# **Calculation of Uncertainty in the Variogram1** Julián Ortiz C.<sup>2</sup> and Clayton V. Deutsch<sup>2</sup>

*There are often limited data available in early stages of geostatistical modeling. This leads to considerable uncertainty in statistical parameters including the variogram. This article presents an approach to calculate the uncertainty in the variogram. A methodology to transfer this uncertainty through geostatistical simulation and decision making is also presented.*

*The experimental variogram value*  $2\hat{v}(\mathbf{h})$  *for a separation lag vector* **h** *is a mean of squared differences. The variance of a mean can be calculated with a model of the correlation between the pairs of data used in the calculation. The "data" here are squared differences; therefore, we need a measure of a 4-point correlation. A theoretical multi-Gaussian approach is presented for this uncertainty assessment together with a number of examples. The theoretical results are validated by numerical simulation. The simulation approach permits generalization to non-Gaussian situations.*

*Multiple plausible variograms may be fit knowing the uncertainty at each variogram point,*  $2\gamma(\mathbf{h})$ *. Multiple geostatistical realizations may then be constructed and subjected to process assessment to measure the impact of this uncertainty.*

**KEY WORDS:** multi-Gaussian, multipoint statistics, decision making.

## **INTRODUCTION**

Variogram modeling is a critical step in any geostatistical study; however, a reliable variogram is difficult to infer in presence of sparse data. This is particularly true in the early exploration stages of an ore deposit or petroleum reservoir. A quantitative model of the uncertainty in the variogram would allow an assessment of uncertainty from geostatistical simulation.

Notwithstanding robust procedures to calculate variograms and other measures of spatial correlation (Cressie, 1991; Cressie and Hawkins, 1980; Genton, 1998), there is unavoidable uncertainty in the variogram. There are many references on the calculation and use of the variogram (including Goovaerts; 1997, Olea, 1995; Omre, 1984); however, there is little on the calculation of the unavoidable uncertainty in the variogram.

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We show how to calculate the pointwise uncertainty in the variogram. This pointwise uncertainty must be translated to joint uncertainty, that is, into uncertainty in the variogram *model*. Within the bounds of pointwise uncertainty, we propose to establish different scenarios, ranging from small continuity to great continuity. The importance of the variogram can be assessed by creating realizations and passing them through a transfer function.

### **POINTWISE VARIOGRAM UNCERTAINTY**

The variogram is defined as

$$
2 \cdot \gamma(\mathbf{h}) = \text{Var}\{Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})\}
$$
(1)

where  $Z(\cdot)$  is an element of a random field  $\{Z(\mathbf{u}) : \mathbf{u} \in D\}$ .

A method of moments estimator of the variogram  $2\gamma$  (**h**) is the average of squared differences between data separated exactly by that distance vector **h** (in practice, we define angle and lag tolerances, so that  $n(\bf{h})$  is the number of pairs approximately **h** apart):

$$
2 \cdot \hat{\gamma}(\mathbf{h}) = \frac{1}{n(\mathbf{h})} \cdot \sum_{i=1}^{n(\mathbf{h})} [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2
$$
 (2)

where  $n(\mathbf{h})$  is the number of data pairs approximately **h** apart.

Consider  $X_i = [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2$ , the squared difference between the values at locations  $(\mathbf{u}_i)$  and  $(\mathbf{u}_i + \mathbf{h})$ . The variogram is the mean of the  $X_i$ s:

$$
\bar{X} = 2 \cdot \hat{\gamma}(\mathbf{h}) = \frac{1}{n(\mathbf{h})} \cdot \sum_{i=1}^{n(\mathbf{h})} X_i
$$
 (3)

From classical statistics, we know that the uncertainty in the mean  $\bar{X}$  is defined as

$$
Var\{\bar{X}\} = E\{(\bar{X} - E\{\bar{X}\})^2\} = E\{\bar{X}^2\} - (E\{\bar{X}\})^2
$$
 (4)

