Mathematical Geology, Vol. 21, No. 3, 1989

To Be or Not to Be . . . Stationary? That Is the Question[1]

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Stationarity in one form or another is an essential characteristic of the random function in the practice of geostatistics. Unfortunately it is a term that is both misunderstood and misused. While this presentation will not lay to rest all ambiguities or disagreements, it provides an overview and attempts to set a standard terminology so that all practitioners may communicate from a common basis. The importance of stationarity is reviewed and examples are given to illustrate the distinctions between the different forms of stationarity.

KEY WORDS: stationarity, second-order stationarity, variograms, generalized covariances, drift.

Frequent references to stationarity exist in the geostatistical literature, but all too often what is meant is not clear. This is exemplified in the recent paper by Philip and Watson (1986) in which they assert that stationarity is required for the application of geostatistics and further assert that it is manifestly inappropriate for problems in the earth sciences. They incorrectly interpreted stationarity, however, and based their conclusions on that incorrect definition. A similar confusion appears in Cliff and Ord (1981); in one instance, the authors seem to equate nonstationarity with the presence of a nugget effect that is assumed to be due to incorporation of white noise. Subsequently, they define ''spatially stationary,'' which, in fact, is simply second-order stationarity.

Both the role and meaning of stationarity seem to be the source of some confusion. For that reason, the editor of this journal has asked that an article be written on the subject. We begin by noting that stationarity (at least as it is defined in the following section) refers to the random function and not to the data. It is this interchange that is the source of much of the confusion that appears in the literature. Moreover, different forms of stationarity, or perhaps we should say nonstationarity, are recognized. In some instances, authors have neglected to indicate which form they are using.

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STATIONARITY

In all of the following, assume that $Z(x)$ is a random function defined in 1, 2, or 3 space (also referred to as a random field in some literature); x is a point in space, not just the first coordinate.

(Strong) Stationarity

$Z(x)$ is stationary if, for any finite number n of points $x_1, \ldots x_n$ and any h, the joint distribution of $Z(x_1), \ldots, Z(x_n)$ is the same as the joint distribution of $Z(x_1 + h), \ldots, Z(x_n + h)$ (Cox and Miller, 1965, p. 273–276).

This is not the form of stationarity that is usually referred to in the geostatistical literature, but it is essentially this form that is required for the application of nonlinear techniques such as disjunctive kriging and indicator and probability kriging. Note that this form of stationarity does not imply the existence of means, variances, or covariances. In nearly all instances, the data are represented as a (nonrandom) sample from one realization of the random function and hence can not be tested for stationarity. To refer to the stationarity (or nonstationarity) of the data implies a misunderstanding or a different definition from that given above. Lest we conclude that stationarity is too strong in all circumstances, most of statistics is based on at least a weak form of stationarity.

Second-Order Stationarity

Both because of the difficulty of testing for strong stationarity and the fact that it does not imply the existence of moments, a weaker form known as second-order stationarity often is used instead.

$Z(x)$ is second-order stationary if $\mathrm{cov}[Z(x + h), Z(x)]$ exists and depends only on h. This implies that $\mathrm{var}[Z(x)]$ exists and does not depend on x; furthermore, $E[Z(x)]$ exists and does not depend on X (Cox and Miller, 1965, p. 277, for details).

Obviously, stationarity does not imply second-order stationarity. Conversely, a stationary random function may not be second-order stationarity, as its first two moments may not be defined. Examples to illustrate this are given in Appendix A. Because stationarity is essentially untestable, as weak a form as possible is desirable to utilize and, as will be seen from a later example, even second-order stationarity may be strong. We turn to forms introduced by Matheron (1971, 1973).

