIC values.

Another remark in Output 124.1.6 is that despite submitting 12 model combinations for fitting, the table shows only 10. You can easily see that the combinations MAT-GAU and MAT-MAT are not among the listed models in the fit summary. This results from the behavior of the VARIOGRAM procedure in the following situation: A parameter optimization takes place during the fitting process. In the present case the optimizer keeps increasing the Matérn smoothness parameter ν in the MAT-GAU model. At the limit of an infinite ν parameter, the Matérn form becomes the Gaussian form. For that reason, when the parameter ν is driven towards very high values, PROC VARIOGRAM automatically replaces the Matérn form with the Gaussian. This switch converts the MAT-GAU model into a GAU-GAU model. However, a GAU-GAU model already exists among the specified forms; consequently, the duplicate GAU-GAU model is skipped, and the fitted model list is reduced by one model. A similar explanation justifies the omission of the MAT-MAT model from the fit summary table.

In our example, the nested Gaussian-Gaussian model is the fitting selection of the procedure based on the default ranking criteria. Output 124.1.7 displays additional information about the selected model. In particular, you see the table with general information about the Gaussian-Gaussian model, the initial values used for its parameters, and information about the optimization process for the fitting.

Output 124.1.7 Fitting and Optimization Information for Gaussian-Gaussian Model

Semivariogram Model Fitting	
Name	Gaussian-Gaussian
Label	Gau-Gau

Model Information	
Parameter	**Initial Value**
Nugget	0.0903
GauScale1	0.6709
GauRange1	100.0
GauScale2	0.6709
GauRange2	50.0230

Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	5
Lower Boundaries	5
Upper Boundaries	0
Starting Values From	PROC

The estimated parameter values of the selected Gaussian-Gaussian model are shown in Output 124.1.8.

Output 124.1.8 Parameter Estimates of the Fitting Selected Model

Parameter Estimates					
Parameter	Estimate	Approx Std Error	DF	t Value	Approx Pr > |t|
Nugget	0.08308	0.05097	36	1.63	0.1118
GauScale1	0.3277	0.2077	36	1.58	0.1234
GauRange1	62.3127	19.8488	36	3.14	0.0034
GauScale2	1.2615	0.2070	36	6.10	<.0001
GauRange2	21.4596	3.2722	36	6.56	<.0001

By default, when you specify more than one model to fit, PROC VARIOGRAM produces a fit plot that compares the first five classes of the successfully fit candidate models. The model that is selected according to the specified fitting criteria is shown with a thicker line in the plot.

You can modify the number of displayed equivalence classes with the NCLASSES= suboption of the PLOTS=FIT option. When you have such comparison plots, PROC VARIOGRAM displays the representative model from each class of equivalence.

The default fit plot for the current model comparison is shown in Output 124.1.9. The legend informs you there is one more model in the first class of equivalence, as the fitting summary table indicated earlier in Output 124.1.6.

Output 124.1.9 Fitted Theoretical and Empirical logAs Concentration Semivariograms for the Specified Models

In the present example, all fitted models in the first five classes have very similar semivariograms. The selected Gaussian-Gaussian model seems to have a relatively larger range than the rest of the displayed models, but you can expect any of these models to exhibit a near-identical behavior in terms of spatial correlation. As a result, all models in the displayed classes are likely to lead to very similar output, if you proceed to use any of them for spatial prediction.

In that sense, semivariogram fitting is a partially subjective process, for which there might not exist only one single correct answer to solve your problem. In the context of the example, on one hand you might conclude that the selected Gaussian-Gaussian model is exactly sufficient to describe spatial correlation in the arsenic study. On the other hand, the similar performance of all models might prompt you to choose instead a more simple non-nested model for prediction like the Matérn or the Gaussian model.

Regardless of whether you might opt to sacrifice the statistically best fit (depending on your selected criteria) to simplicity, eventually you are the one to decide which approach serves your study optimally. The model fitting features of PROC VARIOGRAM offer you significant assistance so that you can assess your options efficiently.

Example 124.2: An Anisotropic Case Study with Surface Trend in the Data

This example shows how to examine data for nonrandom surface trends and anisotropy. You use simulated data where the variable is atmospheric ozone (O_3) concentrations measured in Dobson units (DU). The coordinates are offsets from a point in the southwest corner of the measurement area, with the east and north distances in units of kilometers (km). You work with the ozoneSet data set that contains 300 measurements in a square area of 100 km × 100 km.