Now, using expression (4) we can calculate the uncertainty in the variogram assuming that we have a "reference" variogram model fitted to the experimental points.  $\bar{X}$  is replaced by 2 ·  $\hat{\gamma}$ (**h**) and the variance of squared differences around the model is calculated as follows:

$$
\sigma_{2\cdot\hat{\gamma}(\mathbf{h})}^2 = E\{(2\cdot\hat{\gamma}(\mathbf{h}))^2\} - (E\{2\cdot\hat{\gamma}(\mathbf{h})\})^2
$$
  
= 
$$
E\left\{\left(\frac{1}{n(\mathbf{h})}\cdot\sum_{i=1}^{n(\mathbf{h})}[Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2\right)^2\right\} - (E\{2\cdot\hat{\gamma}(\mathbf{h})\})^2
$$

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$$
= E\left\{ \left( \frac{1}{n(\mathbf{h})^2} \cdot \sum_{i=1}^{n(\mathbf{h})} \sum_{j=1}^{n(\mathbf{h})} [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2 \times [Z(\mathbf{u}_j) - Z(\mathbf{u}_j + \mathbf{h})]^2 \right) \right\} - (2 \cdot \hat{\gamma}(\mathbf{h}))^2
$$
(5)

$$
\sigma_{2\cdot\hat{\gamma}(\mathbf{h})}^2 = \frac{1}{n(\mathbf{h})^2} \cdot \sum_{i=1}^{n(\mathbf{h})} \sum_{j=1}^{n(\mathbf{h})} E\{ [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2 \cdot [Z(\mathbf{u}_j) - Z(\mathbf{u}_j + \mathbf{h})]^2 \}
$$

$$
- (2 \cdot \hat{\gamma}(\mathbf{h}))^2
$$
(6)

This can be simplified by using the definition of the covariance:

$$
C_{ij}(\mathbf{h}) = \text{Cov}\{X_i, X_j\} = E\{(X_i - E\{X_i\}) \cdot (X_j - E\{X_j\})\}
$$
  
=  $E\{X_i \cdot X_j\} - E\{X_i\} \cdot E\{X_j\}$   
=  $E\{X_i \cdot X_j\} - \bar{X}^2$  (7)

Now, replacing  $X_i$  and  $X_j$  by the squared differences  $[z(\mathbf{u}_i) - z(\mathbf{u}_i + \mathbf{h})]^2$  and  $[z(\mathbf{u}_i) - z(\mathbf{u}_i + \mathbf{h})]^2$ , respectively, and  $\bar{X}$  by the variogram 2 ·  $\gamma(\mathbf{h})$ ,

$$
C_{ij}(\mathbf{h}) = E\{ [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2 \cdot [Z(\mathbf{u}_j) - Z(\mathbf{u}_j + \mathbf{h})]^2 \} - (2 \cdot \hat{\gamma}(\mathbf{h}))^2 \tag{8}
$$

A simple formula for the variance of a particular variogram value is obtained replacing the covariance (8) in expression (6):

$$
\sigma_{2\cdot\hat{\gamma}(\mathbf{h})}^2 = \frac{1}{n(\mathbf{h})^2} \cdot \sum_{i=1}^{n(\mathbf{h})} \sum_{j=1}^{n(\mathbf{h})} C_{ij}(\mathbf{h}) \tag{9}
$$

where  $C_{ij}(\mathbf{h})$  is calculated as in Eq. (8). To avoid confusion, note that  $C_{ij}(\mathbf{h})$  is the covariance between pair  $i[Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2$  and  $j[Z(\mathbf{u}_j) - Z(\mathbf{u}_j + \mathbf{h})]^2$ (Fig. 1).

Expression (9) tells us that the uncertainty in the variogram at a distance **h** is the average covariance between "pairs of pairs" used to calculate the variogram for that particular lag.

The covariance between "pairs of pairs" can be calculated theoretically under a multi-Gaussian assumption. The following section presents this approach. The next sections present the local and global simulation methods to check the results given by the theoretical approach. The global simulation method is more general in the sense that it gives the whole distribution of uncertainty in the variogram

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**Figure 1.** Calculation of fourth order covariances  $C_{ij}(\mathbf{h})$ . For a given lag vector **h**, the fourth order covariance corresponds to the covariance between the squared differences of pairs *i* and *j*.

values for each lag. Although the shape of the pointwise uncertainty distribution is unknown and we know that the variogram values must be nonnegative, a Gaussian shape was assumed to present the confidence intervals calculated using the variance in the theoretical approach and the local simulation method. Theory says that if all the squared random variables are independent (which is clearly not the case) the distribution of uncertainty in a variogram point should be  $\chi^2$ (chi square). The global simulation method shows in few cases asymmetric distributions; however, a Gaussian distribution is a good approximation in most of the cases.

