On the Problem of Permissible Covariance and Variogram Models

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The covariance and variogram models (ordinary or generalized) are important statistical tools used in various estimation and simulation techniques which have been recently applied to diverse hydrologic problems. For example, the efficacy of kriging, a method for interpolating, filtering, or averaging spatial phenomena, depends, to a large extent, on the covariance or variogram model chosen. The aim of this article is to provide the users of these techniques with convenient criteria that may help them to judge whether a function which arises in a particular problem, and is not included among the known covariance or variogram models, is permissible as such a model. This is done by investigating the properties of the candidate model in both the space and frequency domains. In the present article this investigation covers stationary random functions as well as intrinsic random functions (i.e., nonstationary functions for which increments of some order are stationary). Then, based on the theoretical results obtained, a procedure is outlined and successfully applied to a number of candidate models. In order to give to this procedure a more practical context, we employ "stereological" equations that essentially transfer the investigations to one-dimensional space, together with approximations in terms of polygonal functions and Fourier-Bessel series expansions. There are many benefits and applications of such a procedure. Polygonal models can be fit arbitrarily closely to the data. Also, the approximation of a particular model in the frequency domain by a Fourier-Bessel series expansion can be very effective. This is shown by theory and by example.

Introduction

A recurring problem of geostatistical investigations in hydrosciences as well as in many other geophysical sciences is to judge whether a particular function can be used as a covariance or variogram model, ordinary or generalized [e.g., Matern, 1960; Matheron, 1965, 1973]. The practitioner frequently faces data which are not satisfactorily approximated by any known covariance or variogram model. Instead, some other function not included in the known models may offer a much better fit. Also, the practitioner may modify a known model so that a better fit to the data is achieved, but it is possible that the model so "improved" is not a covariance or a variogram any more.

The use of the function best fitted to the data is very important in the context of problems such as estimation and simulation of hydrologic random functions. The reasons for this are related to both the understanding of the underlying hydrologic processes [e.g., Mejia and Rodriguez-Iturbe, 1974; Chiles, 1977] and to the effectiveness of the estimation procedures [e.g., Delfiner and Delhomme, 1973; Delhomme, 1978].

Consequently, criteria capable of testing, in an analytically and computationally tractable way, whether a function is permissible as a covariance or variogram model may be of practical importance. This article will try to give an answer to the problem, based on spectral analysis [Bochner, 1959; Jenkins and Watts, 1968]. More specifically, we will first establish the theoretical support to the criteria testing the permissibility, and then we will develop procedures to perform this testing in a more practical context. Within this framework we will consider models for ordinary random functions described by Yaglom [1962] as opposed to generalized random functions in the sense of Gelfand and Vilenkin [1964].

We will examine models for both stationary random functions (in the weak sense, see Yaglom [1962] and Bartlett

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[1975]) and intrinsic random functions (intrinsicalness is used herein as an alternative term for random functions with stationary increments in the sense of Kolmogoroff [1941]; see also Yaglom and Pinsker [1953], Yaglom [1957], and Matheron [1973]). The latter class of random functions could be viewed as a generalization of the former, and this view involves significant advantages concerning statistical inferences. Actually, while searching for permissibility, we will keep the advantages linked to the intuitive idea of stationarity, but at the same time we will enlarge the application range of the theory to cover practical cases where the stationarity is a physically inadmissible assumption.

The difficulty of examining the permissibility of candidate covariance and variogram models is in general greater in more than one dimension, and this is due to obstacles of mathematical and technical nature. Then the operation of space transformations may be very helpful in calculations involving isotropic models.

Before this presentation, a brief review of the mathematical concepts and terminologies used in the article is given, in order to make it as self-contained as possible. In addition, numerous references are given for the reader who wishes a more detailed study.

It must be understood that in this article we will not deal with the problem of fitting a function (candidate model) to the data available. This is a problem related to the structural analysis of the phenomenon under study (familiarity with the nature of the phenomenon, the data, etc.; see *Matern* [1960] or *Whittle* [1954]) and also to the fitting techniques [e.g., *Daniel et al.*, 1971].

REVIEW OF GEOSTATISTICAL INFERENCES

The main tools of geostatistical inferences for random functions (RF) associated with spatiotemporal phenomena are either the traditional covariance function

$$c(x_i, x_j) = E[Z(x_i)Z(x_j)] - E[Z(x_i)] E[Z(x_j)]$$
 (1)

or the variogram function

$$\gamma(x_i, x_j) = \frac{1}{2} \text{Var} [Z(x_i) - Z(x_j)]$$
 (2)

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where $x_i = (x_{i,1}, \dots, x_{i,n})$ represents a point in the *n*-dimensional space R^n , $Z(x_i)$ is the associated RF, E[] is the expectation operator, and Var[] is the variance operator. The function (2) is a second-order statistical moment introduced by Kolmogoroff [1941], under the name of structural function. Since then, (2) has appeared in the literature as the serial variation function [Jowett, 1955] or as the variogram function [Matheron, 1965, 1971]. For many workers in the area the variogram function is the preferable tool for statistical inferences [e.g., Delhomme, 1976, 1978; Chiles, 1977]. This happens because it has a number of advantages over the covariance function (1). Some of them, especially important in practical applications, are (1) it is mean free, (2) its empirical calculation is subject to smaller errors, and (3) it may offer a better characterization of the spatial variability.

In practice, one may work with stationary covariance or variogram functions in one or more dimensions, such that

$$c(x_i, x_i) = c(x_i - x_i) = c(h)$$
 (3a)

or

$$\gamma(x_i, x_i) = \gamma(x_i - x_i) = \gamma(h) \tag{3b}$$

respectively, where $h = x_i - x_j$ is the vector difference between the two points x_i , x_j . It is interesting to note that while (3a) requires the assumption that the RF $Z(x_i)$ is stationary [see Yaglom, 1962], (3b) requires a weaker assumption, the so-called intrinsic hypothesis, (i.e., that $Z(x_i)$ is an RF with stationary increments $Z(x_i + h) - Z(x_i)$ but not necessarily stationary itself; see Yaglom [1957] and Matheron [1971]. Obviously, a stationary RF is also an intrinsic one, but the reverse is not always true. In the case of a stationary RF it follows from (1) and (2) that

$$\gamma(h) = c(0) - c(h) \tag{4}$$

where c(0) is the variance, also called sill in geostatistics. Equation (4) does not hold in general for an intrinsic RF, where c(0) may not exist (e.g., $\gamma(h) = |h|$).

Many times in hydrosciences, one faces the problem of modeling or estimating a nonstationary spatial phenomenon with a complex trend (e.g., hydraulic heads in a hilly aquifer). Then one may generalize the intrinsic hypothesis and employ the more sophisticated model of the κ th-order intrinsic random functions (IRF- κ ; see Yaglom and Pinsker [1953] and Matheron [1973]). An IRF- κ is an RF which requires a κ + 1-th order increment to achieve stationarity. More specifically, a linear combination

$$Y = \sum_{i} \lambda_{i} Z(x_{i})$$

is a so-called generalized kth order increment if

$$\sum_{i} \lambda_{i} x_{i,1}^{b_{1}} x_{i,2}^{b_{2}} \cdots x_{i,n}^{b_{i}} = 0$$
 (5)

for all integers $b_1, b_2, \cdots, b_n \ge 0$ such that

$$\sum_{i=1}^n b_i \leq \kappa$$

and $(x_{i,1}, x_{i,2}, \dots, x_{i,n})$ are the coordinates of the point x_i . Next it is possible to define the κ th-order generalized covariance k(h) (or GC- κ) as the stationary part of the nonstationary covariance $c(x_i, x_i)$ associated with the IRF- κ , $Z(x_i)$. For the case of first-order increments, i.e., IRF-0, we simply have $k(h) = -\gamma(h)$. It is very important that in the context of nonstationary estimation and simulation, the variance of any increment

$$\sum_{i} \lambda_{i} Z(x_{i})$$

depends only on the GC- κ , k(h). Consequently, we only need to know k(h), which is considered as the ordinary covariance of IRF- κ .

Under the above circumstances the covariance, variogram, and generalized covariance functions should satisfy several preliminary properties, such as the following.

1. They belong to the class of real, even, and continuous (except possibly at the origin) functions, and one can write

$$c(-h) = c(h) \tag{6a}$$

$$\gamma(-h) = \gamma(h) \tag{6b}$$

$$k(-h) = k(h) \tag{6c}$$

for every h in their domains. Hence, we simply deal with positive only values of h, and then several interesting theorems of the class of even functions are utilized.

2. The covariance c(h) always has an upper bound,

$$|c(h)| \le c(0) \tag{7}$$

while only in special cases are the variogram $\gamma(h)$ and generalized covariance k(h) so bounded (e.g., see proposition 5, presented later in the paper).

3. They behave at infinity according to the laws

$$\lim \frac{c(h)}{|h|^{(1-n)/2}} = 0 \qquad |h| \to \infty$$
 (8a)

$$\lim \frac{\gamma(h)}{|h|^2} = 0 \qquad |h| \to \infty \tag{8b}$$

$$\lim \frac{k(h)}{|h|^{2\kappa+2}} = 0 \qquad |h| \to \infty \tag{8c}$$

where

$$h = \left(\sum_{i} h_{i}^{2}\right)^{1/2}, h_{i}$$

are the coordinates of vector h in R^n . Equations (8) are related to the requirements that c(h), $\gamma(h)$, and k(h) can be expanded in a Fourier integral, and they are proven in proposition 6 (presented later in the paper). The equations (6a) through (8c), while necessary, are not sufficient conditions for a function to be a covariance, variogram, or generalized covariance. For example, consider the function $\gamma(h) = 1 - \exp(-|h|^d)$, d > 2. Despite the fact that it satisfies all the above conditions, we will prove in a following section that it is not a variogram in R^1 . Throughout this presentation we will discuss additional necessary conditions, which may be very useful in deleting models that cannot be considered as covariance, variogram, or generalized covariance functions, rather than in identifying models that could be so.