The following statements read the data set:

```
title 'Semivariogram Analysis in Anisotropic Case With Trend Removal';

data ozoneSet;
   input East North Ozone @@;
   datalines;
34.9 68.2 286  39.2 12.5 270  44.4 37.7 275  90.5 27.0 282
91.1 40.8 285  98.6 61.6 294  61.8 26.7 281  64.0 11.5 274
22.4 26.5 274  89.3 18.3 279  32.3 28.3 274  31.1 53.1 279
43.0 17.5 272  79.3 42.3 283  99.9 57.9 291   1.8 24.1 273
81.7 73.5 294  22.9 32.0 273  64.9 67.5 292  76.5 56.3 285
78.7 11.7 276  61.8 99.3 307  49.1 86.6 299  40.0 35.8 273
69.3  3.8 278  23.4  9.3 270  66.3 94.3 304  71.3  6.5 275
 9.7 54.4 280  85.2 81.7 300  30.3 60.9 284  94.6 94.3 309
10.6 10.3 271  73.0 43.0 280   4.9 50.7 280  19.0 79.4 289
 2.4 73.1 287  77.7 25.2 278   8.4 27.1 276  93.5 19.7 279
 0.2 34.5 275  50.4 91.3 302  55.7 26.2 279  50.3  2.3 274
16.3 84.4 293  19.0  6.9 272  57.1 92.3 303  61.0  0.4 275
10.7 18.7 271  15.2 43.5 277  67.0 87.4 301  79.0 54.0 285
36.0 53.3 279  58.3 52.1 282  56.6 79.7 294  40.4 32.4 275
48.9 64.1 286  54.0 54.9 281  27.5 48.5 279  36.4 30.3 275
10.5 31.0 273  87.0 39.4 283  47.9 37.5 274  64.7 63.4 288
 0.5 90.8 294  22.8 22.4 275  31.1 78.8 291  93.6 49.8 290
 2.5 39.3 273  83.6 25.6 282  49.8 24.1 278  73.1 91.8 305
30.5 90.6 297  26.0 61.2 284  58.4 66.2 289  30.5  4.3 273
38.3 85.6 298  89.2 96.6 309  53.4  6.3 275  27.3 12.8 271
43.4 56.5 281  99.5 86.9 305  85.8 22.8 281  83.0 10.9 278
24.8 16.7 271  51.1 18.8 275  59.0 54.3 283  35.5 91.4 298
18.1 56.0 279  78.0 36.4 277  56.8  6.9 275  21.1 44.5 277
73.9 75.9 296  54.2  0.1 274  33.2 75.1 290  38.2  3.3 274
15.2 14.7 272  15.9 84.2 292  60.2 95.2 304   9.8 27.2 276
91.2 56.4 289  94.7 86.9 303  56.7 49.6 281  24.2  9.5 270
43.0 17.0 272  85.9 10.7 278  53.9 41.1 276  30.4 63.4 286
62.8 86.3 299  76.8 24.6 279  31.6 94.0 300  26.9 73.8 287
18.9 68.4 284  99.4 37.2 285  79.1  3.3 277  34.9 74.7 289
 6.4 33.8 277  48.4 82.2 294  86.0 58.0 289  92.0 60.4 293
50.2 91.6 300  12.2 38.3 275  72.7 48.9 283  82.7 34.1 279
77.0 51.0 286  86.6 15.8 278  42.0 42.7 277  99.3  8.2 278
17.4 70.6 286  11.2 92.4 295  60.2 28.8 280  92.0 73.3 297
25.3 30.6 273  36.6  8.9 274  34.2  4.4 273  26.6 54.7 278
 1.7 27.4 278  49.6  1.1 275  62.8 89.3 301  28.0 49.3 279
51.2 75.1 293  59.3 93.5 304  83.6 90.5 304  79.4 87.0 302
78.0 28.3 281  16.8 19.1 272   9.1 81.2 292  23.7 55.8 277
```

```
75.5 21.3 279  64.4 43.3 279  38.9 98.9 303  22.5 87.9 293
96.7 37.9 285  92.3 93.9 308  16.9 25.4 273  15.2 61.5 283
73.8 94.0 306  57.4 97.2 305  73.2  4.9 276  39.2 82.3 294
95.7 99.4 315  66.0 98.4 306  95.3 26.9 283  45.4 75.3 291
64.8 15.4 276  69.8 55.4 284  36.3 74.9 290   9.9 22.2 276
65.8 13.9 276  13.0 82.0 293  95.6 77.2 301  32.5 55.6 279
45.8 35.5 275  62.2  6.6 274  25.2 51.2 279  92.4  8.1 277
40.5 35.3 273   9.9  3.9 271  43.5 44.0 278  68.6 61.3 287
64.2 77.5 296  57.6 81.6 294  69.5 64.7 291  64.3 95.1 304
 2.8 62.4 283  33.2 83.3 294  10.7 71.0 285  24.3 88.2 294
94.5 32.2 283  21.0 67.6 286  20.1 71.6 286  85.2 71.3 296
94.8 30.7 283  53.4 92.0 301  81.0 50.0 287  54.6 29.9 277
71.1 90.1 303  15.2  2.9 271  83.6 17.8 278  76.0 21.8 279
55.6 37.4 275  86.7 83.7 303  43.6 83.6 295  44.2 31.7 274
90.0 83.3 300   6.2  0.5 270  42.2 87.7 298  31.7  4.3 273
91.4 41.2 285  78.0 50.6 286  27.1 56.1 278  72.6 63.9 291
29.3 49.9 281  49.0 36.9 275  13.9 53.5 280  93.1 83.2 300
73.0 61.6 289  63.1 27.5 280  38.3 72.5 287  72.7 34.2 277
 6.9 32.3 274  17.1 58.6 280  19.6 94.6 297   2.7 36.5 276
34.5  5.5 275  98.6 95.9 313   9.1 71.1 285  88.6 55.8 287
26.8 78.5 289  64.8 66.6 292  59.7 25.7 280  47.3 70.2 288
 6.1 94.4 296  50.5 82.7 296   9.1 41.6 276  86.0 71.0 296
75.2 69.8 293  73.3 84.8 300  42.5 15.9 274  56.1 76.1 292
87.9 41.2 285  65.1  9.8 274  79.0 41.2 282  44.6 65.1 287
54.7 68.3 289  57.0 26.8 279   8.7 12.3 270  33.7 61.9 286
25.0 55.8 278  69.3 94.9 306  49.2 64.6 287  78.2 93.7 307
47.9 26.6 277  96.9 51.4 292  39.6 73.4 287  37.9 66.1 285
94.5 71.4 296  51.6 18.3 276  37.6 73.2 287  68.5 10.7 274
46.7  9.6 273  87.4 38.9 282  45.6 43.9 277  70.7 76.9 296
82.8 53.6 287  82.5 55.4 286  37.8  5.1 275  89.8 96.1 309
63.9  4.9 276   2.0 11.7 270  31.3 59.2 282  93.9 65.3 296
47.9 93.0 301  29.9 36.0 274  14.6 28.3 274  17.5 70.1 286
 2.6 68.5 282  23.1 12.0 268  36.8 20.4 273  80.9  9.0 276
39.2  0.0 274  26.2 44.3 276  81.9 12.9 277   3.2 21.4 272
76.9 76.7 297  88.6  7.7 277   9.7  8.4 273  26.7 91.5 296
73.8  6.1 276  33.7 39.3 276  64.0 58.4 286   5.7 91.2 295
85.8 93.8 307  85.8 39.1 281  93.9 63.4 295  53.1 46.3 278
51.9 42.9 277  16.8 75.7 288  29.2 66.9 285  37.4 72.5 287
;
```

The initial step is to explore the data set by inspecting the data spatial distribution. Run PROC VARIOGRAM, specifying the NOVARIOGRAM option in the COMPUTE statement as follows:

```
ods graphics on;

proc variogram data=ozoneSet;
   compute novariogram nhc=35;
   coord xc=East yc=North;
   var Ozone;
run;
```

The result is a scatter plot of the observed data shown in Output 124.2.1. The scatter plot suggests an almost uniform spread of the measurements throughout the prediction area. No direct inference can be made about the existence of a surface trend in the data. However, the apparent stratification of ozone values in the northeast–southwest direction might indicate a nonrandom trend.