The following steps are required for all three methodologies

- 1. Transform data to normal space: Any data distribution can be easily transformed to a Gaussian univariate distribution. In the following examples the program nscore in GSLIB (Deutsch and Journel, 1998) was used to perform the transformation. This transformation is commonly done to allow Gaussian simulation.
- 2. Check multigaussianity: To fulfil the multi-Gaussian condition, one should assure that not only the univariate distribution is Gaussian, but also the bivariate and all multivariate distributions. In practice, some tests can be done to the transformed distribution in order to accept bigaussianity; however, they are not often applied, especially in presence of sparse data.
- 3. Calculate the experimental variogram: The location of the sampled points and the values of the variable under study at these locations are used to calculate the experimental variogram,  $2 \cdot \hat{\gamma}$ **(h)**.
- 4. Fit a variogram model: The fitted variogram model is critical for subsequent stages of uncertainty evaluation. The requirement for a variogram model to assess uncertainty in the variogram is of some concern. Nevertheless, a model assumption is required to proceed.

The difference between the theoretical approach and the numerical methods lies in how the variance for each lag is calculated.

### **THEORETICAL APPROACH**

Assuming that the regionalized variable is multi-Gaussian, the variogram uncertainty can be calculated from theory. Expanding expression (8), the covariance can be written as a sum of fourth order moments:

$$
C_{ij}(\mathbf{h}) = E\{ [Z(\mathbf{u}_i) - Z(\mathbf{u}_i + \mathbf{h})]^2 \cdot [Z(\mathbf{u}_j) - Z(\mathbf{u}_j + \mathbf{h})]^2 \} - (2 \cdot \hat{\gamma}(\mathbf{h}))^2
$$
  
\n
$$
= E\{Z(\mathbf{u}_i)^2 \cdot Z(\mathbf{u}_j)^2 - 2 \cdot Z(\mathbf{u}_i)^2 \cdot Z(\mathbf{u}_j) \cdot Z(\mathbf{u}_j + \mathbf{h})
$$
  
\n
$$
+ Z(\mathbf{u}_i)^2 \cdot Z(\mathbf{u}_j + \mathbf{h})^2 - 2 \cdot Z(\mathbf{u}_i) \cdot Z(\mathbf{u}_i + \mathbf{h}) \cdot Z(\mathbf{u}_j)^2
$$
  
\n
$$
+ 4 \cdot Z(\mathbf{u}_i) \cdot Z(\mathbf{u}_i + \mathbf{h}) \cdot Z(\mathbf{u}_j) \cdot Z(\mathbf{u}_j + \mathbf{h})
$$
  
\n
$$
- 2 \cdot Z(\mathbf{u}_i) \cdot Z(\mathbf{u}_i + \mathbf{h}) \cdot Z(\mathbf{u}_j + \mathbf{h})^2 + Z(\mathbf{u}_i + \mathbf{h})^2 \cdot Z(\mathbf{u}_j)^2
$$
  
\n
$$
- 2 \cdot Z(\mathbf{u}_i + \mathbf{h})^2 \cdot Z(\mathbf{u}_j) \cdot Z(\mathbf{u}_j + \mathbf{h}) + Z(\mathbf{u}_i + \mathbf{h})^2 \cdot Z(\mathbf{u}_j + \mathbf{h})^2 \}
$$
  
\n
$$
- (2 \cdot \hat{\gamma}(\mathbf{h}))^2
$$
  
\n(10)

This covariance is called a *quadratic covariance* (Matheron, 1965), and it can be calculated if  $Z(\mathbf{u}_i)$ ,  $Z(\mathbf{u}_i + \mathbf{h})$ ,  $Z(\mathbf{u}_i)$ , and  $Z(\mathbf{u}_i + \mathbf{h})$  have a multivariate Gaussian distribution. In such case, any fourth order moment can be calculated using the pairwise covariance values as follows:

$$
E\{Z_1 \cdot Z_2 \cdot Z_3 \cdot Z_4\} = C_{12} \cdot C_{34} + C_{13} \cdot C_{24} + C_{14} \cdot C_{23} \tag{11}
$$