In general, for a continuous function chosen as a covariance, variogram, or generalized covariance model, it is necessary and sufficient to satisfy the nonnegative definite-

ness properties which ensure that the variance of certain linear combinations,

$$Y = \sum_{i=1}^{n} \lambda_i Z(x_i)$$
 (9)

is not negative. More specifically, and assuming herein continuous functions,

1. The covariance c(h) of a stationary RF $Z(x_i)$ must be nonnegative definite, i.e.,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j c(h) \ge 0 \qquad h = x_i - x_j \qquad (10a)$$

for all n and any complex number λ_i .

2. The variogram $\gamma(h)$, since it exists when the RF $Z(x_i)$ is only intrinsic, must be such that $-\gamma(h)$ is conditionally nonnegative definite, i.e.,

$$-\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_{i}\lambda_{j}\gamma(h)\geq0$$
 (10b)

when

$$\sum_{i=1}^{n} \lambda_{i} = 0 \qquad \forall n$$

3. The generalized covariance k(h) must be conditionally nonnegative definite, i.e.,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j k(h) \ge 0$$
 (10c)

for all combinations of (5).

If, and only if, a function satisfies (10a), (10b), or (10c) it will be called a permissible covariance, variogram, or generalized covariance model, respectively (some authors, instead of the term "permissible," prefer the term "admissible" which, however, is not used in this article because of its connotations in game theory). The validity of (10) immediately implies other properties of the covariance and variogram models (ordinary or generalized). For example, from (10a) for n=2, $\lambda_1=c(h)$, $\lambda_2=-|c(h)|$, it is trivial to show the validity of (7). Permissibility in R^n implies permissibility in R^m for m < n. The reverse is not true. For example, the variogram $\gamma(h)=1-\cos(h)$ is permissible in R^1 but not in R^2 or R^3 .

Practically speaking, it is difficult to apply (10) in order to test if a proposed model is nonnegative definite and therefore a permissible model. What is actually done in current practice is to fit models which are known to be permissible or are derived from permissible ones to the data. Essentially, one utilizes the closure properties of each class of statistical moments in the R^n and uses mainly linear combinations of permissible models [Matern, 1960; Journel and Huijbregts, 1978]. For most of the applications we may favour isotropic models which depend only on the vector length

$$|h| = r = \left(\sum_{i} h_{i}^{2}\right)^{1/2}$$

We will therefore concentrate on such models, and then we can write

$$c(h) = c(|h|) = c(r)$$
(11a)

$$\gamma(h) = \gamma(|h|) = \gamma(r) \tag{11b}$$

$$k(h) = k(|h|) = k(r) \tag{11c}$$

for the isotropic covariance, variogram, and generalized covariance, respectively.

Matern [1960], presents a number of ways to produce permissible isotropic covariances, which, when properly modified, lead to permissible variograms as well. For instance, one may utilize the theorem that if $\mu(a)$ is a measure in a space U and c(r; a) is a covariance integrable over the subspace V of U for every r, then the function

$$c(r) = \int_{V} c(r; a) d\mu(a)$$
 (12)

is also a covariance. The measure $\mu(a)$ may be an arbitrary distribution function in R^1 , and in many cases c(r;a) belongs to the family $\exp(-r/a)$. A well-known group of covariances derived as above is $c_n(r) = \operatorname{const} r^{\vee} \mathsf{K}_{\vee}(r/a)$. When using (4), the corresponding variogram is $\gamma(r) = \operatorname{const} [1 - \operatorname{const} r^{\vee} \mathsf{K}_{\vee}(r/a)]$, where $a, \, \vee \geq 0$, and K_{\vee} is the modified Bessel function of the second kind [see *Gradshteyn and Ryzhik*, 1965]. For $\nu = 0.5$, we obtain the exponential model, while for $\nu = 1$, we find $\gamma_n(r) = \operatorname{const} [1 - (r/a) \mathsf{K}_1(r/a)]$, which is a model widely used in geosciences [see *Veneziano*, 1980].

Matheron [1973] suggested an effective way to construct an isotropic covariance in \mathbb{R}^n . First, assume that $Z_1(x_i)$ is a stationary RF in \mathbb{R}^1 with a covariance $c_1(r)$. Then, by the turning bands operator, the covariance of \mathbb{R}^n will be

$$c_n(r) = 2G\left(\frac{n}{2}\right) \pi^{-1/2} \left[G\left(\frac{n-1}{2}\right) \right]^{-1}$$

$$\cdot \int_0^1 c_1(ur) [1 - u^2]^{(n-3)/2} du \qquad (13)$$

where G is the gamma function. Formula (13) can be also used for both the cases of variogram (after taking (4) in to account) and generalized covariance functions. For example, starting from $c_1(r) = (1 - r/a) \exp(-r/a)$, one derives a covariance useful in hydrology:

$$c_{2}(r) = \operatorname{const}\left\{I_{0}\left(\frac{r}{a}\right) - L_{0}\left(\frac{r}{a}\right) + \left(\frac{r}{a}\right)\left[I_{1}\left(\frac{r}{a}\right) - L_{-1}\left(\frac{r}{a}\right)\right]\right\}$$

in R^2 , where I_0 , I_1 are modified Bessel functions of the first kind and orders zero, one, respectively, and L_0 , L_1 are modified Struve functions of orders zero, one, respectively [see *Mantoglou and Wilson*, 1982; *Gradshteyn and Ryzhik*, 1965]. For the one-dimensional generalized covariance $k_1(r) = r^{2c+1}$, c > 0, the corresponding generalized covariance in R^2 is found to be $k_2(r) = (c!) \pi^{-1/2} [G(c + 3/2)]^{-1} r^{2c+1}$.

Difference or differential equations can lead to several classes of isotropic models. Consider the difference equation in R^2 (useful for soil patterns)

$$Z(x_i, x_j) = b[Z(x_{i+1}, x_j) + Z(x_{i-1}, x_j) + Z(x_i, x_{j+1}) + Z(x_i, x_{j-1})] + a(x_i, x_j)$$
(14)

where $a(x_i, x_j)$ is usually white noise and b is a deterministic coefficient. Equation (14) leads to variograms of the form

$$\gamma(r) = \text{const} \left[1 - \frac{r}{a} \, \mathsf{K}_1 \left(\frac{r}{a} \right) \right]$$

For more discussion and examples in soil sciences, see Whittle [1954], Bartlett [1975], and Christakos [1982; also a manuscript in preparation, 1983]. Another method of constructing isotropic models will be discussed at the end of this article.

However, it is obvious that all the above methods, while providing rich sources of isotropic models, are not totally satisfactory from the practical viewpoint discussed in the introduction. In fact, in most of the cases encountered in practice, the functions fitted to the experimental data are neither included among the known permissible models nor derived from them by a method like the ones described before. Such situations deserve to be studied, especially because of their interest regarding applications. This is the task carried out by the remaining sections.

Analysis in Frequency Domains

The covariance and variogram models presented in the introduction are real and even functions. So are their n-fold Fourier transforms (FT) when they exist. The transform corresponding to the covariance c(h) is usually called spectral density function, and we may establish the FT pair

$$c(h) = \int_{\mathbb{R}^n} \cos(wh) C(w) dw$$
 (15)

$$C(w) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \cos(wh) \, c(h) \, dh \tag{16}$$

where wh is the inner product $\sum_i w_i h_i$, and

$$\int_{\mathbb{R}^n} = \int_{\mathbb{R}^1} n \operatorname{times} \int_{\mathbb{R}^1}$$

holds for the *n*-fold integration [see *Sneddon*, 1972].

Note that, in general, instead of the ordinary Fourier integral (15), the covariance c(h) may be expressed in the form of the Fourier-Stieltjes integral

$$c(h) = \int_{R^n} \cos(wh) dQ(w)$$

where the distribution function Q(w) is not necessarily differentiable. However, the presentation (15) is very convenient and also more than adequate for the purposes of this study. The matter will be again considered below.

Similar representations and comments hold for the FT pairs

$$\gamma(h) \leftrightarrow \Gamma(w)$$
 (17)

$$k(h) \leftrightarrow K(w)$$
 (18)

where $\Gamma(w)$ K(w) are the spectral functions of the variogram $\gamma(h)$ and the generalized covariance k(h), respectively.

The spectral functions may exist in the sense of ordinary or in the sense of generalized functions [Gelfand and Vilen-

kin, 1964]. Usually, for C(w) to exist, it is sufficient to have a c(h) tending to zero fast enough as $|h| \to \infty$.