Output 124.2.1 Ozone Observation Data Scatter Plot

You need to define the size and count of the data classes by specifying suitable values for the LAGDISTANCE= and MAXLAGS= options, respectively. Compared to the smaller sample of thickness data used in "Getting Started: VARIOGRAM Procedure" on page 10027, the larger size of the ozoneSet data results in more densely populated distance classes for the same value of the NHCLASSES= option. After you experiment with a variety of values for the NHCLASSES= option, you can adjust LAGDISTANCE= to have a relatively small number. Then you can account for a large value of MAXLAGS= so that you obtain many sample semivariogram points within your data correlation range. Specifying these values requires some exploration, for which you might need to return to this point from a later stage in your semivariogram analysis. For illustration purposes you now specify NHCLASSES=35.

Your choice of NHCLASSES=35 yields the pairwise distance intervals table in Output 124.2.2 and the corresponding histogram in Output 124.2.3.

Output 124.2.2 Pairwise Distance Intervals Table

Pairwise Distance Intervals				
Lag Class	Bounds		Number of Pairs	Percentage of Pairs
0	0.00	2.01	52	0.12%
1	2.01	6.03	420	0.94%
2	6.03	10.06	815	1.82%
3	10.06	14.08	1143	2.55%
4	14.08	18.10	1518	3.38%
5	18.10	22.12	1680	3.75%
6	22.12	26.15	1931	4.31%
7	26.15	30.17	2135	4.76%
8	30.17	34.19	2285	5.09%
9	34.19	38.21	2408	5.37%
10	38.21	42.24	2551	5.69%
11	42.24	46.26	2444	5.45%
12	46.26	50.28	2535	5.65%
13	50.28	54.30	2487	5.55%
14	54.30	58.33	2460	5.48%
15	58.33	62.35	2391	5.33%
16	62.35	66.37	2302	5.13%
17	66.37	70.39	2285	5.09%
18	70.39	74.41	2079	4.64%
19	74.41	78.44	1786	3.98%
20	78.44	82.46	1640	3.66%
21	82.46	86.48	1493	3.33%
22	86.48	90.50	1243	2.77%
23	90.50	94.53	925	2.06%
24	94.53	98.55	710	1.58%
25	98.55	102.57	421	0.94%
26	102.57	106.59	274	0.61%
27	106.59	110.62	200	0.45%
28	110.62	114.64	120	0.27%
29	114.64	118.66	55	0.12%
30	118.66	122.68	35	0.08%
31	122.68	126.71	14	0.03%
32	126.71	130.73	11	0.02%
33	130.73	134.75	2	0.00%
34	134.75	138.77	0	0.00%
35	138.77	142.80	0	0.00%

Notice the overall high pair count in the majority of classes in Output 124.2.2. You can see that even for higher values of NHCLASSES= the classes are still sufficiently populated for your semivariogram analysis according to the rule of thumb stated in the section "Choosing the Size of Classes" on page 10087. Based on the displayed information in Output 124.2.3, you specify LAGDISTANCE=4 km. You can further experiment with smaller lag sizes to obtain more points in your sample semivariogram.

You can focus on the MAXLAGS= specification at a later point. The important step now is to investigate the presence of trends in the measurement. The following section makes a suggestion about how to remove surface trends from your data and then continues the semivariogram analysis with the detrended data.

Output 124.2.3 Distribution of Pairwise Distances for Ozone Observation Data

Analysis with Surface Trend Removal

You can use a SAS/STAT predictive modeling procedure to extract surface trends from your original data. If your goal is spatial prediction, you can continue processing the detrended data for the prediction tasks, and at the end you can reinstate the trend at the prediction locations to report your analysis results.

In general, the exact form of the trend is unknown, as discussed in the section "Empirical Semivariograms and Surface Trends" on page 10091. In this case, the spatial distribution of the measurements shown in Figure 124.2.1 suggests that you can use a quadratic model to describe the surface trend like the one that follows:

$$T(\text{East}, \text{North}) = f_0 + f_1\,[\text{East}] + f_2\,[\text{East}]^2 + f_3\,[\text{North}] + f_4\,[\text{North}]^2$$

The following statements show how to invoke the GLM procedure for your ozone data and how to extract the preceding trend from them:

```
proc glm data=ozoneSet plots=none;
   model ozone = East East*East North North*North;
   output out=gmout predicted=pred residual=ResidualOzone;
run;
```

Among other output, PROC GLM produces estimates for the parameters $f_0, \ldots, f_4$ in the preceding trend model. Output 124.2.4 shows the table with the parameter estimates. In this table, the coefficient f_0 corresponds to the intercept estimate, and the rest of the coefficients correspond to their matching variables; for example, the estimate in the line of "East*East" refers to f_2 in the preceding model. For more information about the syntax and the PROC GLM output, see Chapter 47, "The GLM Procedure."

Output 124.2.4 Parameter Estimates for the Surface Trend Model

Semivariogram Analysis in Anisotropic Case With Trend Removal

The GLM Procedure

Dependent Variable: Ozone

Parameter	Estimate	Standard Error	t Value	Pr > |t|
Intercept	270.6798273	0.40595731	666.77	<.0001
East	0.0065148	0.01360281	0.48	0.6323
East*East	0.0010726	0.00012987	8.26	<.0001
North	-0.0369159	0.01297491	-2.85	0.0047
North*North	0.0035587	0.00012659	28.11	<.0001

The detrending process leaves you with the GMOUT data set, which contains the ResidualOzone data residuals. This time you run PROC VARIOGRAM again with the NOVARIOGRAM option to inspect the detrended residuals, and with a request only for the observations plot, as follows:

```
proc variogram data=gmout plots(only)=observ;
   compute novariogram nhc=35;
   coord xc=East yc=North;
   var ResidualOzone;
run;
```

The requested observations plot is shown in Output 124.2.5.

Output 124.2.5 Ozone Residual Observation Data Scatter Plot

Before you proceed with the empirical semivariogram computation and model fitting, examine your data for anisotropy. This investigation is necessary to portray the spatial structure of your SRF accurately. If anisotropy exists, it manifests itself as different ranges or sills or both for the empirical semivariograms in different directions.

