Variogram Models Based on the Intersection of Geometric Shapes

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Abstract

Geostatistical models often require a semivariogram or covariance model for kriging and kriging-based simulation. Next to the initial decision of stationarity, the choice of an appropriate variogram model is the most important decision in a geostatistical study. Common practice consists of fitting experimental variograms with a nested combination of proven models such as the spherical, exponential, and Gaussian models. These models work well in most cases; however, there are some "shapes" found in practice that are difficult to fit. Greater flexibility is available through the application of geometric semivariogram models.

We introduce a family of semivariogram models that are based on geometric shapes, analogous to the spherical semivariogram, that are known to be conditionally negative definite and that provide additional flexibility to fit semivariograms encountered in practice. A methodology to calculate the associated geometric shapes to match semivariograms defined in any number of directions is presented.

Introduction

Semivariogram-based geostatistics is important for the modeling of continuous and categorical geologic properties. The random function paradigm of geostatistics involves three main steps: (1) definition of the variable and the stationary domain for the variable $\{Z(u), u \in A\}$, which involves the definition of rock types/facies and large scale trends, (2) establish a semivariogram model for the variable, $\gamma(h)$, that is valid for all distances and directions found in the domain A, and (3) make inferences with kriging and Monte Carlo simulation. The reasonableness of the inferences depends on the first two steps. The expert site-specific decision of a stationary domain is arguably the most important; however, the calculation and fitting of a semivariogram model is also very important. The inference step is largely automatic once the first two steps are taken. This paper is aimed at the second step of establishing a valid semivariogram model. The conventional method of modeling semivariograms by nested structures is reviewed. While this method guarantees a semivariogram model that is conditionally negative definite in all directions, it may be viewed as restrictive. A suite of geometric semivariograms and a method for constructing new geometries that match custom continuity styles are presented. These geometric semivariogram models allow for greater flexibility in the generation of permissible semivariogram models.

Conventional Semivariogram Modeling

The semivariogram of traditional geostatistics characterizes heterogeneity or predictability of the variable under consideration. Semivariogram models must be conditionally negative definite. This property ensures that the semivariogram is an appropriate measure of distance and that all resulting variances will be non-negative for all possible configurations of conditioning data (Journel and Huijbregts, 1978, p. 35).

Experimental semivariogram points are calculated in the principal directions allowing for some distance and direction tolerance to find sufficient pairs. The experimental points are fitted with a sum of nested structures.

$$\gamma(\mathbf{h}) = \sum_{i=0}^{nst} C_i \Gamma_i(\mathbf{h}) \tag{1}$$

where *nst* is the number of nested structures, $i = 0$ is commonly reserved for the nugget effect, and $\Gamma_i(\mathbf{h})$ functions are valid semivariogram functions defined by a shape (spherical, exponential, etc.), rotation angles to allow $\mathbf{h}$ to be represented in the principal directions of continuity ($\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3$), and range parameters to account for anisotropy. A geometric transformation is applied to convert the 3-D distance vector, **h**, to a scalar distance *h* [Eq.(2)].

$$h = \sqrt{\left(\frac{\mathbf{h}_1}{a_1}\right)^2 + \left(\frac{\mathbf{h}_2}{a_2}\right)^2 + \left(\frac{\mathbf{h}_3}{a_3}\right)^2} \tag{2}$$

Semivariogram modeling has relied on fitting known conditionally negative definite functions such as spherical, exponential and Gaussian models. Some additional flexibility is available since linear combinations and products of conditionally negative definite covariance models are known to be conditionally negative definite (Deutsch and Journel, 1998, p. 24). While this provides a workable mechanism for modeling continuity, there are some cases that are not well fit with this framework (see Figure 1 for an example structure commonly observed in experimental semivariograms).

The application of more flexible semivariogram modeling is inhibited by the difficulty in ensuring conditionally negative definiteness. There is a largely unexplored suite of conditionally negative definite models known as *geometric semivariograms* that provides some additional flexibility. They are genetically guaranteed to be conditionally negative definite and therefore avoid the burden of proof required by arbitrary semivariogram functions.

Geometric Semivariograms

Any covariance model based on a moving average of a generalized Poisson process is conditionally negative definite (Matérn, 1960, p. 28). Geometric semivariograms result from the special case of averaging where the weighting function is reduced to a Dirac function of the form:

$$f(\mathbf{u}) = i_v(\mathbf{u}) = \begin{cases} 1, if & \mathbf{u} \in V \\ 0, if & \mathbf{u} \notin V \end{cases}$$
$$F(\mathbf{u}) = K_v(\mathbf{h}) = \int i_v(\mathbf{u}) \cdot i_v(\mathbf{u}+\mathbf{h}) d\mathbf{u} \tag{3}$$
$$\gamma(\mathbf{h}) = 1 - \frac{K_v(\mathbf{h})}{K_v(0)}$$

This amounts to the volume of intersection $K_v(\mathbf{h})$ of any geometric object with itself offset by a lag vector, $\mathbf{h}$ scaled by the volume of the geometric object, $K_v(0)$. Construction of a geometric semivariogram is illustrated in Figure 2.