If c(h) is an impulse or a periodic function, then C(w) still exists in the sense of generalized functions. To demonstrate this, consider in \mathbb{R}^1 the impulse function defined as

$$\int_{R^1} \delta(h - h_0) f(h) dh = f(h_0)$$

where $f(h_0)$ is an arbitrary function continuous at h_0 . By using this definition, the spectral function of the covariance $c(h) = \delta(h)$ is easily found to be $C(w) = 1/2\pi$. Such a spectral function corresponds to the so-called white noise process (which is equivalent to the so-called pure nugget effect in geostatistics). A random function with a covariance as above experiences zero correlation for h values different than zero. Another sound example is the covariance $c(h) = c(0) \cos(ah) \ln R^1$, and after the introduction of the impulse

$$\delta(w) = \frac{1}{2\pi} \int_{R^1} \cos(wx) \, dx$$

the "extended" spectral function will be $C(w) = \text{const } \{\delta(w + a) + \delta(w - a)\}.$

As we will see later, the intrinsic variograms and the generalized covariances may also exist in the sense of generalized functions (e.g., in R^1 , $\gamma(h) = |h|$, $\Gamma(w) = \text{const } w^{-2}$).

The proposition that follows is fundamental as it relates the spectral functions C(w) and $\Gamma(w)$ in the case of stationary RF.

Proposition 1

For a stationary RF with a variance c(0), the relationships below are valid:

$$\Gamma(w) = c(0) \delta(w) - C(w)$$
 (19)

$$\int_{R^n} \Gamma(w) \ dw = \gamma(0) = 0 \tag{20}$$

where $\delta(w)$ is the *n*-dimensional impulse function such that

$$\delta(w \neq 0) = 0 \qquad \int_{\mathbb{R}^n} \delta(w) \ dw = 1 \tag{21}$$

Proof

To prove (19), take the FT of (4). Next, using (19) together with (21) and (15) for h = 0, i.e.,

$$c(0) = \int_{\mathbb{R}^n} C(w) \ dw \tag{22}$$

we derive (20). Note that the area under C(w) gives the variance c(0), while (22) imposes a limitation in the increase of C(w) with that of |w|. The $\Gamma(w)$ itself contains an impulse at w = 0 whose area is equal to c(0), while from $w \ge 0^+$ it starts following the relationship $\Gamma(w) = -C(w)$. In practice, one may work with $w \ge 0^+$, so as to avoid the impulse of (19).

An immediate result of proposition 1 is that the existence of $\Gamma(w)$ may be derived from the existence of C(w) and vice versa. Moreover, another interesting result is presented by the following corollary.

Corollary 1

For a stationary RF it is valid that

$$\gamma(h) = \int_{R^n} \left[1 - \cos\left(wh\right)\right] C(w) \ dw \tag{23}$$

where the C(w) satisfies (19).

Proof

This is a simple consequence of combining (4), (15), and (22).

It is important to see that (23) may exist when (15) does not. To show this, consider the one-dimensional case of expressions (15) and (23): the $\gamma(h)$ converges when C(w) has a singularity at zero of the form w^{-e} , e < 3, while at the same time, c(h) does not converge. Also, one may define (23) in the case of intrinsic only RF, which is characterized from the nonexistence of c(h) (e.g., in R^n , $\gamma(h) = |h|^d$, d > 0, c(h) does not exist but $C(w) = \text{const } |w|^{-d-n}$). These are significant advantages, contributing to the use of the variogram for many practical situations.

For an IRF-0 (i.e., first-order stationary increments) the relationship $k(h) = -\gamma(h)$ immediately implies

$$K(w) = -\Gamma(w) \tag{24}$$

and consequently the $\gamma(h)$ and k(h) are equivalent statistical moments (note that in this case there is no impulse involved in the presentation (24)).

Isotropy of c(r), $\gamma(r)$, or k(r) (see (11)) implies isotropy for the corresponding spectral functions

$$C(w) = C(|w|) = C(\omega) \tag{25a}$$

$$\Gamma(w) = \Gamma(|w|) = \Gamma(\omega)$$
 (25b)

$$K(w) = K(|w|) = K(\omega) \tag{25c}$$

respectively, where

$$\omega = |w| = \left(\sum_{i} w_{i}^{2}\right)^{1/2}$$

In the present study we will concentrate on isotropic covariance and variogram models, which are continuous everywhere. The study of the so-called nugget effect (discontinuity at the origin) is not included in this presentation.

CRITERIA OF PERMISSIBILITY

In this section we will discuss some necessary and sufficient criteria concerning the permissibility of covariance and variogram models (ordinary and generalized). These criteria are equivalent to the nonnegative definite conditions (10a), (10b), and (10c), but they have the advantage of being convenient in their application. Furthermore, a sufficient only criterion, but with a particularly simple enunciation, is also discussed.

Bochner [1959] proved that a continuous function f(h) is nonnegative definite if and only if it can be expressed as the FT of a nonnegative bounded measure ϕ , i.e.,

$$f(h) = \int_{\mathbb{R}^n} \exp(iwh) \ d\phi(w) \tag{26}$$

where $i = \sqrt{-1}$ and wh is the inner product $\sum_i w_i h_i$. For engineering practice, ϕ is usually differentiable, so that (26) will take the more convenient form

$$f(h) = \int_{R^n} \exp(iwh) F(w) dw$$

(see also comments following (15)).

The first criterion concerns stationary and isotropic RF and is a straightforward application of the Bochner's theorem for the case of real-valued and isotropic functions f(r) and $F(\omega)$.

First Criterion of Permissibility (COP-1)

A continuous function c(r) is a permissible covariance model in \mathbb{R}^n , i.e., satisfies condition (10a), if and only if it is the FT of a nonnegative bounded measure $C_n(\omega)$, usually called spectral density function (SDF); i.e., we must have

$$C_n(\omega) \ge 0$$
 on R^n (27)

where, because of isotropy, the *n*-fold FT is reduced to a Hankel transform (see *Sneddon* [1972] and next section). In this case we have a finite variance (sill), i.e., the corresponding variogram is of transitive type [see *Journel and Huijbregts*, 1978]. Of course, the permissibility of c(r) immediately implies the permissibility of the variogram $\gamma(r)$ (see corollary 1). Furthermore, with the aid of proposition 1, (27) gives

$$c(0) \delta(\omega) - \Gamma_n(\omega) \ge 0 \quad \forall \omega$$
 (28a)

ог

$$c(0) \delta(\omega) - \Gamma_n(\omega) \ge 0 \qquad \omega \ge 0^+$$
 (28b)

where $\Gamma_n(\omega)$ is the isotropic spectral function of the variogram $\gamma(r)$.

The representation (28b) may be preferable sometimes, because it avoids the impulses at the origin. However, in most of the situations it may be easier to check the permissibility of the covariance c(r) for several reasons (e.g., it vanishes after some distance). Consider the model $c(r) = \exp(-r^2/a^2)$ in \mathbb{R}^n , where

$$r^2 = \sum_{i=1}^{n} r_i^2$$

It can be written as the product

$$c(r) = \prod_{i=1}^{n} \exp(-r_i^2/a^2) = \prod_{i=1}^{n} c(r_i)$$

and, consequently, its spectral function will be

$$C_n(\omega) = \prod_{i=1}^n C_1(\omega_i) = \prod_{i=1}^n a (2\sqrt{\pi})^{-1} \exp(-\omega_i^2 a^2/4)$$
$$= a^n (2\sqrt{\pi})^{-n} \exp(-\omega^2 a^2/4) \ge 0$$

We can now safely conclude that the above model may be considered as a permissible covariance. So does the corresponding variogram $\gamma(r) = 1 - \exp(-r^2/a^2)$. The associated RF is mean square continuous and differentiable of any order, and one can predict deterministically its realization, everywhere, from knowledge of it only over regions of any finite size. The criterion which follows, despite the fact that

it is only sufficient and deals with rather specific classes of models, is very convenient because it imposes conditions directly on the covariance or the variogram and not on their spectral functions.

Second Criterion of Permissibility (COP-2)

A continuous function c(r) is a permissible covariance model in \mathbb{R}^n , i.e., it satisfies the condition (10a), if (1) it has a negative derivative at zero:

$$c'(0) < 0 \tag{29}$$

while, at infinity, (8a) holds, and (2) for all positive r it satisfies the inequalities below:

in R^1

$$c''(r) \ge 0 \tag{30a}$$

in R^2

$$\int_{r}^{\infty} u (u^{2} - r^{2})^{-1/2} dc''(u) \ge 0$$
 (30b)

in R^3

$$c''(r) - r c'''(r) \ge 0 \tag{30c}$$

where c''(r) and c'''(r) are the second and third derivatives of c(r). The expressions corresponding to the variogram $\gamma(r)$ are derived easily, with the aid of (4).

To prove the COP-2, we use some results concerning moving average models with stochastic weight functions, furnishing realizations of isotropic RF, as have been presented by *Matern* [1960]. A wide class of covariance models (e.g., any completely monotonic covariance) can be expressed as

$$c(r) = \text{const} \int_{r}^{\infty} u^{n} H(r/u) dP(u)$$
 (31)

where

$$H(r/u) = \int_{r/u}^{1} (1 - v^2)^{(n-1)/2} \left[B\left(\frac{n+1}{2}, \frac{1}{2}\right) \right]^{-1} dv$$

B is the beta function [see Gradshteyn and Ryzhik, 1965], and P(u) is a nondecreasing measure. This last fact gives the idea of solving (31) with respect to dP(u)/du, requiring it to be nonnegative. Doing so, we derive (30a), (30b), and (30c) for n = 1, 2, and 3, respectively. Consequences of (31) are (29) and also the recursive equation

$$-c_{n-2}'(r) = \text{const } r^{-1} c_n''(r)$$
 (32)

which is satisfied by the classes of models for which COP-2 holds.