Intrinsic Hypothesis

The form of stationarity implied by the intrinsic hypothesis is essentially second-order stationarity—not for the random function $Z(x)$, but rather for the first-order difference, $Z(x + h) - Z(x)$. Differences have been used in a number of places in statistics as well as in time series analysis (see, for example, von Neumann et al., 1941) wherein successive differences were used for estimating variance in the presence of an unknown and nonconstant mean. The first-order difference is analogous to a first derivative in that the first-order difference will filter out a constant mean and first-order derivatives of constants are zero. As given by Matheron, $Z(x)$ satisfies the intrinsic hypothesis if

(i) $E[Z(x + h) - Z(x)] = 0$ for all x and h

(ii) $\gamma(h) = 0.5 \operatorname{var}[Z(x + h) - Z(x)]$ exists and depends only on h

where $\gamma(h)$ denotes the variogram as usual. An example of a random process that satisfies the intrinsic hypothesis without being second-order stationary is presented in Appendix A.

Of course, if first-order differences filter out constants, one would expect higher-order differences to filter out higher-order polynomials. Unfortunately, the problem is not so simple. Essentially, only one first-order difference exists and only the vector separation of points $x + h$ and x is relevant, but, even in one dimension, higher-order differences are not unique and not all higher-order differences filter out polynomials. (In particular, when sample locations are not on a regular grid, coefficients in the higher-order difference depend on the actual coordinates of locations as well as on the sample location pattern.) At least two ways of codifying a weaker form of stationarity, generally known as universal kriging and intrinsic random functions of order k, are common. Although these are not modes of stationarity per se, they indicate the approach. Both were introduced by Matheron and some disagreement remains as to advantages and disadvantages of each.

Weakly Stationary with Drift

This is not a term that has been used before, but that is being introduced to distinguish the approach followed in connection with universal kriging and that followed with IRFs.

Here, $Z(x)$ is weakly stationary with drift if

$$Z(x) = Y(x) + m(x) \tag{1}$$

where $Y(x)$ satisfies the intrinsic hypothesis and $E[Z(x)] = m(x)$ with $m(x)$ representable as a linear combination of known linearly independent functions. In some instances, authors have assumed that $Y(x)$ was second-order stationary, but that is not necessary. The problem then is determination of the variogram of $Y(x)$. The essential point when using this form of stationarity is to remove $m(x)$, and then to proceed with $Y(x)$ using the intrinsic hypothesis.

Intrinsic Hypothesis Order k

Because of difficulties resulting from simultaneous estimation/modeling of the variogram and $m(x)$, Matheron put forth a second definition of weak stationarity (1973). Specifics are described in Delfiner (1976). One must first define authorized linear combinations of higher orders; that is, linear combinations that filter out polynomials up to order $k - 1$. These generalized differences are obtained as linear combinations whose coefficients satisfy the familiar universality or unbiasedness conditions. These generalized differences must define second-order stationary random functions; that is, stationarity is defined in terms of translation on weights in the generalized difference. For an intrinsic function $Z(x)$ (order 0), the difference $Z(x + h) - Z(x)$, considered as a function of x, is to be stationary. Similarly for an IRF $- k$ and a given authorized linear combination, the global translation of this combination is to be stationary. In turn, generalized covariances are defined and, in particular, the negative of a variogram is a generalized covariance of order zero.

Both weak stationarity with drift (universal kriging) and IRFs implicitly define a weak form of stationarity or rather a not too troublesome form of nonstationarity. In the case of the former, the function representing the mean must be characterized at least in terms of linear combinations of known linearly independent functions and, hence, one attempts to remove the nonstationarity to obtain a residual that is nearly stationary. In the case of IRF $- k$s, the nonstationarity is resolved in the generalized covariance. Both approaches still lead to some practical difficulties when attempting to model the variogram or generalized covariance.

AMBIGUITIES

Drift or Trend?

When referring to one of the forms of nonstationarity, both terms, "drift" and "trend," appear in the literature, often interchangeably. It may be preferable to distinguish between them to identify two slightly different concepts. The term "trend" has a well-known usage in the context of trend surface analysis wherein a model like Eq. (1) is used, but the coefficients in $m(x)$ are fitted by least squares.

