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Variograms with Zonal Anisotropies and Noninvertible Kriging Systems[1]

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Zonal anisotropies are usually simply defined as those that are not geometric (i.e., that cannot be removed by an affine transformation). Such anisotropies have often been associated with zonations and models have been proposed to reflect that association. It is shown by example that such models can lead to noninvertible coefficient matrices in kriging systems, because the models are only (conditionally) semidefinite instead of positive definite. The relationship to the construction used in turning bands algorithm and also to spatial-temporal models is discussed.

KEY WORDS: variogram, anisotropies, positive definiteness, invertibility.

INTRODUCTION

Geometric anisotropies are defined in terms of invertible affine transformations, and zonal anisotropies are commonly defined as those that are not geometric. Physically, the latter are thought of as being related to some form of zonation; and the corresponding variograms or covariance function models commonly have been modeled with a nested structure, with some components being dependent on only some coordinates. An example is presented to show that such a construction may lead to a kriging system that is not invertible.

THE EXAMPLE

Consider a problem in two dimensions with sample locations at the corners of a rectangle. To simplify the discussion, assume that the sample locations are

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at $(x_1, y_1) = (0, 0)$, $(x_2, y_2) = (h, 0)$, $(x_3, y_3) = (0, l)$, and $(x_4, y_4) = (h, l)$. Suppose that $\gamma(x, y)$ is a variogram having a nested structure as follows:

$$\gamma(x, y) = \gamma_1(x) + \gamma_2(y) \tag{1}$$

where γ_1, γ_2 are valid (in 2D space) isotropic variograms, such that $\gamma_1(h) = a$, $\gamma_2(l) = b$. Consider the left-hand side coefficient matrix for an ordinary kriging system, using these four sample locations. The matrix is (assume the points are numbered in the order listed)

$$\begin{bmatrix} 0 & a & b & a+b & 1 \\ a & 0 & a+b & b & 1 \\ b & a+b & 0 & a & 1 \\ a+b & b & a & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

It is obvious that the sum of rows one and four is the same as the sum of rows two and three; hence, the four rows are linearly dependent and thus the matrix is singular. The problem is that $-\gamma$ is only conditionally semidefinite, rather than positive definite. This is easy to see if weights of 1, -1, -1, 1 are assigned to the four points; then the quadratic form

$$- \Sigma \, \Sigma \, \lambda_i \lambda_j \gamma(x_i - x_j, y_i - y_j) \tag{2}$$

is zero, whereas it should be positive if $-\gamma$ were (strictly) conditionally positive definite. Note that analogous observations could be made if covariances were used instead of variograms.

There are several aspects of this (counter) example worth noting:

1. No assumptions have been made about the type of models used to represent γ_1, and γ_2.
2. No assumptions have been made about the numbers a, b, h, l, except that if $h > 0$ then $a > 0$ and if $l > 0$ then $b > 0$. If one or the other of the variograms were periodic, then the conditions on a, b might not be satisfied for all positive h, l. Hence, the coefficient matrix will be singular for (nearly) any four points that are the vertices of a rectangle with sides parallel to the coordinate axes of the model (1).

3. Strict positive definiteness of $-\gamma$ is a sufficient condition for the coefficient matrix to be nonsingular for all sample location patterns (assuming that no sample location appears twice), but semidefinite functions can have singular coefficient matrices for some sample location patterns. For a generalization of this result, see Myers (1988).
4. The singularity of the coefficient matrix in the kriging system is a consequence of the sample location pattern and is not dependent on the location to be estimated (or in the case of block kriging, the location or shape of the block). Whereas the vector of weights used in the kriging estimator is indeterminate, and hence the estimated value is also indeterminate, the kriging variance is constant. Using the example given above, if $\gamma(h/2, l/2) = d$ and the point to be estimated is the center of the rectangle, then the "solution" vector is

$$\begin{aligned}
\lambda_1 &= \lambda_4 \\
\lambda_2 &= 0.5 - \lambda_4 \\
\lambda_3 &= 0.5 - \lambda_4 \\
\lambda_4 &= \lambda_4 \\
\mu &= d - (a + b)/2
\end{aligned}$$

From the symmetry one would expect all the weights to be 0.25, this would correspond to $\lambda_4 = 0.25$. However, for any choice of the arbitrary variable, λ_4, the kriging variance is the same—namely, $2d - (a + b)/2$.

A PARADOX?

While the example given above makes no explicit assumptions about the random function, the construction of a variogram or covariance of the form given in (1) seems very plausible since one way to obtain such a variogram representation is to construct a random function as follows:

$$Z(x, y) = Z_1(x) + Z_2(y) \tag{3}$$

where (x, y) is a point in 2D space (note that it could equally well be x in n-space and y representing time). The representation given in (3) could correspond to a zonation in a deposit. If Z_1, Z_2 are uncorrelated, then the variogram would have the form given in (1). In general, one expects that the sum of two valid models (i.e., strictly positive definite models would result in a strictly positive definite model). The example shows that this does not always happen in this kind of construction.

As pointed out by one of the referees, the construction in (3) results in four random variables being linearly dependent, i.e.,

$$Z(h, l) + Z(0, 0) = Z(h, 0) + Z(0, l) \tag{4}$$

In this case, then, it is not unexpected that the variogram or covariance is poorly behaved.