A conditionally negative definite model in n-D is valid in any less or equal dimensional space; for example, the spherical semivariogram, based on a 3-D geometry, is valid in 3, 2 and 1 dimensions, a circular semivariogram, based on a 2-D geometry, is valid in 2 and 1 dimensions and the triangular semivariogram, based on a 1-D geometry, is valid only in 1 dimension.

In some cases analytical equations may be available for the volumes of intersection. Numerical integration can always be used for complicated geometric objects. The volume of intersection could be efficiently calculated as:

$$\gamma(\mathbf{h}) = \underbrace{\sum_{i_z}^{n_z}\sum_{i_y}^{n_y}\sum_{i_x}^{n_x} i(\mathbf{u}_x,\mathbf{u}_y,\mathbf{u}_z)}_{K'_V(0)} - \underbrace{\sum_{i_z}^{n_z}\sum_{i_y}^{n_y}\sum_{i_x}^{n_x} i(\mathbf{u}_x,\mathbf{u}_y,\mathbf{u}_z)\cdot i(\mathbf{u}_x+\mathbf{h}_x,\mathbf{u}_y+\mathbf{h}_y,\mathbf{u}_z+\mathbf{h}_z)}_{K'_V(\mathbf{h})} \tag{4}$$

where $i(\mathbf{u}_x,\mathbf{u}_y,\mathbf{u}_z)$ and $i(\mathbf{u}_x+\mathbf{h}_x,\mathbf{u}_y+\mathbf{h}_y,\mathbf{u}_z+\mathbf{h}_z)$ are indicators set to 1 if within the object and 0 if without the object and $K'_V(0)$ is the discretized volume of the geometry and $K'_V(\mathbf{h})$ is the volume of intersection given the component lag vectors $\mathbf{h}_x,\mathbf{h}_y,\mathbf{h}_z$ of lag vector $\mathbf{h}$. The result is a discrete covariance model for kriging or simulation. This discrete covariance model may be represented as a covariance table that may be loaded directly into a kriging or kriging based simulation algorithm.

Limitations of Geometric Semivariogram Models

Geometric semivariogram models have a couple of significant limitations in their form: (1) the sill cannot be exceeded, (2) the semivariogram is linear at small lag distance and (3) the semivariogram model is only known at discrete lag distances, unless the analytical solution is known (i.e. spherical semivariogram model). Since the covariance model (see Equation 3) must be positive, it is not possible to model negative covariance or a semivariogram above the sill. This precludes the modeling of trend and hole effect continuity structures. The linear feature at small lag distances prevents geometric semivariogram models from reproducing high short range continuity as seen with the Gaussian semivariogram model (Deutsch and Journel, 1998).
The geometry and covariance table are constructed to match a specific regular grid; therefore, the semivariogram may only be applied to calculate the covariance between points on this grid. These models may be applied to calculate mean covariance values by the generating at a high resolution, such that at least three discretizations exist in each dimension of the smallest grid node. In addition, data must be assigned to the nearest node or the nearest discretization within the node, since the semivariogram is not defined for all lag distances and directions.

Isotropic Geometric Semivariogram Models

Isotropic geometric semivariogram models result from isotropic geometric objects. This is limited to lines (1-D), circles (2-D), spheres (3-D) and hyperspheres (n-D, n > *3*). These geometric models account for anisotropy by scaling the component vectors [Eq. (2)].

Spherical Semivariogram

This semivariogram model is used frequently. The spherical model is based on the standardized volume of intersection of two spheres separated by a lag vector (h) as defined (Serra, 1967).

$$\gamma(\mathbf{h}) = 1 - \frac{volume(\mathbf{h})_{\text{int}}}{volume_{total}} \tag{5}$$

where $volume(\mathbf{h})_{\text{int}}$ is the volume of intersection $volume_{total}$ is the total volume of the geometric object.

Hollowed Spherical Semivariograms

A variety of other isotropic geometric semivariogram models may be calculated by hollowing of the geometric object. For example the circle in 2-D may be changed to an annular region or the sphere in 3-D may be changed to a hollowed sphere. The hollowed sphere results in a novel series of conditionally negative definite 3-D semivariogram models parameterized by the inner radius (r_1) or fraction of hollowing. A series of hollowed spherical semivariogram models are shown in Figure 3.

In the limiting cases this semivariogram is equivalent to the spherical model when r_1 equals 0.0 (the sphere is not hollowed) and approaches the nugget effect as $r_1 \rightarrow r_2$. The difference between the hollowed spherical semivariogram and the spherical semivariogram is equivalent to the volume of intersection lost due to the hollowed inner sphere (Figure 4). An example hollowed sphere (fraction hollowed 0.75) geometry and resulting covariance table are shown in Figure 5.

Anisotropic Geometric Semivariogram Models

Any geometric shape in any dimension leads to a valid semivariogram model. Slices through an approximated shape of a point bar inclined heterolithic strata (IHS) are shown on the top of Figure 6. The covariance table is calculated for this object and is shown on the bottom of Figure 6. This complicated anisotropic geometric object has resulted in a complicated anisotropic covariance table.

There are a variety of geologic geometries that may be applied to calculate semivariogram models. For example, characteristic geometries of architectural elements from fluvial depositional settings such as lateral accretion, downstream accretion, channel fills etc. (Miall, 1999, p. 93) may be suitable.