Matheron (1971) suggested the term "drift" for $m(x)$ to distinguish it from the least-squares estimate of $m(x)$. In the case where $m(x)$ is a polynomial of degree zero, i.e., a constant, some authors refer to zero drift and others to constant drift. With respect to the intrinsic hypothesis, no real distinction is made. The confusion in usage probably results from condition (i) in the intrinsic hypothesis because this essentially requires that $m(x)$ be a constant and hence the difference is zero. In the following, this distinction between drift and trend will be retained. Although commonly the coefficients in $m(x)$ are fit by least squares as a preliminary step in estimating a variogram, this is not the optimal estimator in the presence of a nonstationarity. This introduces a bias in estimation of the variogram.

Drift, Real or Imaginary?

The definition of weakly stationary with drift given above suggests that drift is an intrinsic property of the random function—and theoretically it is—but, as suggested by Cressie (1986b), "What is one person's nonstationarity (in mean) may be another person's random (correlated) variation." The weakly stationary with drift model also matches our predeliction to assume that a deterministic part and a random part exist. In many applications, the deterministic part is viewed as signal and the random part as noise, the objective being to remove the noise. In the context of geostatistics, the random part is not viewed as noise and an obvious deterministic part may or may not be present. As an example of at least a plausible deterministic part, consider the dispersion of a pollutant in the atmosphere in the presence of a prevailing wind. Whether real or imaginary, one often is faced with data sets that appear to be samples from realizations of nonstationary random functions. To ignore an apparent nonstationarity leads to less than satisfactory results. Although problems that may arise are likely all well known, no cohesive discussion in the literature seems to have appeared; thus, an attempt to draw these together in the context of the previous elucidation of nonstationarity will be made.

Histograms, True or False?

Common practice is to construct a histogram early in the process of analyzing data. For example, if the distribution is skewed or multimodal, often the data are transformed or partitioned. In particular, when applying disjunctive kriging, a smoothed version of the histogram is used to obtain the transformation to a normal. The histogram is assumed (at least implicitly) to be an estimate of the marginal STATIONARY distribution. Note that second-order stationarity, or one of the other forms of weak stationarity, is not sufficient; strong stationarity at least must exist for the special case of $n = 1$ (the number of points, not the dimension of the space). If the random function is not stationary, at least to this extent, then the histogram is not an estimate of a distribution related in a known way to the random function. A slightly weaker assumption would be that the distribution of $Y(x) = Z(x) - m(x)$ is independent of x; in that case, the histogram of the true residuals should be constructed.

Spatial or Ensemble?

Even if sampling is continuous, the data are taken from only one realization, and hence ensemble (i.e., probabilistic) averages can not be computed directly. One possible solution is to replace ensemble averages by spatial averages; this is the essential idea underlying the use of the sample variogram. The "equivalence" of these two forms of averaging is the central focus of ergodic theory and an adequate explanation of ergodicity would require too much space to present here (see, for example, Cox and Miller, 1965; Matheron, 1978; or Alfaro, 1979, 1984). An alternative to relying on some form of this equivalence has been proposed in Srivastava (1987); instead of defining the variogram or covariance by ensemble averages and then using spatial averages to construct estimators for ensemble averages, spatial averages are used for defining both the mean function and the covariance function. He presented numerical examples to show that estimators of these behave better than does the sample variogram as an estimator of the ensemble average variogram.

An assumption of the equivalence of ensemble means and spatial means implies additional assumptions about the random function if the probabilistic model is retained. This cannot be totally avoided, but, in some instances, a clear distinction between spatial and ensemble averages should be retained. If we wish to know (i.e., estimate) the grade of a specific selective mining unit, a particular spatial integral is necessary, and to equate it with the ensemble average (assuming some form of weak stationarity) would be very misleading. The latter would be independent of block size and shape, whereas the former definitely is not.

PRACTICE AND THEORY

As was noted above, stationarity or even one of the forms of weak stationarity is defined by properties of the random function—not by a single realization and certainly not by a sample from one realization. This would suggest that stationarity is not scale related, because the above do not explicitly refer to the domain of the random function. However, Matheron (1973) has shown that if the IRF $-$ k has a polynomial generalized covariance, it locally is stationary. Also, common practice is to subdivide a field of study to "avoid" nonstationarities, but, when looking at a data set, whether the field should be subdivided or adjoined is not always clear.