You want detail in your analysis, so you ask for the empirical semivariance in 12 directions by specifying NDIRECTIONS=12. Based on the NDIRECTIONS= option, empirical semivariograms are produced in increments of the base angle $\theta = 180°/12 = 15°$.

You also choose ANGLETOLERANCE=22.5 and BANDWIDTH=20. A different choice of values produces different empirical semivariograms, because these options can regulate the number of pairs that are included in a class. Avoid assigning values that are too small to these parameters so that you can allow for an adequate number of point pairs per class. At the same time, the higher the values of these parameters are, the more data pairs that come from closely neighboring directions are included in each lag. Therefore, values for the ANGLETOLERANCE= and BANDWIDTH= options that are too high pose a risk of losing information along the particular direction. The side effect occurs because you incorporate data pairs from a broader spectrum of angles; thus, you potentially amplify weaker anisotropy or weaken stronger anisotropy, as noted in the section "Angle Classification" on page 10082. You can experiment with different ANGLETOLERANCE= and BANDWIDTH= values to reach this balance with your data, if necessary.

With the following statements you ask to display only the SEMIVAR plots in the specified number of directions. Multiple empirical semivariograms are placed by default in panels, as Output 124.2.6 shows. If you want an individual plot for each angle, then you need to further specify the plot option SEMIVAR(UNPACK).

```
proc variogram data=gmout plot(only)=semivar;
   compute lagd=4 maxlag=16 ndir=12 atol=22.5 bandw=20;
   coord xc=East yc=North;
   var ResidualOzone;
run;
```

Output 124.2.6 Ozone Empirical Semivariograms with $0° \leq \theta < 180°$ and $\delta\theta = 15°$

Output 124.2.6 *continued*

Output 124.2.6 *continued*

The panels in Output 124.2.6 suggest that in some of the directions, such as for $\theta = 0°$, the directional plots tend to exhibit a somewhat noisy structure. This behavior can be due to the pairs distribution across the particular direction. Specifically, based on the LAGDISTANCE= choice there might be insufficient pairs present in a class. Also, depending on the ANGLETOLERANCE= and BANDWIDTH= values, too many pairs might be considered from neighboring angles that potentially follow a modified structure. These are factors that can increase the variability in the semivariance estimate. A different explanation might lie in the existence of outliers in the data set; this aspect is further explored in "Example 124.5: A Box Plot of the Square Root Difference Cloud" on page 10147.

This behavior is relatively mild here and should not obstruct your goal to study anisotropy in your data. You can also perform individual computations in any direction. By doing so, you can fine-tune the computation parameters and attempt to obtain smoother estimates of the sample semivariance.

Further in this study, the directional plots in Output 124.2.6 suggest that during shifting from $\theta = 0°$ to $\theta = 90°$, the empirical semivariogram range increases. Beyond the angle $\theta = 90°$, the range starts decreasing again until the whole circle is traversed at 180° and small range values are encountered around the N–S direction at $\theta = 0°$. The sill seems to remain overall the same. This analysis suggests the presence of anisotropy in the ozone concentrations, with the major axis oriented at about $\theta = 90°$ and the minor axis situated perpendicular to the major axis at $\theta = 0°$.

The multidirectional analysis requires that for a given LAGDISTANCE= you also specify a MAXLAGS= value. Since the ozone correlation range might be unknown (as assumed here), you can apply the rule of thumb that suggests use of the half-extreme data distance in the direction of interest, as explained in the section "Spatial Extent of the Empirical Semivariogram" on page 10089. Following the information displayed in Output 124.2.3, for different directions this distance varies between $99.4/2 = 49.7$ and $140.8/2 = 70.4$ km. In turn, the pairwise distances table in Output 124.2.2 indicates that within this range of distances you can specify MAXLAGS= to be between 12 and 17 lags. In this example you specify MAXLAGS=16.

At this point you are ready to continue with fitting theoretical semivariogram models to the empirical semivariogram in the selected directions of $\theta = 0°$ and $\theta = 90°$. By trying out different models, you see that an exponential one is suitable for your empirical data:

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

For the purpose of the present example, it is reasonable to assume a constant nugget effect equal to zero, based on the empirical semivariograms shown in Output 124.2.6. The same output suggests that the model scale is likely to be above 2, and that the range might be relatively small in $\theta = 0°$. You specify the PARMS statement to set initial values for the exponential model parameters and account for these considerations.

In particular, you assign an initial value of zero to the nugget effect. Then you request a grid search for the range and scale parameters, so that the optimal initial values set is selected for the parameter estimation in each of the two angles $\theta = 0°$ and $\theta = 90°$. By inspecting the empirical semivariograms in Output 124.2.6, you specify the value list 2, 2.5, and 3 for the scale, and the values from 5 to 25 with a step of 10 for the range. In addition, you specify the parameter 1 in the HOLD= option to designate the nugget effect parameter as a constant. According to these specifications, you use the following statements:

```
proc variogram data=gmout plot(only)=fit;
   compute lagd=4 maxlag=16;
   directions 0(22.5,10) 90(22.5,10);
   coord xc=East yc=North;
   model form=exp;
   parms (0.) (2 to 3 by 0.5) (5 to 25 by 10) / hold=(1);
   var ResidualOzone;
run;

ods graphics off;
```

The VARIOGRAM procedure repeats the fitting process for each one of the selected directions. First, in $\theta = 0°$ the parameter search table in Output 124.2.7 shows you which value combinations are tested initially to choose the one that gives the lowest objective function value.

Output 124.2.7 Parameter Search for the Selected Direction $\theta = 0°$

Semivariogram Analysis in Anisotropic Case With Trend Removal

The VARIOGRAM Procedure

Dependent Variable: ResidualOzone
Angle: 0
Current Model: Exponential

Parameter Search

Set	Nugget	Scale	Range	Objective Function
1	0	2	5	391.06593
2	0	2	15	1740.0
3	0	2	25	5167.5
4	0	2.5	5	64.86565
5	0	2.5	15	664.03665
6	0	2.5	25	2480.5
7	0	3	5	72.86743
8	0	3	15	305.53306
9	0	3	25	1305.0

From this search, the combination of scale equal to 2.5 and a range of size 5 is passed as initial values to the model fitting process. This result is reflected in the model information table shown in Output 124.2.8.