There is a limit on the information that geometry may provide with respect to the semivariogram model. For example, the randomly positioned spheres result in the bombing semivariogram model [Eqn. (6)] not the spherical semivariogram model (Deutsch, 87, p. 135).

$$\gamma(\mathbf{h}) = p\left(1 - p^{Sph(\mathbf{h})}\right) \tag{6}$$

Yet the geometry may provide information with respect to the general semivariogram shape and anisotropy. Another approach is to calculate the geometry that will match a target semivariogram model. This target semivariograms are assessed from experimental semivariograms and geologic information.

Sculpted Geometric Semivariograms

A method is presented to calculate the geometry to match a target semivariogram in specified directions. An initial geometry is iteratively eroded and dilated. Changes that improve the match between the current geometric model and the target semivariograms are accepted. The resulting geometry may be applied to calculate covariance tables for application in kriging based estimation and simulation.

The Inputs

Custom geometric semivariograms may be constructed to match continuity structures defined in any set of directions. These continuity structures are represented as tables with the target semivariograms and associated lag distance. The practitioner may freely apply site specific information and professional judgment in assigning these target directional semivariograms. It is anticipated that these models will be fit to at least the principal directions, with additional directions added to further constrain the resulting model.

The Initial Geometry

Initial geometry is coded such that the final model may not have a range greater than the longest identified range nor less than the shortest identified range. The geometry is initialized with a sphere (assuming 3-D) with diameter set to the largest range in all specified directions. Locations outside of this geometry are set static outside (code 0) the geometry. A nested sphere with a diameter equal to the shortest identified range is coded as static inside the geometry (code 1). The remainder of the space may be switched between 1 and 0 iteratively to improve the reproduction of the target directional semivariograms (Figure 7). This approach assumes that the principal continuity directions are included among the identified directions. Also, there is no model assumed for off-diagonal directions, unlike the assumption of an ellipsoidal continuity in the off-diagonal directions in traditional semivariogram models (Figure 8). Multiple sculpted geometric semivariogram models may be calculated to represent this uncertainty in the off-diagonal directions. If adequate information is available, experimental semivariogram fits in off-diagonal directions may be integrated to further constrain the model.
Zonal anisotropy may be included by setting the initial diameter large relative to the size of the covariance lookup table. This may increase the variability of the sculpted semivariogram model in the off-diagonal directions.

The Iterations and Convergence Criteria

An objective function is applied to characterize mismatch between the target and sculpted geometric semivariogram models. This object function is shown below (Deutsch, 1992).

$$O = \sum_{i=1}^{nDir} \sum_{j=1}^{nLag} \left| \gamma^{geo}(\mathbf{h}_{i,j}) - \gamma^{t}(\mathbf{h}_{i,j}) \right| \tag{6}$$

where $\gamma^{geo}(\mathbf{h}_{i,j})$ and $\gamma^{t}(\mathbf{h}_{i,j})$ are the current geometric and target semivariogram models for each indicated direction, i, and lag, j.

The nodes within the modifiable zone (Figure 7) are visited in order from the outside inwards. This ordering is based on the distance function of initial geometry (Vincent, 1993). This amounts to the assignment of the distance to the nearest periphery of the geometry at all nodes within the geometry. The distance function is sorted in ascending order with pointer arrays permuted.

For each location, the geometry code is switched. The location within the current geometry is eroded ($i(u_i) = 1 \rightarrow 0$) or outside the current geometry dilated ($i(u_i) = 0 \rightarrow 1$). The objective function is updated and if the perturbation reduces the objective function it is accepted. The algorithms proceeds until either a maximum number of iterations are performed or until a specified number of iterations occur without acceptance of a perturbation.

Example Sculpted Semivariogram Models

A large suite of sculpted semivariogram models were calculated. Many unconditional 2-D sequential Gaussian simulation models were calculated with a variety of input semivariogram parameters (ranges, nugget effects, anisotropies and structure types). Then the experimental semivariograms were calculated for the 0^0, 45^0, 90^0 and 135^0 azimuths. These experimental semivariograms were applied as input for the construction of 2-D sculpted geometric semivariograms. The resulting covariance tables were each applied in simple kriging 100 times with random data configurations to check for stability of the solutions. None of the trials suggested ill conditioned covariance matrices, since all weights were reasonable [-1,1] and kriging variances were always positive.

An example 2-D sculpted geometric semivariogram model is shown in Figure 9. This example demonstrates the flexibility and some limitations of sculpted semivariogram models. Note that the trend in the input directional variograms is not reproduced since geometric models may not exceed the sill. The zonal anisotropy is not reproduced since the largest range was set to 40 units.

Another example 2-D sculpted geometric semivariogram model is shown in Figure 10. This model represents a phenomenon with a high nugget effect and a high degree of anisotropy. Note that the nugget effect is reproduced by a lack of contiguity in the geometry and the anisotropy results in anisotropy in the geometry.