Notice that those pairwise covariances are different than the  $C_{ii}(\mathbf{u})$  presented earlier, which are fourth order statistics, since they correspond to the covariance between pairs of squared differences (i.e. "pairs of pairs"). Then, the variogram variance is calculated as a sum of fourth order moments minus two times the variogram squared.

A simple program can perform these calculations. For each lag, the location of pairs considered in the experimental variogram calculation is used to determine the fourth order moment as follows:

$$
E\{z(\mathbf{u}_i) \cdot z(\mathbf{u}_i + \mathbf{h}) \cdot z(\mathbf{u}_j) \cdot z(\mathbf{u}_j + \mathbf{h})\}
$$
  
=  $C(z(\mathbf{u}_i), z(\mathbf{u}_i + \mathbf{h})) \cdot C(z(\mathbf{u}_j), z(\mathbf{u}_j + \mathbf{h}))$   
+  $C(z(\mathbf{u}_i), z(\mathbf{u}_j)) \cdot C(z(\mathbf{u}_i + \mathbf{h}), z(\mathbf{u}_j + \mathbf{h}))$   
+  $C(z(\mathbf{u}_i), z(\mathbf{u}_j + \mathbf{h})) \cdot C(z(\mathbf{u}_i + \mathbf{h}), z(\mathbf{u}_j))$  (12)

A valid, positive definite, covariance model is required to perform the calculation presented above. That is the reason to require a first guess of the variogram model.

#### **SIMULATION ALTERNATIVE**

#### **Local Simulation Method**

The idea is to simulate each set of four-point locations in turn and evaluate the fourth order moments in expression (10) by simple averages. Again, the assumption of multigaussianity simplifies the simulation. A matrix or LU simulation approach is very fast and efficient since only four points are considered at a time and there are no conditioning data. All fourth order moments in expression (10) are estimated as averages of products using the simulated values, and the variogram variance is calculated with formula (9).

#### **Global Simulation Method**

The basic idea is to generate nonconditional realizations of the domain using the variogram model, and then calculate the variogram using only the values at the sampled locations. The variance between the variogram values at each lag calculated using these realizations should converge to the same value obtained through any of the other approaches; however, the advantage of this approach is that we can estimate the entire uncertainty distribution of all variogram lags simultaneously, without assuming its shape.

This approach was implemented using the GSLIB program sgsim, that is, unconditional realizations are generated. The sequential path in the program could be modified to only simulate the locations of the original data. Uncertainty in the variogram is directly evaluated by the variability between multiple realizations.

This global simulation method can be viewed as a "spatial bootstrap" or resampling from geostatistical realizations (Journel, 1994).

### **VALIDATION OF THEORETICAL APPROACH BY SIMULATION**

The theoretical approach has the following advantages over the two simulation-based methods (1) implementation is easier since the fourth order

moments are calculated analytically and directly, (2) computer speed is much improved since there is no need for random number generation or multiple realizations, and (3) the simulation methods are approximate, although they converge to the correct result provided the implementation is correct.

The global simulation method has the advantage that the entire distribution of uncertainty is simulated.

# **EXAMPLE 1: CLUSTER.DAT**

Consider the database cluster.dat available in GSLIB (Deutsch and Journel, 1998). The sample locations are on a pseudoregular grid, with clusters in the high value zones (Fig. 2). After normal score transformation, the north–south variogram is calculated for five lags, using a lag separation distance of 4.0 and a lag tolerance of 2.0.