The reader may also be struck by the similarity of (3) with the construction used in the turning bands simulation technique, wherein a random function defined in a higher dimensional space is "simulated" by forming a linear combination of uncorrelated "simulated" random functions defined in 1D space. Each term in the sum corresponds to projecting the point in n-space onto a line, e.g., one of the coordinate axes as is the case in (3). One clear difference is that the covariance function for each of the terms is the one-dimensional covariance corresponding to the original covariance defined in n-space. This example will be discussed subsequently.

EXTENSION TO 3D SPACE

To better understand the counterexample and its relevance to the turning bands construction, it is useful to examine the problem in 3D space; that is, consider 8 sample locations with coordinates $(x_1, y_1, E_1) = (0, 0, 0)$, $(x_2, y_2, E_2) = (h, 0, 0)$, $(x_3, y_3, E_3) = (0, l, 0)$, $(x_4, y_4, E_4) = (0, 0, k)$, $(x_5, y_5, E_5) = (h, l, 0)$, $(x_6, y_6, E_6) = (h, 0, k)$, $(x_7, y_7, E_7) = (0, l, k)$, and $(x_8, y_8, E_8) = (h, l, k)$. Suppose that $\gamma(x, y, E)$ is a variogram having a nested structure as follows:

$$\gamma(x, y, E) = \gamma_1(x) + \gamma_2(y) + \gamma_3(E) \tag{5}$$

where γ_1, γ_2, γ_3 are valid (in 3D space) isotropic variograms, such that $\gamma_1(h) = a$, $\gamma_2(l) = b$, $\gamma_3(k) = c$. Consider the left-hand side coefficient matrix for an ordinary kriging system using these eight sample locations. The matrix is

$$\begin{bmatrix} 0 & a & a+c & c & b & a+b & a+b+c & b+c & 1 \\ a & 0 & c & a+c & a+b & b & b+c & a+b+c & 1 \\ a+c & c & 0 & a & a+b+c & b+c & b & a+b & 1 \\ c & a+c & a & 0 & b+c & a+b+c & a+b & b & 1 \\ b & a+b & a+b+c & b+c & 0 & a & a+c & c & 1 \\ a+b & b & b+c & a+b+c & a & 0 & c & a+c & 1 \\ a+b+c & b+c & b & a+b & a+c & c & 0 & a & 1 \\ b+c & a+b+c & a+b & b & c & a+c & a & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

To see that this matrix is not invertible (i.e., that the rows are linearly dependent), form sums by pairs. Add rows 1 and 7, rows 2 and 8, rows 3 and 5, rows 4 and 6; then it is seen that the resulting four rows are identical and, hence, dependent.

Let v_1, v_2, v_3 be the vectors determined by the points $(x_2, y_2, E_2) = (h, 0, 0)$, $(x_3, y_3, E_3) = (0, l, 0)$, $(x_4, y_4, E_4) = (0, 0, k)$, then the eight points are obtained by the linear combinations

$$c_1 v_1 + c_2 v_2 + c_3 v_3$$

where the coefficients are either 0's or 1's. In this case the vectors are not only linearly independent but also orthogonal; hence, it is sufficient to know the values $\gamma_1(h) = a$, $\gamma_2(l) = b$, $\gamma_3(k) = c$ in order to be able to calculate all the entries in the coefficient matrix above.

More generally let $v_1, v_2, v_3, \ldots, v_m$ be vectors in 3D space and form

$$c_1 v_1 + c_2 v_2 + \cdots + c_m v_m \tag{6}$$

where the coefficients are 0's or 1's. There will be 2^m possible combinations (i.e., possible points in the configuration). To construct a noninvertible coefficient matrix would require that it have $2^m + 1$ rows. Moreover, because the vectors cannot be linearly independent if $m > 3$ and at most three can be mutually orthogonal, to evaluate the variogram constructed as the sum of m terms will require knowing the values at more than m points. In the case of the discretized variogram or covariance in 3D space constructed as the sum of 15 covariances (one-dimensional), singularity of the coefficient matrix would only occur if more than 32,000 points were used in the kriging neighborhood. Since in practice the number of sample locations would always be substantially smaller than 32,000, there is little practical difficulty inherent in the turning bands construction.

DISCUSSION AND CONCLUSIONS

The variogram γ might be thought of as having been constructed by two singular transformations from 2D into 1D space, it is the singularity of these transformations that causes the difficulty. In (3) the variograms (or covariances) are in 1D space, and in general a valid model in a lower dimension is not a valid model in a higher dimension [see Journel and Huijbregts (1978, p. 161)]. As an additional aid to understanding the source of the purported contradiction, consider a plot of either γ_1 or γ_2 but in 2D space; the "surface" is that of a cylinder defined by the isotropic model plotted against distance. In 2D space both γ_1, γ_2 are identically zero along one axis and any function with that property cannot be strictly positive definite. Unfortunately, these examples do not provide insight into a valid way to construct variograms with zonal anisotropies.

These examples are important in another context as well. While there have been few reported examples of modeling variograms in both space and time, Bilonick (1985), those examples have used a construction analogous to the construction of a zonal anisotropy given above. As is shown in Rouhani and Myers (1989), these constructions will fail to be valid for reasons similar to those given above.

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