Output 124.2.8 Model Initial Values for the Selected Direction $\theta = 0°$

Model Information

Parameter	Initial Value	Status
Nugget	0	Fixed
Scale	2.5000	
Range	5.0000	

Fitting is successful, and among the output objects you can see the estimated parameters and the fit summary tables for the direction $\theta = 0°$ in Output 124.2.9.

Output 124.2.9 Weighted Least Squares Fitting Parameter Estimates and Summary for the Selected Direction $\theta = 0°$

Parameter Estimates

Parameter	Estimate	Approx Std Error	DF	t Value	Approx Pr > |t|
Scale	2.6657	0.03830	15	69.60	<.0001
Range	3.7277	0.5609	15	6.65	<.0001

Fit Summary

Model	Weighted SSE	AIC
Exp	43.35103	19.91399

A corresponding parameter search takes place for the direction $\theta = 90°$. The respective table and the choice of initial values for fitting in the direction $\theta = 90°$ are shown in Output 124.2.10.

Output 124.2.10 Parameter Search and Model Initial Values for the Selected Direction $\theta = 90°$

Parameter Search

Set	Nugget	Scale	Range	Objective Function
1	0	2	5	302.54551
2	0	2	15	635.93338
3	0	2	25	1996.0
4	0	2.5	5	95.09939
5	0	2.5	15	104.56776
6	0	2.5	25	662.06813
7	0	3	5	155.50670
8	0	3	15	20.48482
9	0	3	25	190.30599

Model Information

Parameter	Initial Value	Status
Nugget	0	Fixed
Scale	3.0000	
Range	15.0000	

Output 124.2.11 displays the estimated parameters and the fit summary for the direction $\theta = 90°$.

Output 124.2.11 Weighted Least Squares Fitting Parameter Estimates and Summary for the Selected Direction $\theta = 90°$

Parameter Estimates

Parameter	Estimate	Approx Std Error	DF	t Value	Approx Pr > |t|
Scale	2.9199	0.07007	15	41.67	<.0001
Range	14.7576	0.9530	15	15.49	<.0001

Fit Summary

Model	Weighted SSE	AIC
Exp	19.12246	6.00005

The fitted and empirical semivariograms for the selected directions are displayed in the panel of Output 124.2.12.

Output 124.2.12 Fitted Theoretical and Empirical Semivariogram for the Ozone Data in the $\theta = 0°$ and $\theta = 90°$ Directions

Conclusively, your semivariogram analysis on the detrended ozone data suggests that the ozone SRF exhibits anisotropy in the perpendicular directions of N–S ($\theta = 0°$) and E–W ($\theta = 90°$).

The sills in the two directions of anisotropy are similar in size. By inspecting again the empirical semivariograms in Output 124.2.6, you could make the reasonable assumption that you have a case of geometric anisotropy, where the range in the major axis is about 4.5 times larger than the minor axis range. If you would like to use these PROC VARIOGRAM results for predictions, then you would need to specify a single scale value for the geometric anisotropy sill. In this case you could choose an arbitrary value for the constant scale from the narrow interval formed by the estimated scales in the previous results. For example, you can specify the PARMS statement modified as shown in the following statement to approximate a common scale for the semivariance in all directions:

```
parms (0.) (2.7) (5 to 25 by 10) / hold=(1,2);
```

As an alternative, you can use PROC VARIOGRAM to fit an exponential model to all different angles examined in this example, and then select the constant scale value to be the mean of the scales across all directions.

Example 124.3: Analysis without Surface Trend Removal

This example uses PROC VARIOGRAM without removing potential surface trends in a data set in order to investigate a distinguished spatial direction in the data. In doing so, this example also serves as a guide to examine under which circumstances you might be able to bypass the effect of a trend on a semivariogram. Typically though, for theoretical semivariogram estimations you follow the analysis presented in "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122.

As explained in the section "Details: VARIOGRAM Procedure" on page 10072, when you compute the empirical semivariance for data that contain underlying surface trends, the outcome is the pseudo-semivariance. Pseudo-semivariograms are not estimates of the theoretical semivariogram; hence, they provide no information about the spatial continuity of your SRF.

However, in the section "Empirical Semivariograms and Surface Trends" on page 10091 it is mentioned that you might still be able to perform a semivariogram analysis with potentially non-trend-free data, if you suspect that your measurements might be trend-free across one or more specific directions. The example demonstrates this approach.

Reconsider the ozone data presented at the beginning of "Example 124.2: An Anisotropic Case Study with Surface Trend in the Data" on page 10122. The spatial distribution of the data is shown in Figure 124.2.1, and the pairwise distance distribution for NHCLASSES=35 is illustrated in Figure 124.2.3. This exploratory analysis suggested a LAGDISTANCE=4 km, and Figure 124.2.2 indicated that for this LAGDISTANCE= you can consider a value of MAXLAGS=16.

Recall from the section "Empirical Semivariograms and Surface Trends" on page 10091 that you need to investigate the empirical semivariogram of the data in a few different directions in order to identify a trend-free direction. If such a direction exists, then you can proceed with this special type of analysis. The following statements employ NDIRECTIONS=8 to examine eight directions:

```
ods graphics on;

proc variogram data=ozoneSet plot(only)=semivar;
   compute lagd=4 maxlag=16 ndirections=8 robust;
   coord xc=East yc=North;
   var Ozone;
run;
```

By default, the range of 180° is divided into eight equally distanced angles: $\theta = 0°$, $\theta = 22.5°$, $\theta = 45°$, $\theta = 67.5°$, $\theta = 90°$, $\theta = 112.5°$, $\theta = 135°$, and $\theta = 157.5°$. The resulting empirical semivariograms for these angles are shown in Output 124.3.1.

Output 124.3.1 Ozone Empirical Semivariograms with $0° \leq \theta < 180°$ and $\delta\theta = 22.5°$

Output 124.3.1 *continued*

The figures in Output 124.3.1 suggest an overall continuing increase with distance of the semivariance in all directions. As explained in the section "Theoretical Semivariogram Models" on page 10072, this can be an indication of systematic trends in the data. However, the direction of $\theta = 112.5°$ clearly indicates that the increase rate, if any, is smaller than the corresponding rates across the rest of the directions. You then want to search whether there exists a trend-free direction in the neighborhood of this angle.