Proposed Flexible Semivariogram Modeling Procedure

A new methodology for flexible semivariogram modeling is proposed. This methodology requires the following steps: (1) assess the continuity of the modeled phenomenon in at least the principal directions, (2) construct a geometric object either from characteristic geometries or by the iterative method introduced in this paper with a resolution greater than or equivalent to the resolution of the model to be estimated or simulated, (3) calculate a discrete covariance table from this geometry, (4) load this covariance table into the kriging or simulation algorithm. These directional models may be regression fits of the experimental semivariogram points, or even hand drawn. The key is to build models that integrate geologic information.

Conclusion

The choice of semivariogram model has a major affect on kriging and kriging-based simulation. Historically, these models have been limited to nested combinations of proven models. Geometric semivariogram models provide a suite of conditionally negative definite models for improved semivariogram modeling flexibility. A flexible method has been presented for constructing geometries for geometric semivariograms that reproduce spatial continuity identified in principal and additional directions.

The required computer code is straightforward and efficient and is available to all CCG members. All semivariogram models proposed here are guaranteed to be conditionally negative definite;

therefore, there are no issues with implementation. Flexible fitting of semivariogram models allows for greater focus on the available experimental semivariogram and geologic information without the limitation imposed with the traditional method of nested structures.

References

Deutsch, C.V., 1987, A probabilistic approach to estimate effective absolute permeability: unpubl. masters dissertation, Stanford University, 165 p.

Deutsch, C.V., 1992, Annealing techniques applied to reservoir modeling and the integration of geological and engineering well test data: unpubl. doctoral dissertation, Stanford University, 306 p.

Deutsch, C.V. and Journel A.G., 1992, GSLIB: geostatistical software library and user's guide 2nd ed.: Oxford University Press, New York, 369 p.

Deutsch, C.V. and Journel A.G., 1998, GSLIB: geostatistical software library and user's guide 2nd ed.: Oxford University Press, New York, 369 p.

Isaaks, E. H. and Srivastava R.M., 1989. An introduction to applied geostatistics: Oxford University Press, New York, 561 p.

Journel, A.G. and Huijbregts, Ch.J., 1978, Mining geostatistics: Academic Press, New York, 600 p.

Matérn, B., 1960, Spatial variation, volume 36 of lecture notes in statistics 2nd ed.: Springer-Verlag, New York, First edition published by Meddelanden fran Statens Skogsforskningsinstitut, band 49, no. 5, 1960, 151 p.

Miall, A. D., 1996, The geology of fluvial deposits: sedimentary facies, basin analysis and petroleum geology: Springer-Verlag Inc., Berlin, 582 p.

Serra, J., 1967, Un critère nouveau de découvertes de structures: le variogramme: Sciences de la Terre, v. 12, p. 275-299.

Vincent, L., 1993, Morphological Algorithms, In: *Mathematical Morphology in Image Processing*, edited by E.R. Dougherty, Marcel Dekker, Inc., New York.

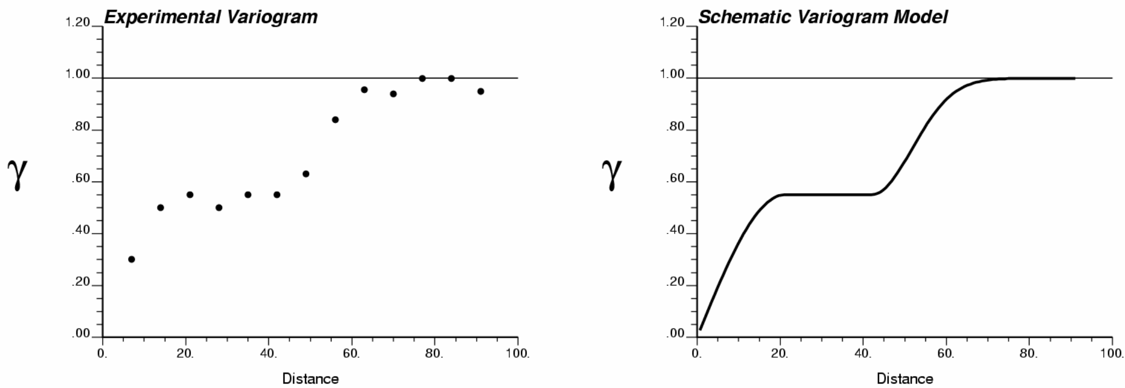

Figure 1 - An example semivariogram that is not well fit by nested sets of traditional variogram models.

