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ANALOGIES AND CORRESPONDENCES BETWEEN VARIOGRAMS AND COVARIANCE FUNCTIONS

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Abstract

Variograms and covariance functions are key tools in geostatistics. However, various properties, characterizations, and decomposition theorems have been established for covariance functions only. We present analogous results for variograms and explore the connections with covariance functions. Our findings include criteria for covariance functions on intervals, and we apply them to exponential models, fractional Brownian motion, and locally polynomial covariances. In particular, we characterize isotropic locally polynomial covariance functions of degree 3.

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1. Introduction

Geostatistical techniques model spatial data as the realizations of random functions. Most analyses rely on a (possibly implicit) assumption of stationarity for the random process $Z = \{Z(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^d\}$, where $Z(\boldsymbol{x})$ is the scalar variable associated with the location $\boldsymbol{x}$.

The process Z is said to be *second-order stationary*, or simply *stationary*, if second moments exist and the expectation $\mathrm{E}\, Z(\boldsymbol{x})$ and the covariance $\mathrm{cov}(Z(\boldsymbol{x}), Z(\boldsymbol{x}+\boldsymbol{h}))$ do not depend on $\boldsymbol{x} \in \mathbb{R}^d$. We may then define the *covariance function*

$$C(\boldsymbol{h}) = \mathrm{cov}(Z(\boldsymbol{x}), Z(\boldsymbol{x}+\boldsymbol{h})), \qquad \boldsymbol{h} \in \mathbb{R}^d. \tag{1}$$

Stationarity is a standard assumption in many applications, such as atmospheric data assimilation. Classical geostatistical theory (Matheron (1973), Chilès and Delfiner (1999)) relies on a weaker assumption, the intrinsic hypothesis. The random function Z is called *intrinsically stationary* if the increment process $I_{\boldsymbol{h}} = \{Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h}) : \boldsymbol{x} \in \mathbb{R}^d\}$ is stationary for all lag vectors $\boldsymbol{h} \in \mathbb{R}^d$. Then $\mathrm{E}(Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h}))$ and $\mathrm{E}(Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h}))^2$ do not depend on $\boldsymbol{x}$, and we may define the *variogram*

$$\gamma(\boldsymbol{h}) = \tfrac{1}{2}\, \mathrm{E}(Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h}))^2, \qquad \boldsymbol{h} \in \mathbb{R}^d. \tag{2}$$

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Any stationary process is intrinsically stationary, but the converse is not true. For example, Brownian motion is an intrinsically stationary but not a stationary process. Thus, variograms are more general than covariance functions. However, covariance functions are better understood theoretically and many important properties, characterizations, and decomposition theorems have been established for covariance functions only. In this paper we present analogous results for variograms, and we explore the relationships between covariance functions and variograms.

In Section 2 we recall the definition of *centered* and *noncentered* variograms, review some fundamental characterization and decomposition theorems, and prove for variograms analogues of recent results for covariance functions. Section 3 is concerned with locally equivalent stationary covariances. If the variogram γ of an intrinsically stationary process Z is bounded, then there exists a stationary process Y with covariance function C such that

$$\gamma(\boldsymbol{h}) = C(\mathbf{0}) - C(\boldsymbol{h}), \qquad \boldsymbol{h} \in \mathbb{R}^d. \tag{3}$$

If γ is unbounded, there is no covariance C for which the correspondence (3) holds. However, a stationary process Y with covariance function C might exist such that the relation holds locally,

$$\gamma(\boldsymbol{h}) = C(\mathbf{0}) - C(\boldsymbol{h}), \qquad \boldsymbol{h} \in \mathbb{R}^d,\ |h| \le r, \tag{4}$$

for some positive r. Then C is said to be a *locally equivalent stationary covariance*; and under suitable conditions Y is a *locally stationary representation* of Z, as defined by Matheron (1973), (1974) and Chilès and Delfiner (1999, pp. 267–270). Locally equivalent covariances have both theoretical and computational interest, because they allow for optimal prediction and fast simulation with genuinely positive definite matrices (Chilès and Delfiner (1999), Stein (2000)). We present various criteria for the existence of locally equivalent stationary covariances. Theorem 8 is a generalization of Pólya's criterion, and Theorems 9 and 10 give necessary and sufficient conditions which are based on functional analytic results of Krein and Langer (1985). The paper closes with applications to exponential variogram models, fractional Brownian motion, and locally polynomial covariances in Section 4. In particular, we characterize isotropic locally polynomial covariance functions of degree 3.

2. Variograms

Our starting point here is the observation that (almost) all major properties of covariance functions carry over to variograms. One of the exceptions is boundedness: it is well known that $|C(\boldsymbol{h})| \le C(\mathbf{0})$ for a covariance function C, whereas variograms need not be bounded. We begin by reviewing the definition of the variogram, proceed with characterization and decomposition theorems, and give sharper results in the isotropic case. Sections 2.1 and 2.2 are largely expository.