For example, one would not normally think of elevation as being stationary; rapid changes such as might occur in proceeding from east to west in the United States come to mind. But suppose that elevation is considered on a global scale; then mountain ranges represent an insignificant part of Earth's surface and, hence, in this instance, a more reasonable view might be to consider elevation as stationary. However, a paradox remains; the data are the only information available to test for stationarity or an appropriate weak form, yet stationarity is a property of the random function, not of the data, and hence untestable. To assume that all applications are stationary or to ignore the advantages of some form of stationarity is not adequate. To compare theory and practice, we begin by considering some data sets with apparent nonstationarities and examine both the purported reasons and methods of attack.

Examples

Example a

Daily readings of SO_2 over an 18-month period (Fig. 1a) show that the (spatial) average over summer periods is not the same as the same averages over winter periods. Also, the spatial variance over winter periods is greater than for summer. This suggests nonstationarity; but, perhaps more importantly, this interpretation is reasonable in terms of what is known about the seasonal effect on production of SO_2. That is, our modeling of nonstationarity is not just an artifact of our interpretation of the data.

Example b

Because of an interpretation of nonstationarity (Example a), first-order differences, $Z(x + 1) - Z(x)$, where the units are in days, were considered. The transformed data (Fig. 1b) show that the distinction between averages for summer and winter is gone, but that the variances are not the same. This suggests that condition (i) of the intrinsic hypothesis is satisfied, but not condition (ii).

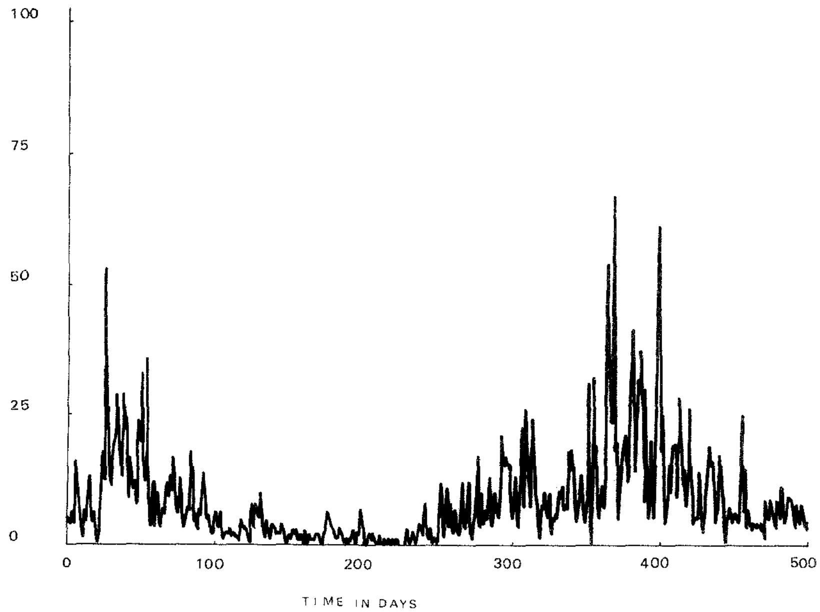

Fig. 1a. Plot of the raw pollution data against time.