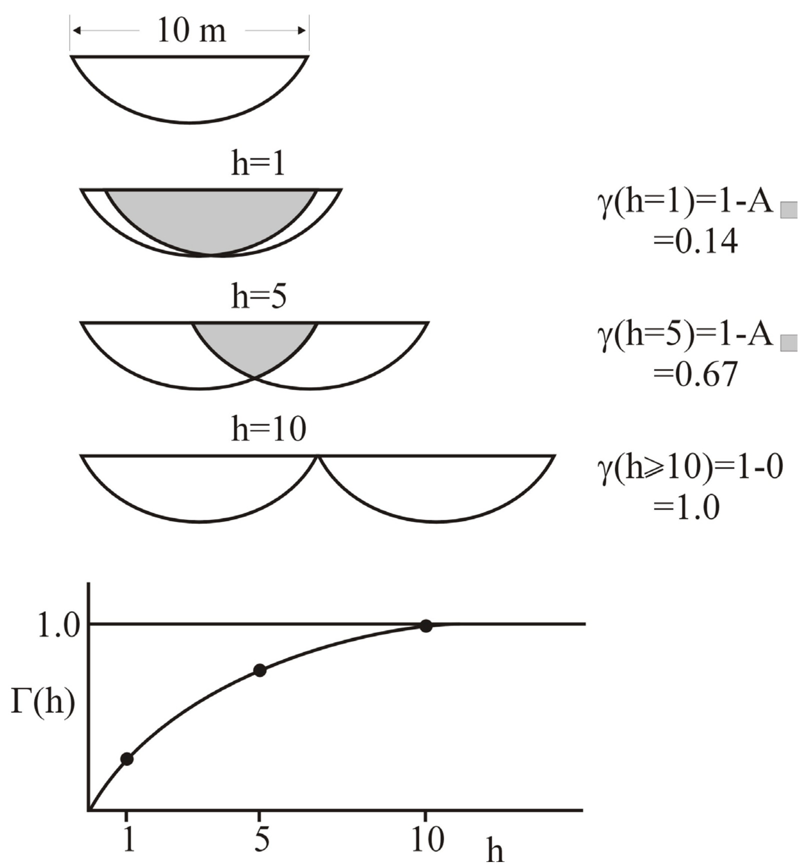

Figure 2 - An example geometric object and the resulting geometric variogram in the horizontal direction. The semivariogram model is anisotropic.

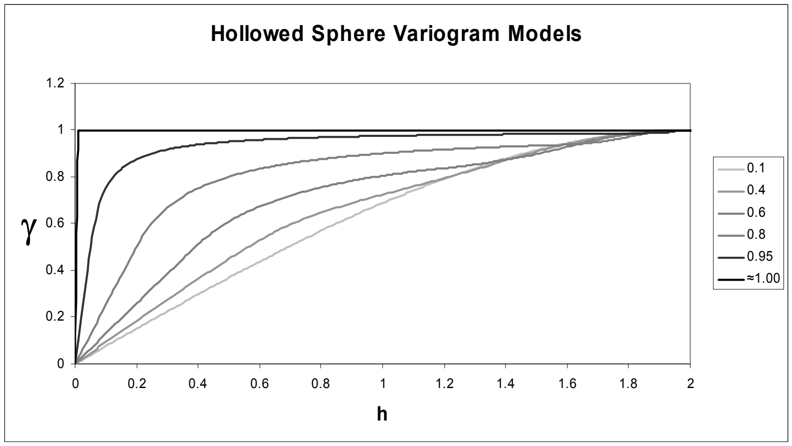

Figure 3 - A series of hollowed sphere semivariogram models. The sphere radius, r2, is set to 1.0 and the radius of the hollowing is varied.

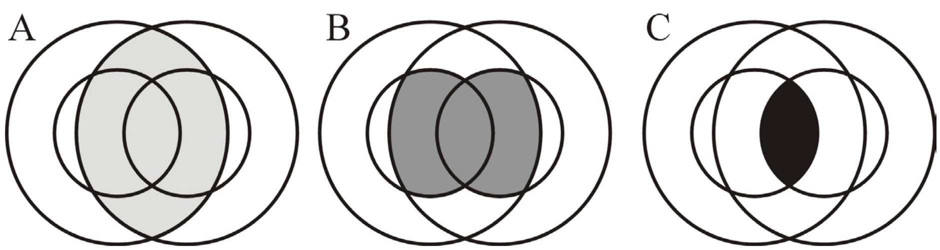

Figure 4 - Volumes v1, v2 and v3 (A, B and C): a traditional spherical variogram model is equal to standardized v1 subtracted from the contribution. The hollowed sphere model is equal to the spherical minus v2 plus v3.

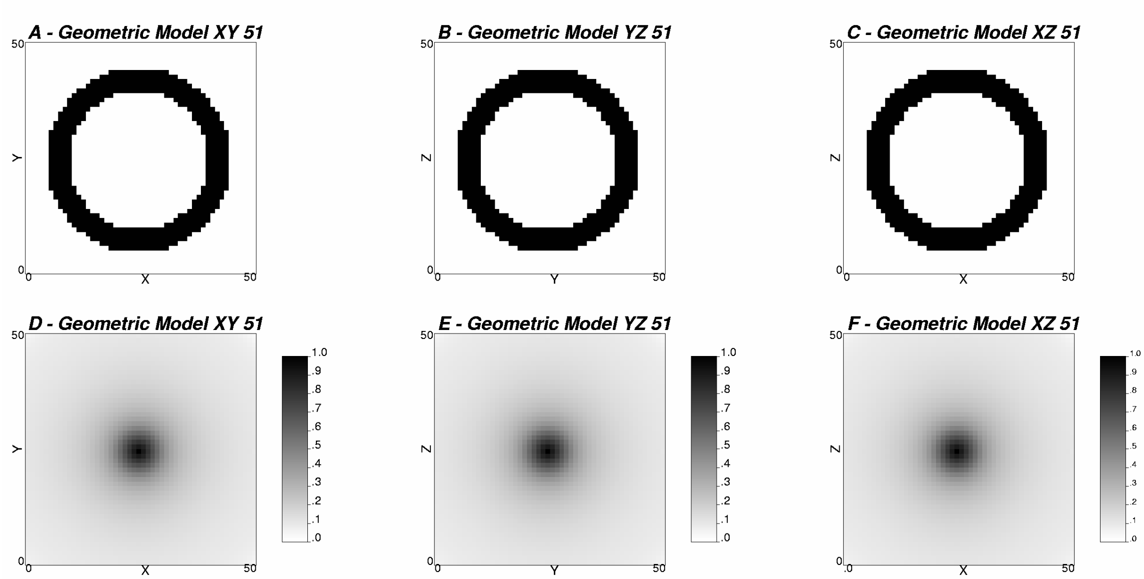

Figure 5 - Center slices through the rasterized geometric object and the resulting covariance table for the hollow spherical model with a hollowed fraction of 0.75.