Run PROC VARIOGRAM again, specifying several directions within an interval of angles where you want to close in and you suspect the existence of a trend-free direction. In the following step you specify ANGLETOL=15°, which is smaller than the default value of 22.5°, and you also specify BANDWIDTH=10 km. The smaller values help with minimization of the interference with neighboring directions, as discussed in the section "Angle Classification" on page 10082.

The aforementioned considerations are addressed in the following statements:

```
proc variogram data=ozoneSet plot(only)=semivar(cla);
   compute lagd=4 maxlag=16 robust;
   directions 100(15,10) 103(15,10)
              106(15,10) 108(15,10)
              110(15,10) 112(15,10)
              115(15,10) 118(15,10);
   coord xc=East yc=North;
   var Ozone;
run;
```

Your analysis has brought you to examine a narrow strip of angles within $\theta = 100°$ and $\theta = 118°$. The pseudo-semivariograms in Output 124.3.2 and Output 124.3.3 indicate that at the boundaries of this strip, the angles display increasing semivariance with distance. On the other hand, within this interval there are directions across which the semivariance is tentatively reaching a sill, and these are potential candidates to be trend-free directions.

Output 124.3.2 Ozone Empirical Semivariograms in 100°, 103°, 106°, and 108°

Output 124.3.3 Ozone Empirical Semivariograms in 110°, 112°, 115°, and 118°

You can further investigate this angle spectrum in more detail. For example, you can monitor additional angles in between, or use a smaller LAGDISTANCE= and increased MAXLAGS= values to single out the most qualified candidate. For the purpose of this example, you can consider the direction $\theta = 108°$ to very likely be the trend-free one you are looking for.

From a physical standpoint, the trend-free direction, if it exists, is expected to be perpendicular to the direction of the maximum dip in the values of the ozone field, as mentioned in the section "Empirical Semivariograms and Surface Trends" on page 10091. If you cross-examine the ozone data distribution in Output 124.2.1, the figure suggests that this direction exists and is slightly tilted clockwise with respect to the E–W axis. This direction emerges from the mild stratification of the ozone values in your data distribution. The ozone concentrations across it are similar when compared to surrounding directions, and as such, it has been identified as a trend-free direction.

Your next step is to obtain the empirical semivariogram in the suspected trend-free direction of $\theta = 108°$ and to perform a theoretical model fit.

The semivariance in Output 124.3.2 exhibits a slow, almost linear rise at short distances and seems to be reaching the sill fast, rather than asymptotically. You can accommodate this behavior by using the spherical model

$$\gamma_z(h) = \begin{cases} c_n + {\sigma_0}^2 \left[\frac{3}{2}\frac{h}{a_0} - \frac{1}{2}(\frac{h}{a_0})^3 \right], & \text{for } 0 < h \le a_0 \\ c_0, & \text{for } a_0 < h \end{cases}$$

where $\gamma_z(0) = 0$ and $a_0 > 0$. The empirical semivariograms also suggest that there does not seem to be a nugget effect. Assume that in this example you are interested in what the fitting process concludes about the nugget effect, so you skip the NUGGET= option in the MODEL statement. You also let PROC VARIOGRAM provide initial values for the rest of the model parameters. Eventually, you use the PLOTS option to inspect the classical and robust empirical semivariograms in the selected direction and to produce a plot of the fitted model. The following statements implement these considerations:

```
proc variogram data=ozoneSet plot(only)=(semivar fit);
   compute lagd=4 maxlag=16 robust cl;
   directions 108(15,10);
   coord xc=East yc=North;
   model form=sph;
   var ozone;
run;

ods graphics off;
```

The classical and robust empirical semivariograms in the selected direction $\theta = 108°$ are displayed in Figure 124.3.4.

Output 124.3.4 Ozone Classical and Robust Empirical Semivariograms in $\theta = 108°$

The output continues with information about the fitting process, which terminates successfully and produces the estimated parameters and the fit summary tables shown in Output 124.3.5. The near-zero nugget parameter estimate indicates that you can consider the process to be practically free of nugget effect.

Output 124.3.5 Weighted Least Squares Fitting Parameter Estimates and Summary in $\theta = 108°$

Parameter Estimates

Parameter	Estimate	Approx Std Error	DF	t Value	Approx Pr > |t|
Nugget	0.006260	0.09449	14	0.07	0.9481
Scale	6.6791	0.1741	14	38.37	<.0001
Range	47.3012	2.0776	14	22.77	<.0001

Fit Summary

Model	Weighted SSE	AIC
Sph	13.13869	1.61991

The fitted and empirical semivariograms for the selected direction $\theta = 108°$ are displayed in Output 124.3.6.

Output 124.3.6 Fitted Theoretical and Empirical Semivariogram for the Ozone Data in $\theta = 108°$

A comparative look at the empirical and fitted semivariograms in Output 124.3.6 and Output 124.2.12 suggests that the analysis of the trend-free ResidualOzone produces a different outcome from that of the original Ozone values. In fact, a more suitable comparison can be made between the semivariograms in the assumed trend-free direction $\theta = 108°$ of the current scenario and the one shown in Output 124.2.6 in the nearly identical direction $\theta = 105°$. It might seem unreasonable that these two semivariograms are produced both in the same ozone study and in a narrow band of directions free of apparent surface trends, yet they bear no resemblance. However, the lack of similarity in these plots stems from operating on two different data sets where the outcome depends on the actual data values.

More specifically, the semivariogram analysis treats the trend-free ozone set and the original ozone measurements as different quantities. The process of detrending the original Ozone values is a transformation of these values into the trend-free values of ResidualOzone. Any existing spatial correlation in the original data is not necessarily retained within the transformed data. Depending on the transformation features, the emerging data set has its own characteristics, as demonstrated in this example.

A final remark concerns the issue of isotropy. Based on the details presented in the section "Empirical Semivariograms and Surface Trends" on page 10091, your knowledge of the spatial structure of the ozoneSet data set is limited to the selected trend-free direction you indicated in the present example. You can generalize this outcome for all spatial directions only if you consider the hypothesis of isotropy in the ozone field to be reasonable. However, you cannot infer the assumption of anisotropy in the present example based on the analysis in the section "Analysis with Surface Trend Removal" on page 10126. Again, the reason is that you currently use the observed Ozone values, whereas the ResidualOzone data in the previous example emerged from a transformation of the current data. Hence, you have essentially two data sets that do not necessarily share the same properties.