Let us next examine the application of the COP-2 to a few well-known covariance and variogram models. A trivial example is the model $c(r) = \exp(-r/a)$. For this model it holds that c'(0) = -1/a < 0 and $c''(r) - r c'''(r) = (r + a)a^{-3} \exp(-r/a) > 0$, and according to the COP-2, it is a permissible covariance in R^3 . It is clear that the same applies in R^1 , R^2 . An interesting counterexample in R^2 is the variogram $\gamma(r) = 1 - \cos t r K_1(r)$, which does not satisfy COP-2 but which is, however, a permissible model, as we saw in a previous section. Indeed, the conditions for variograms

corresponding to (29) and (30b) are

$$-\gamma'(0)<0$$

$$-\int_{r}^{\infty} u (u^{2} - r^{2})^{-1/2} d\gamma''(u) \ge 0$$

respectively. Both of them are not valid for the present variogram. Instead, the first one equals zero, while the second one is equal to

const
$$\{r[K_0^2(r) + K_1^2(r)] - K_0(r) K_1(r)\}$$

which takes negative values for small r (K is the modified Bessel function; see *Gradshteyn and Ryzhik* [1965]).

We now pass to the case of intrinsic only RF, where the variance c(0) may not exist. Then we can use only the variogram $\gamma(r)$, and the corresponding criterion is as follows (necessary and sufficient criterion).

Third Criterion of Permissibility (COP-3)

A continuous function $\gamma(r)$ is a permissible variogram model in \mathbb{R}^n , i.e., it satisfies the condition (10b) if and only if (1) its spectral function $\Gamma_n(\omega)$ exists in the sense of generalized functions; it does not contain any impulses $\delta(\omega)$, while the measure $-\omega^2 \Gamma_n(\omega)$ is a nonnegative one, i.e.,

$$-\omega^2 \, \Gamma_n(\omega) \ge 0 \qquad \text{on } R^n \tag{33}$$

and (2) it increases more slowly than r^2 as $r \to \infty$, i.e.,

$$\lim \gamma(r)/r^2 = 0 \qquad r \to \infty \tag{34}$$

The justification of this COP is based on Bochner's theorem properly extended to take into account the special features of the intrinsic variogram $\gamma(r)$. More specifically, from the definition of the variogram and in accordance with the Gelfand-Vilenkin theory [Gelfand and Vilenkin, 1964; Yaglom, 1957; Matheron, 1973], a function $-\gamma(r)$ is conditionally nonnegative definite in the sense of (10b) if and only if there exists a measure $\chi(dw) \ge 0$ without atom at the origin (i.e., includes no $\delta(w)$) and such that

$$-\gamma(h) = \int_{R^n} \frac{\cos(wh) - 1}{w^2} \chi(dw)$$
 (35)

$$\int_{\mathbb{R}^n} \chi(dw)/(1+w^2) < \infty \tag{36}$$

Equation (36) is the existence condition of integral (35) and is equivalent to (34) above. To show this, assume that (34) is valid. Then, if e is a unit vector in \mathbb{R}^n we find

$$\gamma(eh) = \int_{\mathbb{R}^n} \left[1 - \cos\left(ewh\right)\right] \chi(dw)/w^2 \le ah^2 \qquad a < \infty$$

Taking the Laplace transform of both sides of the above inequality and summing over all axes of $w = (w_1, w_2, \dots, w_n)$, we find, in a trivial way,

$$\int t^2 \, \chi(dw)/(t^2 + w^2) \le 2na$$

(note that the Laplace transform of h^2 is $2/t^3$). Furthermore, $\lim_{t \to \infty} t^2/(t^2 + w^2) = 1$ when $t \to \infty$, and this implies (monotonic continuity)

$$\int \chi(dw) < 2na < \infty$$

Clearly, $\chi(dw)$ is a bounded measure and (36) follows. For the case of isotropic variogram $\gamma(h) = \gamma(|h|) = \gamma(r)$, the isotropic measure associated with $\chi(dw)$ is $-\omega^2 \Gamma_n(\omega)$, where $\Gamma_n(\omega)$ is the FT of $\gamma(r)$, according to well-known properties of FT and assuming that $\Gamma_n(\omega)$ exists and contains no impulses $\delta(\omega)$. Consequently, condition $\chi(dw) \ge 0$ is equivalent to (33), and the COP-3 is fully justified. A typical example is the variogram widely used in application, $\gamma(r) = r$, with $\Gamma_1(\omega) = -2/\omega^2$ in R^1 . Another important counterexample is the function $\gamma(r) = r\{1 + \cos{(ar)}\}$, which is not a permissible variogram in R^1 , because

$$-\omega^2 \Gamma_1(\omega) = 2 + \frac{\omega^2}{(\omega - a)^2} + \frac{\omega^2}{(\omega + a)^2}$$

is not a (finite) measure on R^1 (in the sense of Kolmogoroff and Fomin [1970]). To verify this fact, assume that there exists an intrinsic RF $Z(x_i)$ with a variogram as above. Then, for a=1, $\gamma(\pi)=0$ and $\gamma(2\pi)=4\pi$. But in expressing the variogram in terms of norms (in the sense, again, of Kolmogoroff and Fomin), we have, by definition, $\|Z(2\pi) - Z(0)\| \le \|Z(2\pi) - Z(\pi)\| + \|Z(\pi) - Z(0)\|$, i.e., $\gamma(2\pi) < 2 \gamma(\pi)$. Thus $\gamma(r)$ is not a permissible variogram model.

Some of the results concerning the permissibility of ordinary covariance and variogram models discussed up to now can be properly extended to the case of IRF- κ . This is a task carried out by the following criterion.

Fourth Criterion of Permissibility (COP-4)

A continuous function k(r) is a permissible GC- κ in \mathbb{R}^n , i.e., it satisfies the condition (10c) if and only if (1) its spectral function $K_n(\omega)$ exists in the sense of generalized functions and does not contain any impulses $\delta(\omega)$, while the measure $\omega^{2\kappa+2} K_n(\omega)$ is a nonnegative one, i.e.,

$$\omega^{2\kappa+2} K_n(\omega) \ge 0 \quad \text{on } R^n \tag{37}$$

and (2) it increases slower than $r^{2\kappa+2}$ as $r \to \infty$, i.e.,

$$\lim k(r)/(r^{2\kappa+2}) = 0 \quad \text{when } r \to \infty$$
 (38)

To justify the COP-4, much of the same procedure as with COP-3 is followed. If an RF $Z(x_i)$ is $\kappa + 1$ times differentiable (in the mean square sense), then its GC- κ is $2(\kappa + 1)$ times differentiable and such that

$$k(h) = \int_{R^n} \frac{\cos(wh) - P_{\kappa}(wh)}{w^{2\kappa+2}} \chi(dw)$$
 (39)

$$\int_{\mathbb{R}^n} \chi(dw)/(1+w^2)^{\kappa+1} < \infty \tag{40}$$

where

$$P_{\kappa}(w) = \sum_{p=0}^{\kappa} (-1)^p \ w^{2p}/(2p)! \tag{41}$$

and $\chi(dw)$ is a positive symmetric measure without atom at origin. Equation (38) is a necessary condition for a permissible k(r) (the proof is given in proposition 6) and is equivalent to the condition (40). This can be shown in exactly the same way as before, with (34) and (36). For an isotropic k(h) = k(|h|) = k(r), the spectral measure associated with the measure $\chi(dw)$ is $\omega^{2\kappa+2} K_n(\omega)$, where $K_n(\omega)$ is the spectral

function of k(r) and includes no impulses $\delta(\omega)$. This completes the justification of COP-4.

Consider the model

$$k(r) = (-1)^{l+1} r^{2l+1}$$
 (42)

In R^1 , we find [see Gelfand and Shilov, 1964]

$$K_1(\omega) = \pi^{-2l-2} 2^{-l-1} (l!) [(2l+1)!!] (\omega/2\pi)^{-2l-2}$$

Consequently, $\chi(d\omega) = \omega^{2\kappa+2} K_1(\omega)$ or, after some manipulations, $\chi(d\omega) = 2(2l+1)! \omega^{2(\kappa-l)}$. The measure $\chi(d\omega)$ contains no $\delta(\omega)$ and is nonnegative, satisfying all the conditions of COP-4 if $l \le \kappa$. For l = 0, (42) is GC-0; if l = 1, it is a GC-1, etc. Model (42) belongs to the very important family of polynomial models

$$k(r) = \sum_{l=0}^{m} (-1)^{l+1} a_l r^{2l+1}$$
 (43)

Applying COP 4 to the model (43), we find that $l \le \kappa = m$, and also the restrictions below, imposed on the coefficients ai:

if $\kappa = 0$

$$a_0 \ge 0 \tag{44a}$$

if $\kappa = 1$

$$a_1, a_0 \ge 0 \tag{44b}$$

if $\kappa = 2$

$$a_2, a_0 \ge 0$$
 $a_1 \ge -2 \left[\frac{5}{3} \left(\frac{n+3}{n+1} \right) a_0 a_2 \right]^{1/2}$ (44c)

where n = 1, 2, 3.