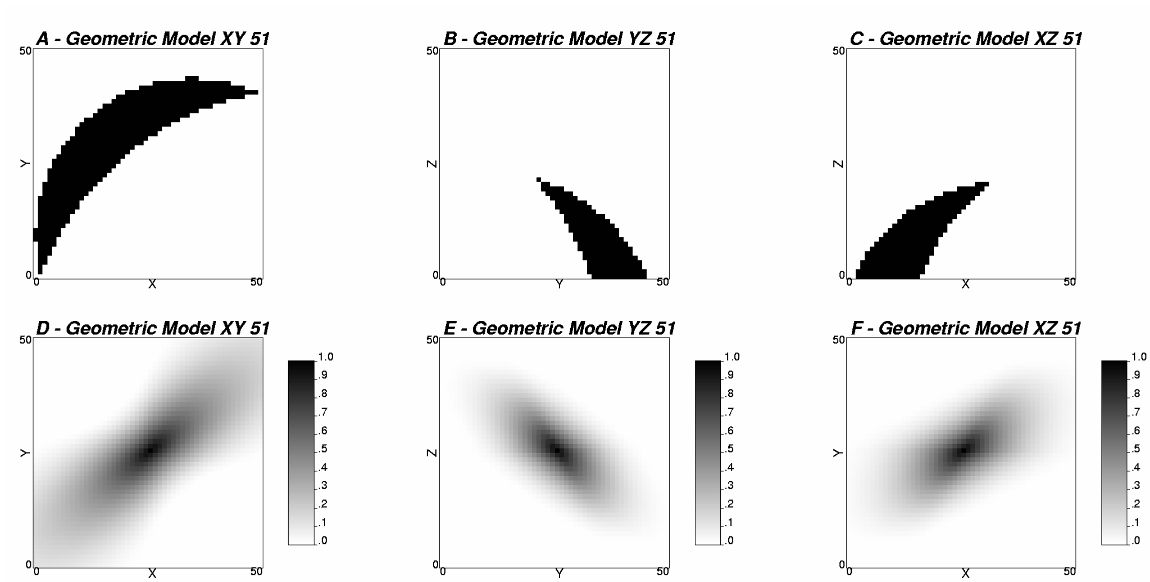

Figure 6 - Center slices through the raster geometric object and the resulting covariance table for a possible IHS point bar variogram.

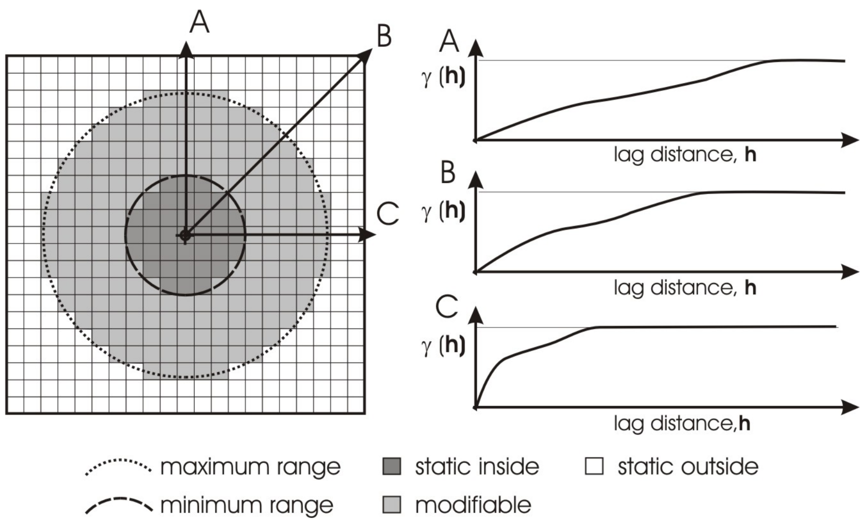

Figure 7 - An initial 2-D geometry based on fit semivariograms in three directions. The area outside a circular geometry with a diameter equal to the longest identified range (direction A) is set as permanently outside the geometry. A circular geometry with a diameter equal to the shortest identified range (direction C) is set as permanently inside the geometry. The remainder may be modified iteratively to fit the semivariograms in each identified direction.

