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Variogram Models Must Be Positive-Definite[1]

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The aim of this short article is to stress the importance of using only positive-definite functions as models for covariance functions and variograms.

The two examples presented show that a negative variance can easily be obtained when a nonadmissible function is chosen for the variogram model.

KEY WORDS: Variograms, geostatistics, positive-definite.

INTRODUCTION

One of the most difficult tasks in teaching geostatistics is to convince students that they *must* choose conditionally positive-definite functions as models for the variogram. Warnings (and threats) about the possibility of ending up with a negative variance go unheeded. The only way to really convince students is to present a few examples.

Since it is not easy to concoct suitable examples, the authors felt that the other teachers of geostatistics may find these two examples useful in their courses.

As is well known, the functions chosen as covariance models must be positive-definite; that is, the function $f(\cdot)$ must satisfy the following relation for all possible λ_i, for all x_i, and for all n

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j f(x_i - x_j) \geqslant 0 \tag{1}$$

Otherwise, the variance of the linear combination $\Sigma \lambda_i Z(x_i)$ of the regionalized variables $Z(x_i)$ would be negative.

Similar restrictions also apply to the choice of variogram models. However, since variogram models can exist when the regionalized variables $Z(x_i)$ satisfy the

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intrinsic hypothesis (which is weaker than stationarity), an additional restriction must be met: the sum of the λ_i must equal 0. The variogram model γ must therefore satisfy

$$-\sum_i \sum_j \lambda_i \lambda_j \gamma(x_i - x_j) \geqslant 0 \tag{2}$$

for all x_i, for all λ_i such that $\Sigma\lambda_i = 0$, and for all n.

FIRST EXAMPLE

For the first example we take a simple linear combination of three regionalized variables $Z(x_1)$, $Z(x_2)$, and $Z(x_3)$. Fig. 1a shows the layout of the three points x_1, x_2, and x_3 and also the associated weighting factors.

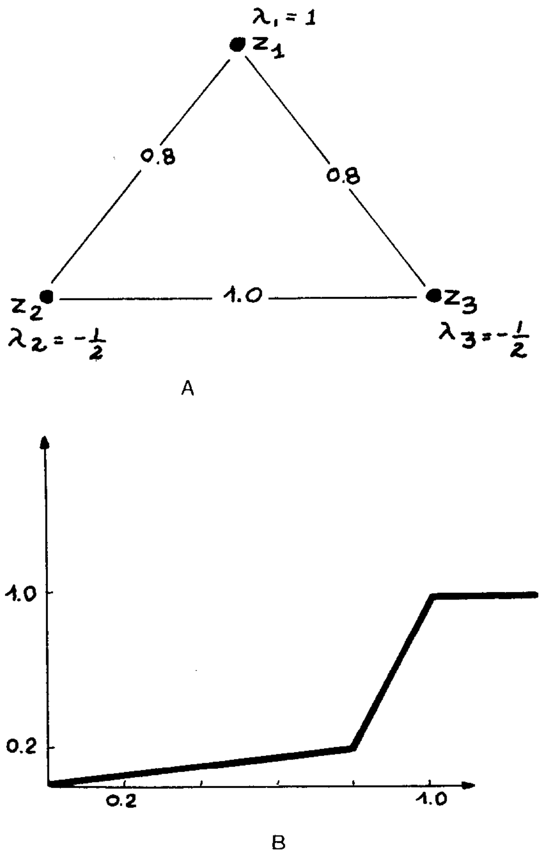

Fig. 1. (a) Layout of the three points, (b) nonauthorized variogram model.

The sum of the λ_i is clearly 0, so we are dealing with an authorized linear combination. The variance of this combination can be evaluated from the formula

$$\mathrm{Var}\left[\sum \lambda_i Z(x_i)\right] = -\sum_i \sum_j \lambda_i \lambda_j \gamma(x_i - x_j) \tag{3}$$

For our model of γ we take the piece-wise linear function shown in Fig. 1(b). Since $\gamma(0.8) = 0.2$ and $\gamma(1) = 1.0$, the variance of $\Sigma\, \lambda_i Z(x_i)$ is -0.1.

At first glance the problem seems to arise because this model does not concave downward. But concavity is neither a necessary nor a sufficient condition for positive definiteness. It is clearly not necessary: the Gaussian variogram model and the models in h^α with $1 < \alpha < 2$ are acceptable models for the variogram, but they are certainly not concave downward. Nor is concavity sufficient, as can be seen from the following example.