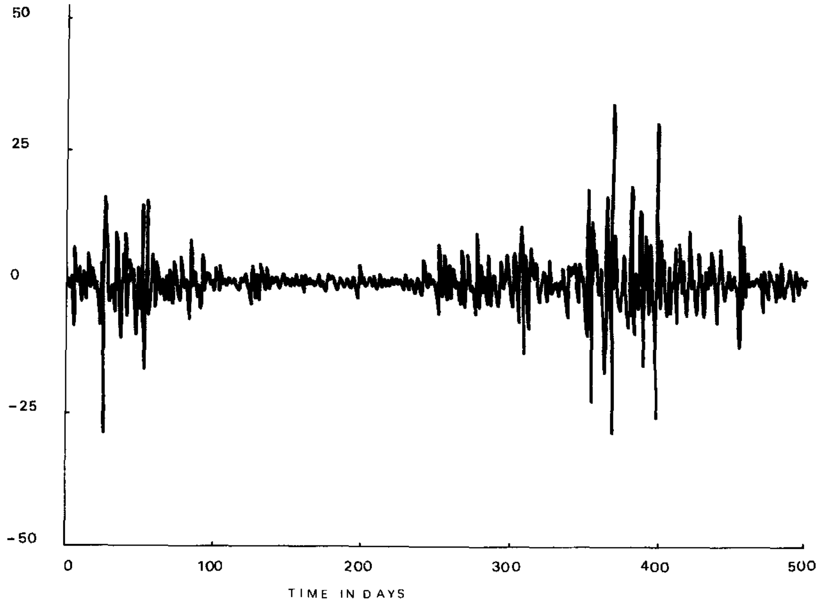

Fig. 1b. Plot of the increments of the pollution data against time.

Example c

Differencing was used to remove an apparent nonstationarity in the first moment. Also the largest values seem to be most variable. This suggests a transformation to equalize variance, such as the logarithm. The result of plotting log $[Z(x)]$ (Fig. 1c) demonstrates that the seasonal difference in variances seems to be gone, but that the first-order moment is not constant.

Example d

Lastly, both approaches are combined by plotting the difference logarithms (Fig. 1d), which seems to produce the desired effect (and we emphasize) on the DATA. If the random function were nonstationary in the same way, these transforms might be expected to have the desired effect on $Z(x)$.

The analysis and interpretation described above would be fairly standard as an approach in applying geostatistics to a data set, but we should consider the practical and theoretical consequences of such an approach as well as possible clues to difficulties that may arise. In particular, we should be careful not to conclude from this example that the phenomena can be reduced to a pure nugget effect on logarithmic differences. In that case, the seasonal behavior would be completely lost as a significant characteristic.

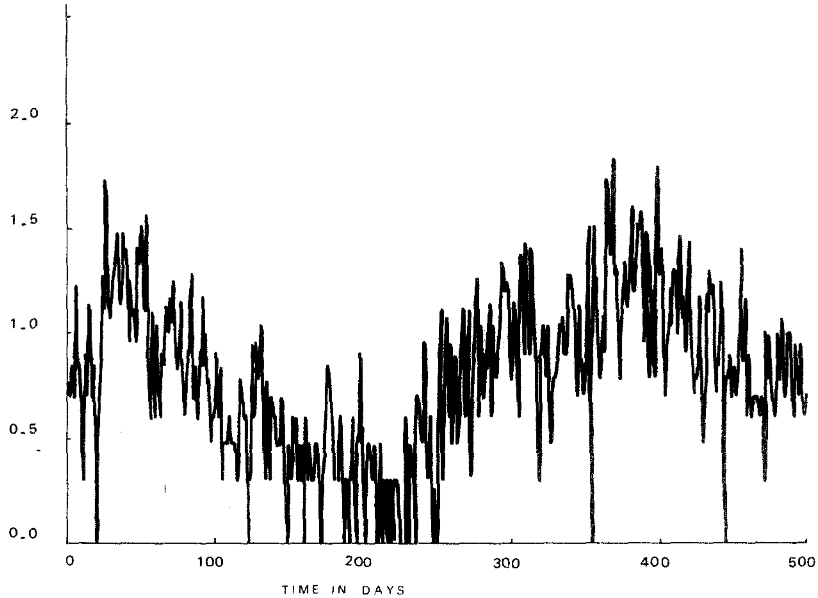

Fig. 1c. Plot of the logarithms of the pollution data against time.