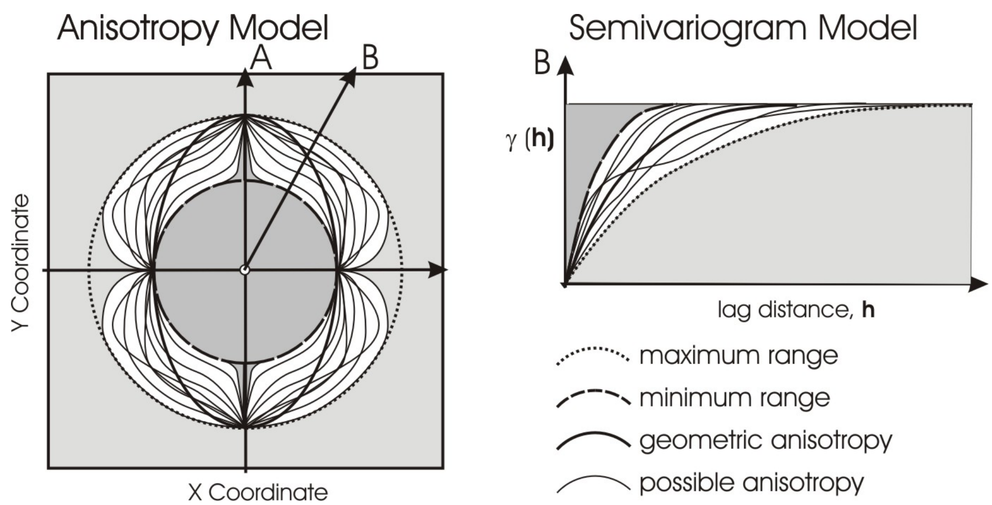

Figure 8 - The constraints on sculpted geometric semivariogram models. The major and minor principal directions (directions A and B respectively) and the traditional anisotropy ellipsoid are shown. The sculpted semivariogram model is constrained such that range in the off diagonal directions (such as direction B) may not exceed the range in the major direction or be exceeded by the range in the minor direction. The anisotropy may be expressed in a various forms within this constraint.