SECOND EXAMPLE

For the second example we have chosen the concave variogram shown in Fig. 2(a). This is an acceptable variogram for data in a 1-D space but not in higher-dimension spaces.

To show this we consider a regular 6×8 square grid with sides of length $a/2^{1/2}$. The weighting factors λ are chosen to be alternately positive and negative (see Fig. 3). Consequently $\Sigma\, \lambda_i = 0$.

The variogram model has been chosen so that the variogram value between adjacent points ($h = a/2^{1/2}$) is calculated using the linear part ($\gamma(h) = h$) of the model, whereas all the other terms equal the sill value. The variance of $\Sigma\, \lambda_i Z(x_i)$ can be calculated using formula (3), but it is much easier to use the corresponding covariance model shown in Fig. 2(b) because all the covariances at distances greater than a equal zero.

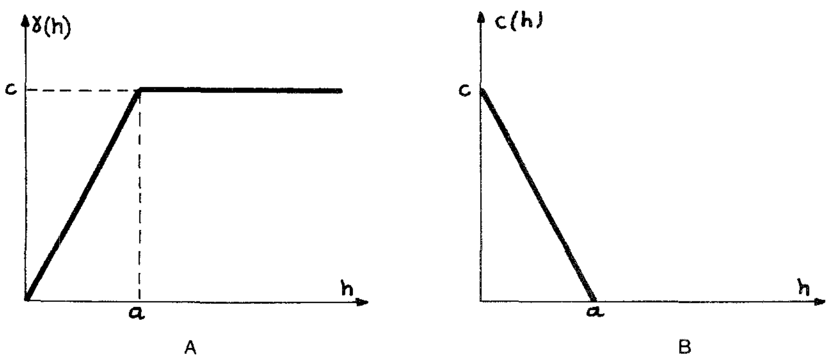

Fig. 2. (a) Variogram, (b) covariance.

Fig. 3. Layout of points.

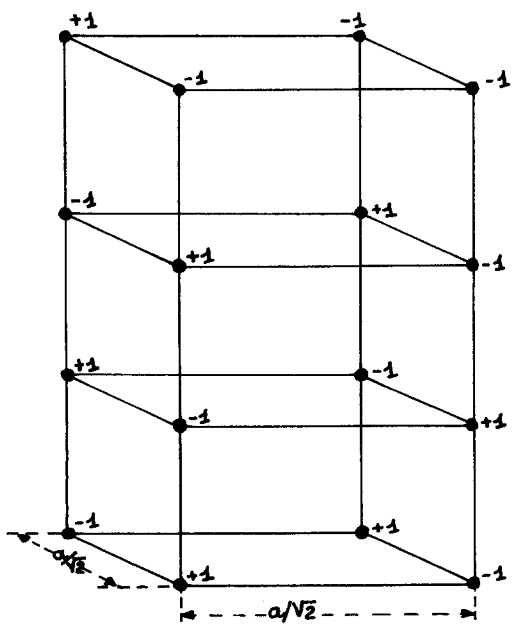

Fig. 4. 3-D configuration.

$$\begin{aligned}\operatorname{Var}\left[\sum \lambda_i Z(x_i)\right] &= \sum \lambda_i^2 C(0) + \sum_{i \neq j}\sum \lambda_i \lambda_i\, C(x_i - x_j)\\ &= 48\lambda^2 C(0) - 2 \times 82\lambda^2 C(a/2^{1/2})\\ &= \lambda^2 C(0)\ [48 - 164\,(1 - (2^{1/2}/2))]\\ &< 0\end{aligned}$$

Negative variances can also be obtained using this model in three dimensions. A suitable configuration of points and weighting factors is shown in Fig. 4.

DISCUSSION

In one sense these examples are rather artificial. The values of λ and the layout of the points have to be chosen with care to get a negative variance. However, it should be remembered that kriging minimizes the estimation variance, so it will unfailingly ferret out the values of λ which minimize the variance, even if this minimum value turns out to be negative.

One problem in dealing with piece-wise linear models is that some of them are positive definite and others are not. What's more, it is time consuming and difficult to test the positive-definiteness of particular models. It is much simpler and safer to stick to the "approved" models.