In practice, we need the GC- κ , k(r) for the kriging equations, but the so-called generalized variogram g(r) (i.e., GV- κ ; see *Chiles* [1979]) may be computed experimentally from the available data. When the data are along lines and sampled at regular intervals, g(r) is defined as

$$g(r) = {2\kappa + 2 \choose \kappa + 1}^{-1}$$

$$\cdot \operatorname{Var} \left\{ \sum_{l=0}^{\kappa+1} (-1)^l {\kappa + 1 \choose l} Z(x + (\kappa + 1 - l)r) \right\}$$
(45)

where

$$\binom{n}{m} = (n!)/[(n-m)!]m!$$

Definition (45) is a generalization of the ordinary variogram $\gamma(r)$ given by (2). The g(r) is well determined as a linear function of k(r), i.e., we can find, by using (45),

$$g(r) = {2\kappa + 2 \choose \kappa + 1}^{-1} \sum_{l = -\kappa - 1}^{\kappa + 1} (-1)^l {2\kappa + 2 \choose \kappa + 1 + l} k(lr)$$
 (46)

The reverse is not true, except for the case of IRF -0, where $g(r) = \gamma(r) = -k(r)$. Therefore while we can determine the corresponding permissible g(r) from a permissible k(r), we cannot, in general, do the reverse. Nevertheless, we can occasionally operate in a rather indirect way to test the permissibility of g(r). If the fitted g(r) is of a polynomial

form, we may start by determining the order κ of the intrinsicalness (i.e., the order of the generalized increment that stationarizes the data). Then we can find the form of k(r) from (43), but the coefficients a_l will still be unknown. To evaluate them, we employ the formula (46), and if the soestimated a_l satisfy the restrictions (44), then the experimental g(r) is permissible. Let us say that we fitted to our data, for $\kappa = 1$, the candidate variogram model

$$g(r) = \frac{2}{3}b_0r + \frac{4}{3}b_1r^3 \tag{47}$$

where b_0 , b_1 are known coefficients. From (46) we find

$$g(r) = -\frac{4}{3}k(r) + \frac{1}{3}k(2r) \tag{48}$$

But k(r) is given from (43) for $\kappa = 1$, whereas

$$k(r) = -a_0 r + a_1 r^3 (49)$$

and then (48), because of (49), gives $g(r) = \frac{2}{3}a_0 \ r + \frac{4}{3}a_1r^3$. Comparing this last equation with (47), we obtain $a_0 = b_0$, $a_1 = b_1$. Thus the GC model is $k(r) = -b_0r + b_1r^3$, which must be next checked to see if it is permissible. Using (44b), we realize that for this we only need to have b_0 , $b_1 \ge 0$.

METHODOLOGICAL AND COMPUTATIONAL ASPECTS

After the theoretical background provided by the proceeding COP's, we now pass to some practical aspects concerning their effective application in practice. First, there are several properties of a stereological nature satisfied by the isotropic spectral functions which deserve to be studied, especially because of their interest regarding applications.

Stereological Properties of Spectral Functions

A very important question in geostatistical practice is, if a statistical model $(c(r), \gamma(r), \text{ or } k(r))$ is permissible in R^1 , is it an isotropic permissible model in R^2 or R^3 ? The proposition below gives an answer to this question by presenting the transformation equations between the one- and two- or three-dimensional spectral functions of the variogram $\gamma(r)$. Similar equations are valid for the ordinary and generalized covariances c(r) and k(r), respectively, and this is shown in the examples to follow.

Proposition 2. The transformation equations between the one- and two- or three-dimensional spectral functions of an isotropic variogram $\gamma(r)$ are as follows:

From R^1 to R^2

$$\Gamma_2(\omega) = \frac{1}{\pi} \int_{\omega}^{\infty} \left\{ \frac{d}{d\bar{\omega}} \left[\frac{1}{\bar{\omega}} \frac{d\Gamma_1(\bar{\omega})}{d\bar{\omega}} \right] \right\} (\bar{\omega}^2 - \omega^2)^{1/2} d\bar{\omega}$$
 (50)

From R^1 to R^3

$$\Gamma_3(\omega) = -\frac{1}{2\pi\omega} \frac{d\Gamma_1(\omega)}{d\omega}$$
 (51)

For the c(r) and k(r) we simply replace Γ with C or K, respectively.

Proof. If $\Gamma_n(\omega)$ is the spectral function in the space W_n of n dimensions $(\omega_1, \omega_2, \cdots, \omega_n)$ and Γ_{n-k} is its projection in the subspace W_{n-k} of n-k dimensions, we have

$$\Gamma_{n-k}(\omega_1, \omega_2, \cdots, \omega_{n-k})$$

$$= \int \Gamma_n(\omega_1, \omega_2, \cdots, \omega_n) d\omega_{n-k+1} \cdots d\omega_n$$

Changing into polar coordinates, we get

$$\Gamma_{n-k}(\omega) = \int \Gamma_n(\omega^2 + y^2)^{1/2} y^{k-1} dS_k dy$$

where ω and y are the radius vectors in the subspaces W_{n-k} and W_k (with coordinates ω_{n-k+1} , ω_{n-k+2} , \cdots , ω_n), respectively, and S_k is the surface of the unit sphere in the k-dimensional subspace, i.e., $S_k = 2\pi^{k/2}$: G(k/2). After integrating over the whole space W_k and putting $\bar{\omega} = (\omega^2 + y^2)^{1/2}$, we find

$$\Gamma_{n-k}(\omega) = \frac{2\pi^{k/2}}{G(k/2)} \int_{\omega}^{\infty} \Gamma_n(\bar{\omega}) (\bar{\omega}^2 - \omega^2)^{k/2-1} \bar{\omega} d\bar{\omega}$$

Moreover, for proper choice of n, k, and solving for $\Gamma_2(\omega)$, $\Gamma_3(\omega)$ we obtain (50) and (51), respectively.

Let us illustrate the above proposition with two examples. First, we consider the variogram $\gamma(r) = 1 - \exp(-r^2/a^2)$. In \mathbb{R}^1 we have

$$-\Gamma_1(\omega) = \frac{a}{2\sqrt{\pi}} \exp\left(-\omega^2 a^2/4\right) \ge 0$$

while in R^2 , R^3 we find, using (50) and (51), respectively,

$$-\Gamma_2(\omega) = \frac{a^2}{4\pi} \exp\left(-\omega^2 a^2/4\right) \ge 0$$

$$-\Gamma_3(\omega) = \frac{a^3}{8\pi^{3/2}} \exp(-\omega^2 a^2/4) \ge 0$$

(i.e., the same result as in the previous section). Next, for the generalized covariance $k(r) = G(-\lambda/2) r^{\lambda}$, the spectral function in R^{1} is (see Gelfand and Shilov, 1964]

$$K_1(\omega) = \pi^{-\lambda - 1/2} \frac{G[(\lambda + 1)/2]}{G(-\lambda/2)} \left(\frac{\omega}{2\pi}\right)^{-\lambda - 1}$$

Using (51), we immediately obtain

$$K_3(\omega) = \pi^{-\lambda - 3/2} \frac{G((\lambda + 3)/2)}{G(-\lambda/2)} \left(\frac{\omega}{2\pi}\right)^{-\lambda - 3}$$

This expression for $K_3(\omega)$ is the same with the one obtained from Gelfand and Shilov [1964] for n = 3.

It is obvious that the last proposition allows us to work in R^1 , where we calculate the spectral function using the available transform tables, as did *Gradshteyn and Ryzhik* [1965] or *Gelfand and Shilov* [1964]. Then we can employ the (50) and (51) to calculate the spectral functions in R^2 and R^3 , respectively. Note that given the spectral function in R^1 , it may be more convenient to check the permissibility of the statistical models in R^3 , even if the field of interest is the R^2 , because the permissibility in R^3 immediately implies the one in R^2 .

Because of isotropy, the FT in R^2 and R^3 is reduced to a Hankel transform [see *Sneddon*, 1972]. Then the following corollaries are immediate applications of proposition 2.

Corollary 2. The spectral function $\Gamma_n(\omega)$ is given, when it exists:

in R^2

$$\Gamma_2(\omega) = \frac{1}{2\pi} \int_0^\infty J_0(\omega r) \ r \ \gamma(r) \ dr \tag{52}$$

in R^3

$$\Gamma_3(\omega) = \frac{1}{2\omega\pi^2} \int_0^\infty \sin(\omega r) \, r \, \gamma(r) \, dr \tag{53}$$

where J_0 is the Bessel function of first kind and zero order. *Proof.* Starting from

$$\Gamma_1(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \cos(\omega r) \gamma(r) dr$$

we apply (50) and (51) to get, in a trivial way, the formulas (52) and (53), respectively.

By using Hankel transforms, we find, from (52) and (53), respectively:

in R2

$$\gamma(r) = 2\pi \int_0^\infty J_0(\omega r) \ \omega \ \Gamma_2(\omega) \ d\omega \tag{54}$$

in R^3

$$\gamma(r) = 4\pi \int_0^\infty \frac{\sin(\omega r)}{\omega r} \, \omega^2 \, \Gamma_3(\omega) \, d\omega \tag{55}$$

Similar expressions are, of course, valid for the covariance functions, and the matter will be considered again, later on in the presentation.

Moreover, when taking into consideration corollary 1, proposition 2 may offer additional expressions for the variogram functions. More specifically, it may take the following forms:

in R^2

$$\gamma(r) = 2\pi \int_0^\infty \left[1 - J_0(\omega r)\right] \omega C_2(\omega) d\omega \qquad (56a)$$

in R^3

$$\gamma(r) = 4\pi \int_0^\infty \left[1 - \frac{\sin(\omega r)}{\omega r} \right] \omega^2 C_3(\omega) d\omega \qquad (56b)$$

where $C_2(\omega)$ and $C_3(\omega)$ satisfy (19) in the isotropic case.

Corollary 3. For a stationary and isotropic RF with a transitive-type variogram $\gamma(r)$, a sufficient condition for $\gamma(r)$ to be permissible in R^3 is that the function $r[c(0) - \gamma(r)]$ is nonincreasing.