Example 124.4: Covariogram and Semivariogram

The covariance that was reviewed in the section "Stationarity" on page 10079 is an alternative measure of spatial continuity that can be used instead of the semivariance. In a similar manner to the empirical semivariance that was presented in the section "Theoretical and Computational Details of the Semivariogram" on page 10077, you can also compute the empirical covariance. The covariograms are plots of this quantity and can be used to fit permissible theoretical covariance models, in correspondence to the semivariogram analysis presented in the section "Theoretical Semivariogram Models" on page 10072. This example displays a comparative view of the empirical covariogram and semivariogram, and examines some additional aspects of these two measures.

You consider 500 simulations of an SRF $Z(\boldsymbol{s})$ in a square domain of 100×100 (10^6 km^2). The following DATA step defines the data locations:

```
title 'Covariogram and Semivariogram';

data dataCoord;
   retain seed 837591;
   do i=1 to 100;
      East = round(100*ranuni(seed),0.1);
      North = round(100*ranuni(seed),0.1);
      output;
   end;
run;
```

For the simulations you use PROC SIM2D, which produces Gaussian simulations of SRFs with user-specified covariance structure—see Chapter 105, "The SIM2D Procedure." The Gaussian SRF implies full knowledge of the SRF expected value $\mathrm{E}[Z(\boldsymbol{s})]$ and variance $\mathrm{Var}[Z(\boldsymbol{s})]$ at every location $\boldsymbol{s}$. The following statements simulate an isotropic, second-order stationary SRF with constant expected value and variance throughout the simulation domain:

```
proc sim2d outsim=dataSims;
   simulate numreal=500 seed=79750
            nugget=2 scale=6 range=10 form=exp;
   mean 30;
   grid gdata=dataCoord xc=East yc=North;
run;
```

Here, the SIMULATE statement accommodates the simulation parameters. The NUMREAL= option specifies that you want to perform 500 simulations, and the SEED= option specifies the seed for the simulation random number generator. You use the MEAN statement to specify the expected value $\mathrm{E}[Z(\boldsymbol{s})] = 30$ units of Z. You also specify two variance components. The first is the nugget effect, and you use the NUGGET= option to set it to $c_n = 2$. The second is the partial sill ${\sigma_0}^2 = 6$ that you specify with the SCALE= option. The two variance components make up the total SRF variance $\mathrm{Var}[Z(\boldsymbol{s})] = c_n + {\sigma_0}^2 = 8$. You assume an exponential covariance structure to describe the field spatial continuity, where ${\sigma_0}^2$ is the sill value and its range $a_0 = 10$ km (effective range $a_\epsilon = 3a_0 = 30$ km) is specified by the RANGE= option. The option FORM= specifies the covariance structure type.

The empirical semivariance and covariance are computed by the VARIOGRAM procedure, and are available either in the ODS output semivariogram table (as variables Semivariance and Covariance, respectively) or in the OUTVAR= data set. In the following statements you obtain these variables by using the OUTVAR= data set of the VARIOGRAM procedure:

```
proc variogram data=dataSims outv=outv noprint;
   compute lagd=3 maxlag=18;
   coord xc=gxc yc=gyc;
   by _ITER_;
   var svalue;
run;
```

For each distance lag you take the average of the empirical measures over the number of simulations. PROC SORT prepares the input data for PROC MEANS, which produces these averages and stores them in the dataAvgs data set. This sequence is performed with the following statements:

```
proc sort data=outv;
   by lag;
run;

proc means data=outv n mean noprint;
   var Distance variog covar;
   by lag;
   output out=dataAvgs mean(variog)=Semivariance
                       mean(covar)=Covariance
                       mean(Distance)=Distance;
run;
```

The SGPLOT procedure creates the plot of the average empirical semivariogram and covariogram, as in the following statements:

```
proc sgplot data=dataAvgs;
   title "Empirical Semivariogram and Covariogram";
   xaxis label = "Distance" grid;
   yaxis  label = "Semivariance" min=-0.5 max=9 grid;
   y2axis label = "Covariance"   min=-0.5 max=9;
   scatter y=Semivariance x=Distance /
           markerattrs = GraphData1
           name='Semivar'
           legendlabel='Semivariance';
   scatter y=Covariance x=Distance /
           y2axis
           markerattrs = GraphData2
           name='Covar'
           legendlabel='Covariance';
   discretelegend 'Semivar' 'Covar';
run;
```

The plot of the average empirical semivariance and covariance of the preceding analysis is shown in Output 124.4.1. The high number of simulations led to averages of empirical continuity measures that accurately approximate the simulated SRF characteristics. Specifically, the empirical semivariogram and covariogram both exhibit clearly exponential behavior. The semivariogram sill is approximately at the specified variance $\mathrm{Var}[Z(\boldsymbol{s})] = 8$ of the SRF.

The simulated SRF is second-order stationary, so you expect at each lag the sum of the empirical semivariance and covariance to approximate the field variance $\mathrm{Var}[Z(\boldsymbol{s})]$, as explained in the section "Stationarity" on page 10079. This behavior is evident in Output 124.4.1.

This example concludes with a discussion of basic reasons why the empirical semivariogram analysis is commonly preferred to the empirical covariance analysis. A first reason comes from the assumptions that are necessary to compute each of these two measures. The condition of intrinsic stationarity that is required in order to define the empirical semivariogram is less restrictive than the condition of second-order stationarity that is required in order to consider the covariance function as a parameter of the process.

Also, an empirical semivariogram can indicate whether a nugget effect is present in your data sample, whereas the empirical covariogram itself might not reveal this information. This point is illustrated in Output 124.4.1, where you expect to see that $C(\mathbf{0}) = \mathrm{Var}[Z(\boldsymbol{s})]$, but the empirical covariogram cannot have a point at exactly $\boldsymbol{h} = \mathbf{0}$. A practical way to investigate for a nugget effect when you use empirical covariograms is as follows: recall that the OUTVAR= data set provides you with the sample variance (shown in the COVAR column for LAG=–1), as the following statement shows:

```
/* Obtain the sample variance from the data set ----------------*/

proc print data=dataAvgs (obs=1);
run;
```

Output 124.4.1 Average Empirical Semivariogram and Covariogram from 500 Simulations

Output 124.4.2 is a partial output of the dataAvgs data set, which contains averages of the OUTVAR= data set and shows the computed average $C(\mathbf{0})$ in the Covariance column. The combination of the empirical covariogram and the $C(\mathbf{0})$ value can help you fit a theoretical covariance model that includes any nugget effect, if present. See also the discussion in Schabenberger and Gotway (2005, section 4.2.2) about the Matérn definition of the covariance function that is related to this issue. In particular, this definition provides for an additional variance component in the covariance expression at $\boldsymbol{h} = \mathbf{0}$ to account for the corresponding nugget effect in the semivariogram.