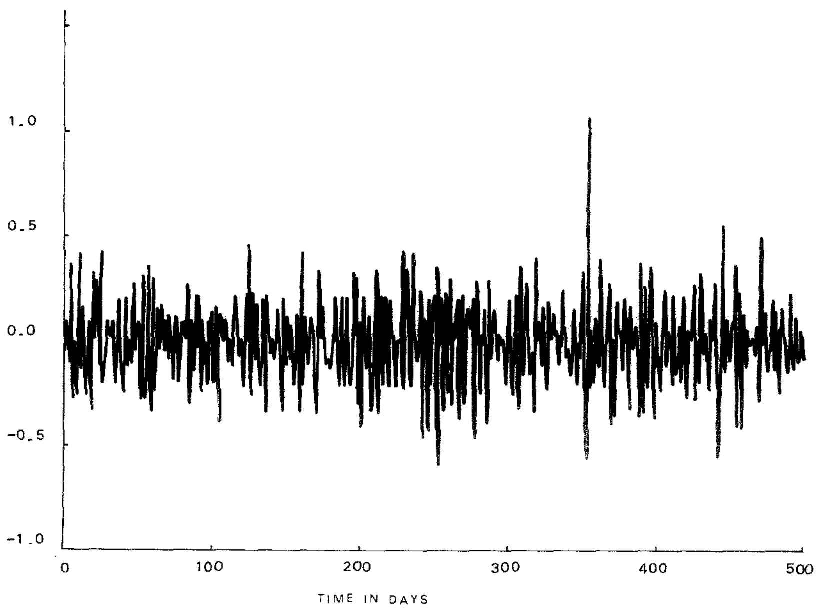

Fig. 1d. Plot of the increments of the logarithms of the pollution data against time.

Common Practice

As is well known, the principal difficulty arising from the presence of an apparent nonstationarity concerns estimation of the variogram. The sample variogram, which is the most commonly used estimator, is in fact an estimator of the expected value of the squared first-order difference rather than of the variance. In the presence of nonstationarity, a critical difference exists between the two, and the variance is needed. As has been noted by a number of authors—for example, Matheron (1971), Chiles (1976), and Starks and Fang (1982b)—if $Z(x)$ is given by model (1) above, then

$$E\left\{\left[Z(x+h) - Z(x)\right]^2\right\} = 2\gamma(h) + \left\{\left[m(x+h) - m(x)\right]^2\right\} \quad (2)$$

and hence the sample variogram is biased. Sabourin (1976) described a method for matching sample variograms against the theoretical model when this bias is present. Unfortunately, the bias is not calculated easily in the general case, *i.e.*, in two or three dimensions with irregularly spaced data and with an unknown variogram model. Because linear drift leads to parabolic growth in Eq. (2), parabolic growth in the sample variogram is interpreted usually as evidence of nonstationarity. But remember that the sample variogram is determined by a sample of $(0.5)[Z(x+h) - Z(x)]^2$ from one realization and is not itself the true expected value. Essentially the same difficulty exists here as in the interpretation of a plot of data against position coordinates; namely, a trend in the data is not necessarily the same as nonstationarity. Often the sample variogram is computed from residuals after a least-squares fit to the trend, and significant differences in the variograms are interpreted as evidence of nonstationarity. This conclusion is plausible, but is not infallible.

In some instances, as was noted in Chiles (1976), the apparent nonstationarity is present for some directions, but not for others. In such cases, one solution is to assume an isotropic variogram modeled from the sample variogram for the directions without drift and then to use that variogram to estimate the drift optimally. This approach is especially plausible when a physical reason supports the modeling in only one direction. Chiles (1976) provides an example of this.

Because the problem of estimating drift and modeling the variogram is a circular one—i.e., each is needed prior to the other—an iterative approach, as supplied by Neuman and Jacobson (1984), would seem to be an appropriate solution. Although this seems eminently reasonable, it still suffers from the theoretical difficulty of identifying drift from only one realization and of adequate estimation of the variogram without at least the intrinsic hypothesis. As noted by Cressie (1986a), this iteration does not remove bias.