Proof. From (28a),

$$c(0) \ \delta(\omega) - \Gamma_3(\omega) = \frac{1}{2\pi^2 \omega} \int_0^{\infty} \left[c(0) - \gamma(r) \right] r$$

$$\cdot \sin(\omega r) \ dr = \frac{1}{2\pi^2 \omega} \sum_{m=0}^{\infty} \int_0^{\pi/\omega} (-1)^m$$

$$\cdot \left[c(0) - \gamma \left(u + \frac{m\pi}{\omega} \right) \right] \left(u + \frac{m\pi}{\omega} \right) \sin(u\omega) du$$

The summation consists of a series with alternatively positive and negative terms, decreasing in absolute value, and since the first term is positive, it follows that $c(0) \delta(\omega) - \Gamma_3(\omega) > 0$, i.e., (28a) is satisfied.

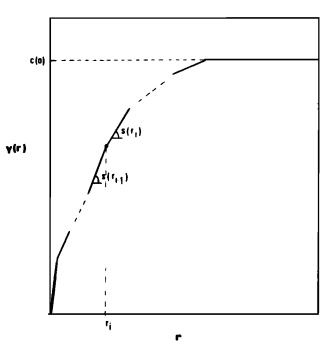


Fig. 1. Variogram model of polygonal form.

Corollary 4. The spectral function $\Gamma_2(\omega)$ of a variogram $\gamma(r)$ in \mathbb{R}^2 is equal to the one-dimensional FT of the function

$$\psi(h_1) = \frac{1}{2\pi} \int_{R^1} \gamma[r = (h_1^2 + h_2^2)^{1/2}] dh_2$$

Proof. By the definition of the FT in R^2 , we have $w_2 = 0$,

$$\Gamma_2(\omega = w_1) = \frac{1}{(2\pi)^2} \int_{R^1} \cos(w_1 h_1) \cdot \left\{ \int_{R^1} \gamma(h_1^2 + h_2^2)^{1/2} dh_2 \right\} dh_1$$

and corollary 4 follows.

Corollary 4 may offer an alternative, and sometimes easier, way for the calculation of $\Gamma_2(\omega)$ to the one suggested by proposition 2. In addition, it can be made valid for the spectral function $C_2(\omega)$, by simply replacing $\gamma(r)$ with c(r). To demonstrate this, take the covariance model

$$c[r = (h_1^2 + h_2^2)^{1/2}] = \exp\left(-\frac{h_1^2 + h_2^2}{a^2}\right)$$

Then the corresponding $\psi(h_1)$ function will be equal to

$$\frac{a}{2\sqrt{\pi}}\exp\left(-\frac{{h_1}^2}{a^2}\right)$$

whose FT in R^1 is $(a^2/4\pi) \exp(-\omega^2 a^2/4)$. The latter is also the spectral function $C_2(\omega)$ in R^2 of the covariance c(r).

Polygonal Models

When applying basic geostatistics, we frequently deal with transitive variogram models which have a polygonal form, as is shown in Figure 1. The proposition that follows offers an easy method to calculate the spectral functions $\Gamma_n(\omega)$.

Proposition 3. If the variogram has a polygonal form, its spectral function in R^1 is given by $(\omega \ge 0^+)$

$$\Gamma_1(\omega) = \frac{1}{\pi \omega^2} \sum_{i=0}^n \{ s(r_i) - s(r_{i-1}) \} \cos(\omega r_i)$$
 (57)

where $s(r_i)$ is the slope of $\gamma(r)$ at the point r_i (see Figure 1). For the spectral functions $\Gamma_2(\omega)$ and $\Gamma_3(\omega)$, one uses (50) and (51) together with (57) above.

Proof. If $\gamma(r)$ is of polygonal form, its second derivative is

$$\gamma''(r) = \sum_{i=0}^{n} \{s(r_i) - s(r_{i-1})\} \delta(r - r_i)$$

Since the FT of $\gamma''(r)$ is $-\omega^2 \Gamma_1(\omega)$ and the FT of the impulse $\delta(r-r_i)$ is known, we find (57).

The frequency ω_c up to which we need to compute $\Gamma_n(\omega)$ is given a priori or determined in some other way. For example, in \mathbb{R}^1 , using the bounds of $-\Gamma_1(\omega)$,

$$b_1 = 2|\Gamma_1(0^+)|$$

$$b_2 = \text{const } \omega^{-2} \sum_{i=0}^n \{ |s(r_i) - s(r_{i-1})| \}$$

 ω_c can be found solving the equation $b_2(\omega_c) = e \ b_1$, where e < 1.

To illustrate the application of proposition 3, consider the model

$$\gamma(r) = ar$$
 $r \le 1/a$
 $\gamma(r) = 1$ $r \ge 1/a$ (58)

In R^1 , we find $-\Gamma_1(\omega) = 2a (\pi \omega^2)^{-1} \sin^2(\omega/2a) \ge 0$, which asserts the permissibility of $\gamma(r)$. In R^2 , by applying (50) we find $(\omega > 0)$

$$- \Gamma_2(\omega) = \frac{1}{2\pi} \int_0^{1/a} J_0(\omega r) (1 - ar) r dr$$

which takes negative values and consequently the $\gamma(r)$ is not permissible in R^2 . It is interesting to note that (57), without the negative sign, gives the spectral function of a polygonal covariance c(r).

Approximation of Spectral Functions

Proposition 3 can be used to evaluate the spectral functions of a curve variogram or covariance model, properly approximated by a polygonal, keeping in mind that we are interested in the sign of the spectral function rather than its exact value. The degree of accuracy of such an approximation can be very satisfactory by proper discretization.

Another way to evaluate spectral functions approximately is to expand them in Fourier-Bessel series. This is an excellent approximation for the common case where they vanish outside the finite frequency ω_c , discussed before. However, even when this does not happen, such an expansion is still usable because, as we already mentioned, we are interested about the sign of the spectral functions and not exact values. The proposition below provides the explicit expressions for the spectral functions $\Gamma_n(\omega)$ of a variogram model $\chi(r)$. The expressions corresponding to a covariance model c(r) can be derived in exactly the same way.

Proposition 4. The Fourier-Bessel approximations of the spectral functions $\Gamma_n(\omega)$ of a variogram model $\gamma(r)$ are as follows:

in R^1

$$\Gamma_1(\omega) \equiv \omega_c^{-1} \sum_{k=0}^{\infty} \gamma(k\pi/\omega_c) \cos(k\pi\omega/\omega_c)$$
 (59a)

in \mathbb{R}^2

$$\Gamma_2(\omega) = (\pi \omega_c^2)^{-1} \sum_{k=1}^{\infty} \cdot \gamma(i_k/\omega_c) J_0(i_k\omega/\omega_c) \{J_1^2(i_k)\}^{-1}$$
 (59b) in R^3

$$\Gamma_3(\omega) = (2\omega_c^2 \ \omega)^{-1} \sum_{k=1}^{\infty} k \ \gamma(k\pi/\omega_c) \cdot \sin(k\pi\omega/\omega_c)$$
 (59c)

where J_v is the Bessel function of vth order (v = 0, 1) and i_k are the zeros of J_0 [see Gradshteyn and Ryzhik, 1965].

Proof. The proof of this proposition is based on the theory discussed by **Watson** [1966, chapter XVIII]. The R^1 case is a trivial expansion of $\Gamma_1(\omega)$ in Fourier series. For the R^2 , we expand the function $2\pi \Gamma_2(\omega)$ assuming $\Gamma_2(\omega > \omega_c) = 0$, v = 0, and we get (59b). In R^3 , we expand the function $4\pi\sqrt{r} \Gamma_3(\omega)$ and we find, for v = 0.5, the expansion (59c). Alternatively, in order to prove (59b) and (59c) one may use proposition 2 together with expansion (59a).

In practice, in order to remove the impulses inherent in the above equations, we may replace $\gamma(k\pi/\omega_c)$ with $\gamma(k\pi/\omega_c)$ – c(0), for $\omega > 0$. Then the value of the later function at origin has to be halved (i.e., at k = 0 of (59a)). Moreover, instead of Σ_k^{∞} , we use the summation Σ_k^N , where N is the number of samples taken. The choice of N as well as the sampling interval of the discretization are very important when programing the equations in a digital computer. A better approximation may be obtained in some cases by multiplying each term of the summation by (1 - k/N). Such a "modification" expresses the approximated spectral function as a weighted average of the actual spectral function with a positive kernel, and consequently it retains the true sign of the spectral function [see also Lanczos, 1966]. These aspects concerning the application in practice of the proposition 4 are to be emphasized in the following section. However, because of space limitations, more details and case studies will be given in a forthcoming paper.

Necessary Conditions

As we already discussed in the introduction, a number of restrictions are placed on the possible behaviour of the covariance, variogram, and generalized covariance models. We now give short proofs for the most important of them, and we also present some more in the form of simple inequalities.

Proposition 5. For a stationary and isotropic RF the associated variogram should satisfy the inequalities below:

in R¹

$$\gamma(r) \le 2 \ c(0) \tag{60a}$$

in R²

$$\gamma(r) \le 1.403 \ c(0) \tag{60b}$$

in R^3

$$\gamma(r) \le 1.218 \ c(0) \tag{60c}$$

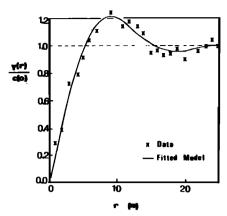


Fig. 2. Calculated and fitted variogram models for some water content data. The fitted model is permissible in a one-dimensional but not in a three-dimensional description of the spatial variability.