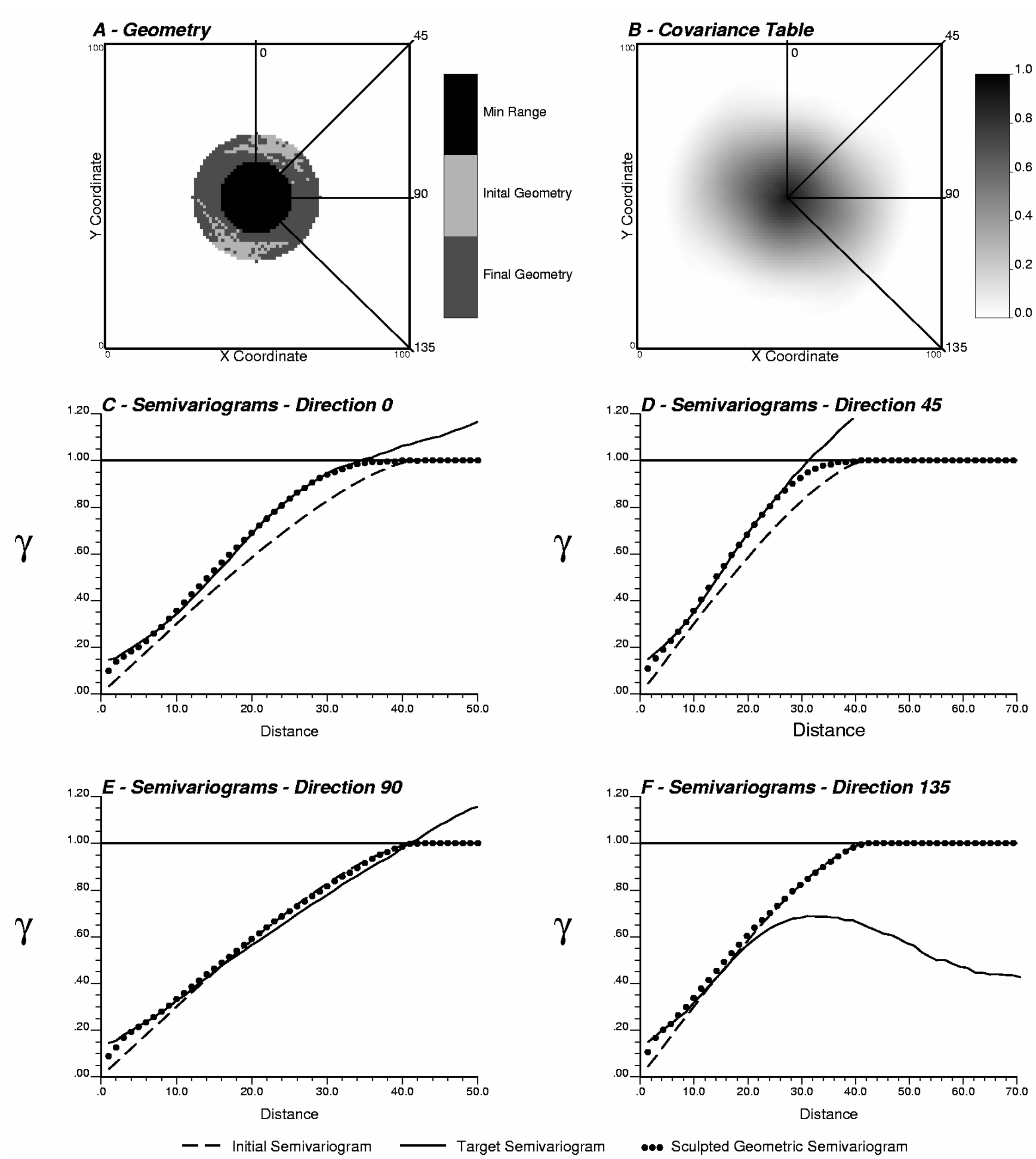

Figure 9 - A 2-D geometry and covariance table for a sculpted geometric semivariogram model based on a phenomenon with high continuity. The initial geometry, the target directional models and resulting sculpted geometric semivariogram models in 0^O, 45^O, 90^O and 135^O directions are shown. The longest range of continuity was assigned as 40 units. The target models are experimental semivariograms from unconditional sequential Gaussian simulation.

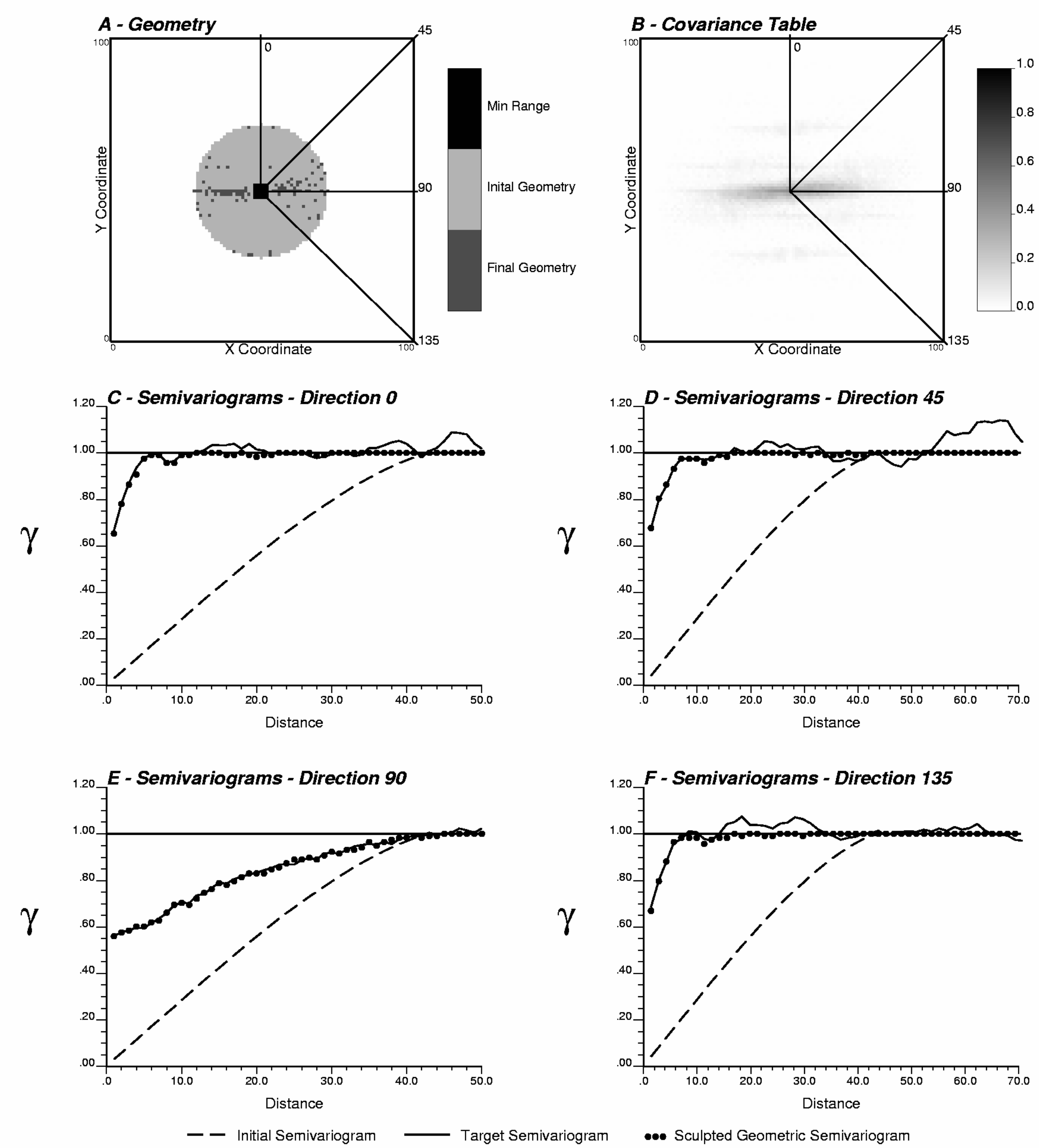

Figure 10 - A 2-D geometry and covariance table for a sculpted geometric semivariogram model based on a phenomenon with high anisotropy and large nugget effect. The initial geometry, the target directional models and resulting sculpted geometric semivariogram models in 0^{O}, 45^{O}, 90^{O} and 135^{O} directions are shown. The target models are experimental semivariograms from unconditional sequential Gaussian simulation.