One variogram model allows us to have our cake and eat it too. Because neither the nugget nor the slope in a linear model affects the weights obtained from the kriging equation and moreover, at least for a regular grid, the bias resulting from least-squares fitting of the drift is computed easily, the variogram can be modeled without first knowing the drift and conversely the model can be used to estimate drift without knowing the coefficients in the model. Care should be taken not to confuse the intercept with the nugget effect. This technique is illustrated in Olea (1972) and in Webster and Burgess (1981). In the latter, the size of the kriging neighborhood is shown to be crucial to the modeling as might be expected from Matheron's theorem on local stationarity for polynomial generalized covariances. Of course, use of small moving neighborhoods for kriging is another method for coping with nonstationarity although it does not avoid the problem as it affects estimation of the variogram. The use of moving neighborhoods, however, also leads to discontinuities in the interpolated surface. Note that, in some cases, nonstationarity, as evidenced in the sample variogram, may not be distinguished easily from anisotropies and, in the modeling process, one may have to choose between the two. In the latter case, how the resulting estimated values and kriging variances are affected by a misspecified variogram should be examined. Journel and Froideveaux (1982) provide an example of a complex anisotropic hole effect model, but conclude that the additional complexity did not substantially affect the resulting estimated values. More general theoretical results are given in Armstrong (1984a), Diamond and Armstrong (1984), and Myers (1985, 1986).

In the previous discussion of nonstationarity, the emphasis has been on difficulties arising from nonconstant drift, particularly with respect to estimation of the variogram. Second-order stationarity and even the intrinsic hypothesis assume that the variance and variogram are not position dependent. However, this may not be the case. Cressie (1985) notes that certain nonlinear transformations are concerned, in fact, primarily with obtaining this property, and that the relative variogram is one such example. The drift is allowed to be nonconstant, but is assumed constant within separate regions; hence, it is of a rather special, but important, form.

GENERALIZED COVARIANCES OR VARIOGRAMS?

The kriging equations are essentially the same whether one uses universal kriging with a variogram or intrinsic random functions order k with generalized covariances; hence, the choice between them is not so much one of theory as of difficulties associated with fitting or estimating these functions.

The variogram has the advantage that the estimator can be plotted and, in case of standard models, the parameters are interpretable on the plot. This is especially advantageous in presenting results to a nonspecialist. Although the covariance would share this advantage, it also would have the disadvantage of requiring separate estimation of the mean, which introduces a bias. The difficulties encountered in the presence of real or apparent nonstationarity have been noted already and, as yet, no adequate solutions to these problems are known. In contrast, modeling of polynomial generalized covariances lends itself to automatic procedures whether by the use of the algorithm in BLUEPACK or a restricted maximum likelihood approach such as has been proposed by Kitanidis (1983).

Chauvet (1984, 1985, 1986) and Cressie (1986a) have both proposed ways to utilize graphical presentations of estimators, but, in both cases, methods are difficult to apply in more than one dimension even if isotropy is assumed. Although variograms are generalized covariances (with a change in sign), and hence in theory, the use of variograms should be subsumed as a special case of generalized covariances; in practice, it is not because the only known standard models for generalized covariances are the polynomials including the spline term. An anisotropy is not simple to incorporate because the generalized covariance is not a function of the separation vector only in the same sense that the variogram is; in particular, no simple analogue of the sample variogram for generalized covariances of higher order exists and hence there is no easy way to distinguish the behavior in different directions. The difficulty is compounded by use of only polynomial models for generalized covariances. No theoretical difficulties are involved with incorporating anisotropies into generalized covariances, but the practical ones indicated do exist. In general, the generalized covariance estimators, or rather the estimators of the coefficients in the polynomial model, use the data in a global manner whereas the variogram plot provides information both locally as well as for longer ranges.

SUMMARY

Some form of stationarity is needed for geostatistics, but considerable confusion prevails in the literature as to what constitutes stationarity. In particular, the appellation is applied frequently to data when it should be reserved for the random function. This confusion leads to potential misinterpretations in analyzing the data. Unfortunately, no best way of treating or resolving the problem has been discovered.