Output 124.4.2 Partial Outcome of the dataAvgs Data Set

Empirical Semivariogram and Covariogram

Obs	LAG	_TYPE_	_FREQ_	Semivariance	Covariance	Distance
1	-1	0	500	.	7.74832	.

In addition to the preceding points, if the SRF is nonstationary, the empirical semivariogram indicates that the SRF variance increases with distance $\boldsymbol{h}$, as Output 124.3.1 shows in "Example 124.3: Analysis without Surface Trend Removal" on page 10136. In that case it makes no sense to compute the empirical covariogram.

Specifically, the covariogram could provide you with an estimate of the sample variance, which is not sufficient to indicate that the SRF might not be stationary (see also Chilès and Delfiner 1999, p. 31).

Finally, the definitions of the empirical semivariance and covariance in the section "Theoretical and Computational Details of the Semivariogram" on page 10077 clearly show that the sample mean $\bar{Z}$ and the SRF expected value $\mathrm{E}[Z(\boldsymbol{s})]$ are not important for the computation of the semivariance, but either one is necessary for the covariance. Hence, the semivariance expression filters the mean, and this behavior is especially useful when the mean is unknown. On the other hand, if $\mathrm{E}[Z(\boldsymbol{s})]$ is unknown and the empirical covariance is computed based on the sample mean $\bar{Z}$, this can induce additional bias in the covariance computation.

Example 124.5: A Box Plot of the Square Root Difference Cloud

The Gaussian form selected for the semivariogram in the section "Getting Started: VARIOGRAM Procedure" on page 10027 is based on consideration of the plots of the sample semivariogram. For the coal thickness data, the Gaussian form appears to be a reasonable choice.

However, it can often happen that a plot of the sample variogram shows so much scatter that no particular form is evident. The cause of this scatter can be one or more outliers in the pairwise differences of the measured quantities.

A method of identifying potential outliers is discussed in Cressie (1993, section 2.2.2). This example illustrates how to use the OUTPAIR= data set from PROC VARIOGRAM to produce a square root difference cloud, which is useful in detecting outliers.

For the SRF $Z(\boldsymbol{s}), \boldsymbol{s} \in \mathcal{R}^2$, the square root difference cloud for a particular direction $\boldsymbol{e}$ is given by

$$| Z(s_i + he) - Z(s_i) |^{\frac{1}{2}}$$

for a given lag distance h. In the actual computation, all pairs $P_1 P_2$ of points P_1, P_2 within a distance tolerance around h and an angle tolerance around the direction $\boldsymbol{e}$ are used. This generates a number of point pairs for each lag class h. The spread of these values gives an indication of outliers.

Following the example in the section "Getting Started: VARIOGRAM Procedure" on page 10027, this example uses a basic LAGDISTANCE=7, with a distance tolerance of 3.5, and a direction of N–S, with an angle tolerance ATOL=30°.

First, use PROC VARIOGRAM to produce an OUTPAIR= data set. Then use a DATA step to subset this data by choosing pairs within 30° of N–S. In addition, compute lag class and square root difference variables, as the following statements show:

```
title 'Square Root Difference Cloud Example';

proc variogram data=sashelp.thick outp=outp noprint;
   compute novariogram;
   coordinates xc=East yc=North;
   var Thick;
run;
```

```
data sqroot;
   set outp;
   /*- Include only points +/- 30 degrees of N-S -------*/
   where abs(cos) < 0.5;
   /*- Unit lag of 7, distance tolerance of 3.5 --------*/
   lag_class=int(distance/7 + 0.5000001);
   sqr_diff=sqrt(abs(v1-v2));
run;

proc sort data=sqroot;
   by lag_class;
run;
```

Next, summarize the results by using the MEANS procedure:

```
proc means data=sqroot noprint n mean std;
   var sqr_diff;
   by lag_class;
   output out=msqrt n=n mean=mean std=std;
run;
title2 'Summary of Results';

proc print data=msqrt;
   id lag_class;
   var n mean std;
run;
```

The preceding statements produce Output 124.5.1.

Output 124.5.1 Summary of Results

Square Root Difference Cloud Example
Summary of Results

lag_class	n	mean	std
0	5	0.47300	0.14263
1	31	0.77338	0.41467
2	51	1.17052	0.47800
3	58	1.52287	0.51454
4	65	1.68625	0.58465
5	65	1.66963	0.68582
6	80	1.79693	0.62929
7	88	1.73334	0.73191
8	83	1.75528	0.68767
9	108	1.72901	0.58274
10	80	1.48268	0.48695
11	84	1.19242	0.47037
12	68	0.89765	0.42510
13	38	0.84223	0.44249
14	7	1.05653	0.42548
15	3	1.35076	0.11472

Finally, present the results in a box plot by using the SGPLOT procedure. The box plot facilitates the detection of outliers. The statements are as follows:

```
proc sgplot data=sqroot;
   xaxis label = "Lag Class";
   yaxis label = "Square Root Difference";
   title "Box Plot of the Square Root Difference Cloud";
   vbox sqr_diff / category=lag_class;
run;
```

Output 124.5.2 suggests that outliers, if any, do not appear to be adversely affecting the empirical semivariogram in the N–S direction for the coal seam thickness data. The conclusion from Output 124.5.2 is consistent with our previous semivariogram analysis of the same data set in the section "Getting Started: VARIOGRAM Procedure" on page 10027. The effect of the isolated outliers in lag classes 6 and 10–12 in Output 124.5.2 is demonstrated as the divergence between the classical and robust empirical semivariance estimates in the higher distances in Output 124.7. The difference in these estimates comes from the definition of the robust semivariance estimator $\bar{\gamma}_z(\boldsymbol{h})$ (see the section "Theoretical and Computational Details of the Semivariogram" on page 10077), which imposes a smoothing effect on the outlier influence.

Output 124.5.2 Box Plot of the Square Root Difference Cloud

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