Also, in R^1 ,

$$\gamma(2^m r) \le 4^m \gamma(r)$$
 m nonnegative integer (61)

$$|\gamma(r) - \gamma(r + r')| \le [2 \gamma(r')]^{1/2}$$
 (62)

Proof. For (60a), we simply use (4) and (7). For (60b), starting from

$$\gamma(r) = 2\pi \int_0^\infty \left[1 - J_0(\omega r)\right] \omega C_2(\omega) d\omega$$

we see that $\gamma(r)/c(0)$ cannot be larger than

$$1 - \inf_{r} J_0(\omega r) = 1 - (-0.403) = 1.403$$

In an analogous way, (56b) implies restriction (60c). For (61), from the valid inequality $1 - \cos(2\omega r) \le 4[1 - \cos(\omega r)]$, we easily derive $\gamma(2r) \le 4 \gamma(r)$. Then, by induction, we get (61). Finally, for (62), use the inequality of Schwarz [see *Kolmogoroff and Fomin*, 1970]. It is not difficult to derive similar restrictions for the covariance c(r), using the above results together with (4).

Let us next examine a few examples. First, the variogram $\gamma(r) = 1 - \cos(r)$ cannot be a permissible model in more than one dimension, as we see by using (60). The model $\gamma(r) = 1 - \exp(-r^d)$ is not permissible in R^1 if d > 2. This results from the application of restriction (61), together with the expansions

$$\gamma(ar) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(ar)^{kd}}{k!}$$
 $a = 1$ and 2.

Proposition 6. An ordinary covariance c(r) and a generalized one k(r) should behave at infinity, as in expressions (8a) and (8c), respectively.

Proof. Equation (8a) is a straightforward application of the lemma of section 14.41 of Watson [1966], assuming that

$$\int_0^\infty C(\omega) \ \omega^{(1-n)/2} \ d\omega$$

exists. For (8c), from (39) and the well-known inequality $|\cos(x) - P_k(x)| \le x^{2\kappa+2}/(2\kappa+2)!$, we have $|k(r)| \le a_1 + a_2 r^{2\kappa+2}$, when a_1 , a_2 are constants. Then (8c) follows by the dominated convergence theorem. For $\kappa = 0$, we find (8b), keeping in mind that in this case $k(r) = -\gamma(r)$.

The usefulness of all the above restrictions regarding permissibility consists of the preliminary rejection of nonpermissible models before we proceed to the sophisticated analysis described by the COP's.

Procedure

Based on the above results, the procedure below may be useful in judging whether a function fitted to the data is a permissible model:

Step 1. This is a preliminary step. Check if the necessary conditions (propositions 5 and 6) are satisfied.

Step 2.

- 1. If the candidate model is of a "convenient," closed form (i.e., one can find its FT in R^1 by using the existing transform tables), calculate the particular spectral function in R^1 and check its permissibility by using the appropriate COP. If the answer is positive, calculate the spectral function in the field of interest R^2 or R^3 , by using Proposition 2 and the associated corollaries, and apply the COP's again.
- 2. If the candidate model is of a transitive, polygonal form, use proposition 3.
- 3. Finally, if the candidate model is of some arbitrary form, we may have to evaluate the spectral functions approximately by using propositions 3 or 4.

Many practitioners used to fit polygonal or curve functions empirically "by eye." Such a technique allows them to include information and engineering judgement which are not easily quantified (this is an interesting advantage over the statistical fitting techniques). Steps 2.2 and 2.3 would help the workers in the area to check if the fitted model is a permissible one or not and take appropriate action. The applications of the section that follows will illustrate this methodology.

APPLICATIONS

Testing Candidate Models for Permissibility

We will now examine the application of the results of the previous sections to further candidate variogram and covariance models. Some of them are already in use in water resources, while some others are functions occasionally fitted to the available data.

First, consider the model

$$\gamma(r) = 1 - \exp(-r/a)\cos(br)$$
 $a, b > 0$ (63)

It offers a very good fit for many soil properties [see, Lumb, 1975]. However, caution is needed when using (63) because it is not a permissible variogram for arbitrary values of the coefficients a and b. By applying the methodology of the preceding section we can avoid such pitfalls: In R^1 , the spectral function is

$$-\Gamma_{1}(\omega) = \frac{a^{2} + b^{2} + \omega^{2}}{[(\omega - b)^{2} + a^{2}][(\omega + b)^{2} + a^{2}]} > 0$$

But in R^3 we find, by using proposition 2, that the spectral function

$$-\Gamma_3(\omega) = \frac{\omega^4 + 2\beta^2 \ \omega^2 + (2\alpha - \beta^2) \ \beta^2}{\alpha \pi^2 (\omega^4 + 2\alpha \omega^2 + \beta^4)^2}$$
$$\alpha = (1 - a^2 b^2 / a^2) \qquad \beta = (1 + a^2 b^2) / a^2$$

is positive only if ab < 0.577. To illustrate the importance of these restrictions, the model (63) is fitted to the water content data of Figure 2, for a = 6.3 m and b = 0.3 m⁻¹.

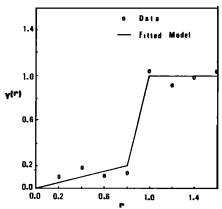


Fig. 3. The fitted model is not a permissible variogram in one or more dimensions.

According to our discussion, the fitted model is permissible in R^1 , but it cannot be used for a three-dimensional description of the spatial variability, since ab = 1.89 > 0.577, leading to erroneous results (negative variances, etc). Note that the model (63) is continuous at r = 0 and thus for all r > 0. However,

$$\left. \frac{d\gamma(r)}{dr} \right|_{r=0} \neq 0$$

and therefore we conclude that the associated RF $Z(x_i)$, while continuous (in the mean square sense), is not mean square differentiable.

For the extensively used exponential variogram

$$\gamma(r) = 1 - \exp(-r/a)$$
 $a > 0$ (64)

the spectral function in R^1 is such that

$$-\Gamma_{\mathsf{I}}(\omega) = \frac{a}{\pi(1+\omega^2 a^2)} > 0$$

and the COP-1 is satisfied. Next, by using proposition 2 we find

in R^2

$$-\Gamma_2(\omega) = \frac{1}{2\pi a[(a^2\omega^2+1)/a^2]^{3/2}} > 0$$

in R^3

$$-\Gamma_3(\omega) = \frac{a^3}{\pi^2(1+\omega^2a^2)^2} > 0$$

and according to COP-1, model (64) is permissible in R^1 , R^2 , or R^3 . Like model (63), it corresponds to a continuous but not differentiable RF.

A covariance model permissible only in R^1 and R^2 is the one below:

$$c(r) = \exp(-r^2/a^2) J_0(br)$$
 (65)

In \mathbb{R}^2 , its spectral function is such that

$$C_2(\omega) = \frac{a^2}{4\pi} I_0(a^2b\omega/2) \exp\left(-\frac{a^2b^2 + a^2\omega^2}{4}\right) > 0$$

and the COP-1 is valid. This is a model for rather strong correlations and tends rapidly to zero, where it oscillates. The underlying RF is mean square differentiable.

The polygonal model shown in Figure 3 is not a permissi-

ble one, even in R^1 , where we get, by using proposition 3,

$$-\Gamma_1(\omega) = \text{const } \omega^{-2} \{1 + 15 \cos (4\omega) - 16 \cos (5\omega)\}$$

which takes negative values. On the other hand, the model of Figure 3 is immediately rejected from the application of the necessary condition (61). For instance, for m=1, r=0.5 we get $\gamma(2\times0.5)=\gamma(1)>4$ $\gamma(0.5)$. The use of proposition 3 in practice may offer some interesting hints concerning the permissibility of polygonal models or models approximated by polygonal functions. For example, a large initial slope seriously contributes to the permissibility in R^1 (in the present model the initial slope is only 0.25, see Figure 3). The same applies to a nonincreasing slope of the variogram (in the present model we have a slope increasing from $r=0.8^-$ to $r=0.8^+$).

In the application to follow, we will use the methodology of proposition 4 to investigate the permissibility of the variogram model

$$\gamma(r) = r^2/(1 + r^2) \tag{66}$$

fitted to the data, as shown in Figure 4. Its spectral function in \mathbb{R}^3 is calculated employing a computer program based on (59c), after replacing $\gamma(k\pi/\omega_c)$ with $\gamma(k\pi/\omega_c) - 1$ (see discussion following proposition 4). A sampling interval of $\Delta r =$ 0.50 and N = 16 samples, with a highest frequency of $\omega_c =$ 2π has been used. Such a ω_c value insures no aliasing. In Figure 5 are shown both the calculated and the theoretical spectral functions for comparison. Obviously, the $-\Gamma_3(\omega)$ is always nonnegative and hence the model (66) is permissible in \mathbb{R}^3 (and also, of course, in \mathbb{R}^2 and \mathbb{R}^1). When programing proposition 4 to the computation of spectral functions, care is needed in some details, such as the choice of Δr and N (a large Δr or a small N may lead to poor approximation of the spectral function at higher frequencies ω) and also the correct interpretation of the results (the approximated spectral function may be symmetrical about N/2, related to negative frequencies, and this follows because it is an even function).