APPENDIX A

Strict Stationarity Versus Second-Order Stationarity

As noted earlier in the text, the definition of strict stationarity (Cox and Miller, 1965, p. 272–276) requires that the joint distribution of any n points be invariant under translation. So, if the moments exist, they must be invariant under translation, but, of course, they need not exist. One might expect that second-order stationarity would require merely that the bivariate distribution be invariant under translation. However, this is not the case. Cox and Miller (1965) define it in terms of the first two moments:

$$E[Z(x)] = m \text{ (constant)}$$
$$\text{cov}\,[Z(x+h), Z(x)] = C(h)$$

That is, the covariance depends on the distance h but not on x.

(i) Strictly Stationary, But Not Second Order Stationary

To see this, consider a process $Z(x)$ defined in the following way. At each point x, a value $z(x)$ is drawn at random from the Cauchy distribution whose density function is

$$f(z) = \frac{1}{\pi(1+z^2)} \quad -\infty < z < \infty$$

Clearly, none of the moments (mean, variance) exist because the corresponding integrals do not converge absolutely, but the distribution is exactly the same at all points and is translation invariant. Hence, the process is strictly stationary, but does not satisfy the definition of second-order stationarity given above.

(ii) Second-Order Stationary, But Strict Stationary

In this case, consider a point process defined on the integers n 0, ± 1, ± 2, ± 3, . . . etc. For each point n, let $Z(n)$ be drawn at random from a three-parameter lognormal distribution such that

$$\log\,[Z(n) + \alpha_n] \sim N(\mu_n, \sigma_n^2)$$

where

$$\alpha_n = -1 - \frac{1}{n}$$
$$\mu_n = -0.5 \ln(2) \qquad \text{if } n = 0$$
$$= \ln(|n|) - 0.5 \ln(n^2+1) \qquad \text{otherwise}$$
$$\sigma_n^2 = \ln(n^2+1)$$

Because

$$E[Z(x) + \alpha] = \exp(\mu + \sigma^2/2)$$
$$\text{var}[Z(x) + \alpha] = \exp(2\mu + \sigma^2)[\exp(\sigma^2) - 1]$$

then,

$$E[Z(x)] = 1$$
$$\text{var}[Z(x)] = 1$$
$$\text{cov}[Z(x + h), Z(x)] = 0$$

Thus, the moments of the process are independent of n, as required by definition, but the distribution (even the marginal ones) depends on the location n and so are not strictly stationary.

Intrinsic, But Not Second-Order Stationary

The best-known example of a process that is intrinsic, but not second-order stationary, is the Wiener–Levy process or, as it is often called, Brownian movement.

For simplicity, consider a point process $Z(n)$. Set $Z(0)$ equal to 0 and take the sum of a set of random increments $Y(i)$ such that

$$Y(i) = +1 \quad \text{with a probability of} \quad 0.5$$
$$Y(i) = -1 \quad \text{with a probability of} \quad 0.5$$

So $Z(n) = \Sigma_n\, Y(i)$ and, hence,

$$E[Z(n)] = 0$$
$$\text{var}[Z(n)] = n/2$$

The process certainly is not second-order stationary, but it does satisfy the intrinsic hypothesis because

$$E[Z(n) - Z(m)] = 0$$
$$\text{var}[Z(n) - Z(m)] = E[Z(n) - Z(m)]^2$$
$$= (n - m)^2$$

ACKNOWLEDGMENTS

Special thanks are due Margaret Armstrong; she was a co-author on the original version of this paper. In particular, the initial impetus for writing the paper as well as examples and the appendix are primarily her contribution. The paper in its present form has also benefited substantially from the careful review and helpful suggestions of Jean-Paul Chiles. Figures were provided by P. Chauvet of the Centre de Geostatistique from data supplied by C. Kirsch of the Freie Universitat Berlin. The author also wishes to acknowledge that portions of this paper were written while on a visiting appointment at the Centre de Geostatistique, Fontainebleau.

Although the research described in this article has been funded in part by the United States Environmental Protection Agency through Cooperative Agreement 811938 to the University of Arizona, it has not been subjected to Agency review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred.

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