An isotropic spherical variogram model with range 15 m and 90% of variance contribution is fitted to the experimental variogram. The nugget effect is 0.1 (10% of variance contribution):

$$
\gamma(\mathbf{h}) = 0.1 + 0.9 \cdot \mathrm{Sph}\left(\frac{h}{15}\right) \tag{13}
$$



**Figure 2.** Location map of samples taken from Cluster database.

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Lag	Lag distance	Experimental variogram	Fitted variogram	Variance theoretical approach	Variance local simulation method	Variance global simulation method
$\overline{c}$	1.395	0.262	0.225	0.004	0.004	0.004
3	4.361	0.431	0.481	0.021	0.019	0.014
$\overline{4}$	7.906	0.716	0.746	0.046	0.042	0.038
5	11.876	1.191	0.946	0.080	0.068	0.068
6	15.796	1.198	1.000	0.096	0.083	0.130

**Table 1.** Pointwise Variogram Uncertainty Calculated Using the Three Methods Presented

The variogram uncertainty is assessed theoretically, using local simulation, and through the global simulation method. The variance has been calculated for each lag using the three methodologies presented above. In the local simulation approach (using LU simulation), 100 realizations were performed. The results are presented in Table 1.

Results show that with a reasonable number of LU simulations, the local simulation method gives a variance very close to the theoretical result. Assuming normality in the uncertainty distribution, the confidence intervals can be calculated. The variogram, its model and the central confidence intervals at 95, 75, 50, and 25% for each lag are shown in Figure 3.



**Figure 3.** The experimental variogram, along with the variogram model fitted and the central confidence intervals at 95, 75, 50, and 25% for each lag (Cluster database).

#### **EXAMPLE 2: RED.DAT**

This database contains samples of a vertical north–south tabular deposit, where thickness and gold, silver, copper, and zinc concentrations were measured. The variogram uncertainty is calculated for thickness and gold content using the theoretical approach and both numerical methods. The sample locations are presented in Figure 4. The normal score transformation is performed for each variable. The following isotropic variogram model is fitted to the omnidirectional experimental variogram of thickness:

$$
\gamma(\mathbf{h}) = 0.15 + 0.85 \cdot \text{Exp}\left(\frac{h}{250}\right) \tag{14}
$$

For gold content, the variogram model is:

$$
\gamma(\mathbf{h}) = 0.45 + 0.55 \cdot \text{Sph}\left(\frac{h}{250}\right) \tag{15}
$$



**Figure 4.** Location map of samples and gold content taken from the database red.dat.



**Figure 5.** The experimental variogram, along with the variogram model fitted and the central confidence intervals at 95, 75, 50, and 25% for each lag (red.dat database). Left: Variogram for thickness; Right: Variogram for gold content.

The calculation of confidence intervals was performed for each variable, and the results are shown in Figure 5.

The global simulation method was used to obtain the entire uncertainty distribution for each lag. 100 nonconditional realizations of a Gaussian random variable were generated using sgsim. The simulated values at the sampled locations (obtained from the database red.dat) were extracted for each realization. The experimental variogram was calculated using the simulated values at the sampled locations and the same parameters that were used to find the experimental points shown in Figure 5.

The experimental variograms calculated for each realization using the entire simulated field (showing ergodic fluctuations) and those calculated using only the simulated data at the sample locations (now considering the effect of ergodic fluctuations and "sampling fluctuations") are shown in Figure 6 for thickness and gold content.

Table 2 shows the variogram variance for each variable and lag, calculated using the theoretical approach, the local simulation method, and the global simulation method. Hundred realizations were generated for the numerical methods.

The results obtained from the theoretical approach and the local simulation method are similar; however, the global simulation method gives lower variance for all the lags. The main difficulty of this approach is to ensure correct use of the variogram for all distances when a limited number of nearby samples is used (Tran, 1994). The variogram calculated for each realization (using all the simulated nodes) was presented in Figure 6 (Left). The variability in the variograms calculated using all the nodes in the grid is lower than the expected variability.

Histograms showing the entire uncertainty distribution for the corresponding lags are presented in Figure 7. All the histograms generated through the global simulation method are slightly asymmetric with a tail to the right. This asymmetry was expected since the variogram is nonnegative.