The variogram

$$\gamma(r) = r^m \qquad m \ge 0 \tag{67}$$

is a nonbounded one, and for the associated RF only the intrinsic hypothesis is valid. In R^3 it satisfies the COP-3 only if $0 \le m < 2$, when

$$-\omega^2 \Gamma_3(\omega) = \frac{G[(m+3)/2]}{G(-m/2)} \pi^{-(m+3/2)} \omega^{-m-1} > 0 \qquad \omega > 0$$

$$\lim_{r \to \infty} \gamma(r)/r^2 = 0 \qquad r \to \infty$$

Consequently, it is permissible in \mathbb{R}^3 , and it is not difficult to show that the same applies in \mathbb{R}^n , n > 3. The model (67) is continuous but not always differentiable, depending on the value of m.

The GC-1 spline model

$$k(r) = r^m \log (r) \qquad m > 0 \tag{68}$$

is a very useful model for nonstationary spatial phenomena, and it is derived from the family (43). When applying COP-4, we find

$$K(\omega) = \frac{dC_m}{dm} (\omega/2\pi)^{-m-n} + C_m(\omega/2\pi)^{-m-n} \log (\omega/2\pi)$$

where $C_m = 2^{m+n} \pi^{n/2} G[(m+n)/2]/G(-m/2)$ [see Gelfand and Shilov, 1964]. For $\omega^4 K(\omega) \ge 0$, we need 0 < m < 2. The

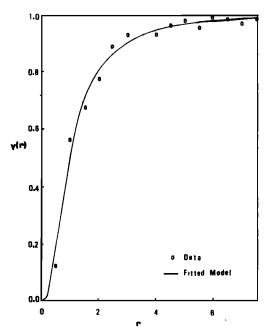


Fig. 4. Calculated and fitted variogram models in \mathbb{R}^3 .

value m = 2 is also included because the k(r) may be derived as the limit of the first-order generalized covariance

$$r^{2+c} - r^2$$
 $0 < c < 2$

i.e.,

$$k(r) = \lim_{c \to 0} \frac{r^{2+c} - r^2}{c}$$

and the limit of a generalized covariance is still a generalized covariance. On the other hand, condition (38) is satisfied for m < 4. Hence the spline model (68) is permissible as a GC-1 in \mathbb{R}^n , for $0 < m \le 2$.

Finally, a remarkable generalized covariance model, resulting from the combination of the models (43) and (68), is

$$k(r) = -a_0 r + a_1 r^2 \log(r) + a_2 r^3$$
 (69)

In R^3 the COP-4 leads to the following constrains for the parameters a_0 , a_1 , and a_2 :

$$a_0, a_2 \ge 0$$
 $a_1 \ge -1.47(a_0 a_2)^{1/2}$

For R^2 and R^1 the constraints on a_1 are less severe, being -1.50 and -1.56, respectively.

A Spectral Method for Generating Covariance and Variogram Models

So far we have concentrated on the problem of testing a given function to see if it is a permissible statistical moment (covariance, variogram, or generalized covariance). Next, we will discuss how the same theory as above can be applied to create several families of isotropic models. The idea is to work in the opposite direction and try to construct variogram or covariance models from properly chosen spectral functions. If $p_n = c_n(r)/c(0)$ is the correlation function, similar to (54) and (55), expressions may be established, i.e., we can write

$$\rho_n(r) = \frac{c_n(r)}{c(0)} = \frac{(2\pi)^{n/2}}{r^p} \int_{R_+^1} J_p(\omega r) \ \omega^{n/2} \frac{C_n(\omega)}{c(0)} d\omega \tag{70}$$

where p = (n-2)/2. Equation (70) implies that the "normalized" spectral function $C_n(\omega)/c(0)$ can be viewed as the probability function $P_v(v)$ of an *n*-dimensional random vector, i.e., $P_v(v) = C_n(\omega)/c(0)$. Furthermore, $P_v(v)$ is isotropic (i.e., it is fully defined by the probability density function of |v|, say, $P_{|v|}(\omega)$, where |v| is in ω units). The necessary and sufficient conditions for $c_n(r)$ to be a permissible covariance model is that it can be expressed by (70) where $C_n(\omega)$ is nonnegative and summable (see COP's). Based on this fact, and since it is easier to construct a probability density function P_v than a nonnegative definite covariance $c_n(r)$, a convenient way to generate covariance and (consequently) variogram functions in R^n may be as follows:

- 1. Construct a probability density function P_v for a random vector v.
- 2. Substitute P_v into (70) to obtain the corresponding covariance $c_n(r)$.
- 3. Substitute $c_n(r)$ into (4) to find the corresponding variogram $\gamma_n(r)$.

Let us examine a few examples. Suppose that the random vector v is uniformly distributed on the surface of an n-dimensional sphere with radius u. The probability density function of v will be

$$P_v(v = \omega) = \frac{G(n/2)}{2\pi^{n/2}\omega^{n-1}}\delta(\omega - u)$$

and the spectral function $C_n(\omega) = P_v(\omega) c(0)$ is nonnegative for all ω . Hence we can substitute it into (70), and then by using (4), derive the variogram model below:

$$\gamma_n(r) = c(0) \left\{ 1 - 2^p G(n/2) (ur)^{-p} J_p(ur) \right\}$$
 (71)

The model (71) for n = 1, gives $\gamma_1(r) = c(0) [1 - \cos(ur)]$; for n = 2, gives $\gamma_2(r) = c(0) \{1 - J_0(ur)\}$; and finally, for n = 3; gives $\gamma_3(r) = c(0) \{1 - [\sin(ur)/ur]\}$.

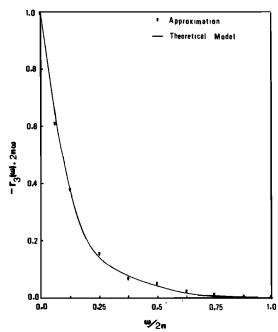


Fig. 5. Calculated and theoretical spectral functions for the variogram model of Figure 4.

Following the same procedure, if we take the P_v to be of (74) for n = 5, we obtain the model exponential form, the corresponding variogram will be

$$\gamma_n(r) = c(0) \left\{ 1 - \left(1 + \frac{r^2}{a^2} \right)^{-(n+1)/2} \right\}$$
 (72)

which may be a useful model in geotechnical applications. Also, if we take

$$P_v(\omega) = \left(1 + \frac{\omega^2}{a^2}\right)^{-l} \qquad l > n/2$$

it is not difficult to prove that the corresponding variogram will be

$$\gamma_n(r) = \text{const } \{1 - \text{const } r^{\vee} \mathsf{K}_{\vee}(r/a)\}$$

where v = (1 - n)/2. A convenient class of models is generated by assuming that

$$P_{v}(\omega) = (2/\omega)^{n} \left\{ \frac{n}{2}! J_{n/2}(\omega) \right\}^{2}$$
 (73)

In this case we may derive the following models:

for n = 1

$$\gamma_1(r) = \text{const } r$$
 $r \le 1/\text{const}$
 $\gamma_1(r) = c(0)$ $r > 1/\text{const}$

for n = 2

$$\gamma_2(r) = 2 \frac{c(0)}{\pi} \left\{ cr(1 - c^2 r^2)^{1/2} + \arcsin(cr) \right\} \qquad r \le 1/c$$

$$\gamma_2(r) = c(0) \qquad r > 1/c$$

for n = 3

$$\gamma_3(r) = c(0) \left\{ \frac{3}{2} cr - \frac{1}{2} c^3 r^3 \right\} \qquad r \le 1/c$$

$$\gamma_3(r) = c(0) \qquad r > 1/c$$

Such models have the advantage that data points can be ignored after the distance 1/c and so the computations are reduced.

We can apply the same method as above to find models for n > 3. For example, a common fourth dimension may be the time. The models obtained for n > 3 are also valid for $n \le 3$, a fact that further enriches the classes of available isotropic models for the one-, two-, and three-dimensional spaces. For instance, (73) may be used for n = 5 (say) to give

$$\gamma_5(r) = 0.25 \ c(0) \cdot [7.5cr - 5c^3r^3 + 1.5c^5r^5] \qquad r \le 1/c$$

$$\gamma_5(r) = c(0) \qquad r > 1/c$$

which may be a convenient model for n < 5, also.

An alternative method, to produce permissible models for $n \le 3$ from known permissible models in n > 3, is introduced by the recursive formula below:

$$\gamma_{n-2}(r) = \gamma_n(r) + \frac{r \, \gamma_n'(r)}{n-2} \qquad \gamma_n'(r) = \frac{d\gamma_n(r)}{dr} \qquad (74)$$

Formula (74) is derived from the combination of (4) and (32). Consider as an example the model $\gamma_5(r)$, above. When using

$$\gamma_3(r) = c(0) \{2.5cr - 2.5c^3r^3 + c^5r^5\}$$
 $r \le 1/c$
 $\gamma_3(r) = c(0)$ $r > 1/c$

which is a model for stronger correlations.

To conclude, the methods discussed in this section may provide a number of variogram and covariance functions useful for a wide range of practical applications. From this point of view, they could be considered as tools of potential usefulness for the geostatistical investigations.

Conclusions

The important problem of judging the permissibility of candidate covariance and variogram models (ordinary or generalized) has been discussed in this article. Several criteria of permissibility, covering the case of stationary random functions as well as the case of kth-order intrinsic random functions, have been introduced for this purpose.

A procedure recommended for testing the permissibility in one or more dimensions may be suitable for a wide range of practical applications. To maintain the proper balance between theory and facts, we have presented numerous examples that have been computed in detail.

The author believes that the problem of identifying permissible models is by no means simple. However, he hopes that the reader of this article will be helped to test efficiently whether a particular function fitted to the data is permissible or not, and also that he will find some new sources of potential models in addition to the ones already used.

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