Lag	Lag distance	Experimental variogram	Fitted variogram	Variance theoretical approach	Variance local simulation method	Variance global simulation method
				Variable: Thickness		
$\overline{c}$	17.497	0.332	0.311	0.013	0.012	0.004
3	51.119	0.687	0.540	0.008	0.001	0.007
$\overline{4}$	99.311	0.669	0.742	0.044	0.041	0.024
5	148.627	0.871	0.857	0.092	0.089	0.052
6	197.746	0.957	0.921	0.152	0.150	0.085
7	250.436	1.178	0.958	0.176	0.177	0.112
8	297.843	0.969	0.976	0.264	0.258	0.160
9	345.356	0.992	0.986	0.289	0.270	0.193
				Variable: Gold content		
$\overline{2}$	17.497	0.493	0.554	0.044	0.041	0.014
3	54.099	0.706	0.712	0.015	0.001	0.008
4	99.435	0.715	0.833	0.030	0.005	0.015
5	149.221	0.865	0.908	0.053	0.043	0.028
6	198.912	1.065	0.949	0.078	0.075	0.056
7	249.254	1.216	0.972	0.096	0.092	0.066
8	297.879	0.961	0.985	0.134	0.140	0.079
9	345.618	1.088	0.991	0.160	0.161	0.110

**Table 2.** Theoretical Approach to Calculate the Variogram Confidence Intervals

# **TRANSFERRING POINTWISE UNCERTAINTY INTO THE JOINT MODEL**

Several alternative variogram models could be fitted within the confidence limits generated above. In order to achieve more realistic predictions, we can assume different scenarios within those confidence limits. It is important to note that variogram models fitted using the 97.5 and the 2.5 quantile variogram values for all lags (Fig. 8) do not fairly represent extreme cases in the joint uncertainty. The correlation between the lags and the "continuity" of alternative variogram models should be accounted for when fitting models to represent extreme "joint" cases.

Our proposal is to evaluate the consequences of using our first guess (the one used to calculate the pointwise uncertainty), plus two extreme scenarios showing high and low continuity, within the pointwise confidence limits (Fig. 9). Simulation can be done using those three scenarios to determine the sensitivity of the results to variogram uncertainty. Notice that we do not just have to modify the parameters (range and sill contribution) of the variogram model, but the type of structure to account for high and low continuity scenarios.

Uncertainty in the variogram sill can be addressed by fitting models with different sill. This uncertainty can be due to uncertainty in the reference statistics.



**Figure 6.** The experimental variogram values for each lag calculated using (Left) all the simulated data and (Right) only the simulated values at sampling locations (red.dat database). Top: Thickness; Bottom: Gold.

### **COMMENTS**

A variogram model is required in all approaches. Ideally, one could determine the uncertainty using the experimental points before fitting a model. The assessment of uncertainty, however, requires a positive definite covariance model (i.e. a nonnegative variogram model); therefore a variogram must be fitted before evaluating the uncertainty. This seems circular, however, it is the only way to solve the problem: the authorized model is assumed as the expected value of the variogram at each lag and then the variance is calculated.

The variogram uncertainty can be transferred to subsequent stages of a geostatistical study. The theoretical approach and the local simulation method generate the same results. The global simulation method requires more computer time and should give the same result, since the idea is basically the same as the local method; however, it is difficult to honor the variogram precisely for large distances and consequently, the variance may be lower. The advantage of the global simulation method is that it estimates the shape of the joint uncertainty in the variogram for all lags.



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Figure 8. An example of an incorrect interpretation of joint uncertainty, given the pointwise uncertainty. Scenarios 1 and 2 do not represent quantiles 97.5 and 2.5 in the joint model.



Figure 9. An example of a correct interpretation of joint uncertainty: Scenarios 1 and 2 represent low and high continuity (extremes of the joint model).

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Confidence intervals for each experimental variogram value can be determined from the variance assuming normality. This is approximate since the histogram of variogram values obtained for each lag must be nonnegative. All methods require multigaussianity, which could be relaxed with non-Gaussian simulation methods. This has not been explored in this article.

The difference between the pointwise uncertainty and joint uncertainty must be addressed: the procedures presented in this article allow calculation of the pointwise uncertainty. Within this uncertainty, several variogram models (joint models) can be fitted. The confidence intervals for the joint model will be different since we are interested in finding the uncertainty in the continuity of the variable. Several joint models with different degrees of continuity should be used in the subsequent kriging and simulation stages of a geostatistical study to account for the uncertainty in the variogram model.

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