2.1. Centered and noncentered variogram

The definition (2) of the variogram may appear clear-cut but calls for comments. The factor $\frac{1}{2}$ has led to the notion of a *semivariogram*, and some authors distinguish variogram (defined without the factor) and semivariogram (defined with the factor). We retain the definition with the factor and nevertheless talk of the *variogram*. However, we distinguish noncentered variograms, or simply variograms, and centered variograms.

Definition 1. Suppose that Z is an intrinsically stationary process in $\mathbb{R}^d$. Then Z has *noncentered variogram* or *variogram*

$$\gamma(\boldsymbol{h}) = \tfrac{1}{2}\,\mathrm{E}(Z(\boldsymbol{x}) - Z(\boldsymbol{x} + \boldsymbol{h}))^2, \qquad \boldsymbol{h} \in \mathbb{R}^d,$$

and *centered variogram*

$$\widetilde{\gamma}(\boldsymbol{h}) = \tfrac{1}{2}\,\mathrm{var}(Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h})), \qquad \boldsymbol{h} \in \mathbb{R}^d.$$

It follows readily that for a given process Z,

$$\gamma(\boldsymbol{h}) = Q(\boldsymbol{h}) + \widetilde{\gamma}(\boldsymbol{h}), \qquad \boldsymbol{h} \in \mathbb{R}^d, \tag{5}$$

where Q is a nonnegative quadratic form, that is, $Q(\boldsymbol{h}) = \sum_{i=1}^{d} a_i h_i^2$ where $\boldsymbol{h} = (h_1, \ldots, h_d)^\top \in \mathbb{R}^d$ and $a_i \geq 0$ for $i = 1, \ldots, d$. Conversely, if $\widetilde{\gamma}$ is a centered variogram and Q is a nonnegative quadratic form, then (5) is a noncentered variogram. The definitions coincide in the standard case when $\mathrm{E}(Z(\boldsymbol{x}) - Z(\boldsymbol{x}+\boldsymbol{h})) = 0$.

2.2. Characterization and decomposition theorems

We first review a fundamental characterization theorem for variograms. Recall that a function $\gamma : \mathbb{R}^d \to \mathbb{R}$ is said to be *conditionally negative definite* if the inequality

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j \gamma(\boldsymbol{x}_i - \boldsymbol{x}_j) \leq 0$$

holds for all finite systems of points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$ and coefficients $a_1, \ldots, a_n$ for which $\sum_{i=1}^{n} a_i = 0$.

Theorem 1. *If γ is a real function in $\mathbb{R}^d$ satisfying $\gamma(\mathbf{0}) = 0$, the following properties are equivalent.*

(a) *There exists an intrinsically stationary Gaussian random function Z with variogram $\gamma(\cdot)$.*

(b) *The function $\gamma(\cdot)$ is conditionally negative definite.*

(c) *For all $t > 0$, $\exp(-t\gamma(\cdot))$ is a covariance function.*

This result is known, and the equivalence of (a) and (b) mimics the characterization of covariances as positive definite functions. However, in the statistical literature, Theorem 1 has been known only under the additional assumption of continuity of γ (cf. Cressie (1993, p. 87), Chilès and Delfiner (1999, pp. 66–67)). This excludes many practically important variogram models which are obtained by adding a *nugget effect*,

$$\gamma_0(\boldsymbol{h}) = \begin{cases} 0, & \boldsymbol{h} = \mathbf{0}, \\ \alpha, & \text{otherwise}, \end{cases} \qquad \alpha > 0,$$

to a continuous variogram. The general result presented here is immediate from Theorem 6.1.9 of Sasvári (1994).

The equivalence of (a) and (c) in Theorem 1 allows us to establish interesting and useful analogies between covariance functions and variograms, that is, between stationary and intrinsically stationary random fields. For instance, Davies and Hall (1999) show that if a stationary process in $\mathbb{R}^2$ satisfies the usual one-dimensional scaling laws, then the fractal dimensions of its line transect processes are the same in all directions, except possibly one, whose dimension may be less than in all others. By Theorem 1, the result carries over to intrinsically stationary processes in $\mathbb{R}^2$. We omit the technical statement and proof.

Any measurable covariance function C admits the decomposition $C = C_c + C_0$ where C_c is a continuous covariance and C_0 is a covariance function which vanishes Lebesgue-almost everywhere (see, for example, Crum (1956) and Sasvári (1994, pp. 92–93)). This result and the equivalence of (a) and (c) in Theorem 1 suggest an analogue for variograms. Indeed, if γ is a measurable variogram on $\mathbb{R}^d$ we can write $\exp(-\gamma(\cdot)) = C_c(\cdot) + C_0(\cdot)$ where $C_c(\cdot) > 0$. Then the decomposition

$$\begin{aligned}\gamma(\boldsymbol{h}) &= \gamma_c(\boldsymbol{h}) + \gamma_0(\boldsymbol{h}) \\ &= \log\frac{C_c(\mathbf{0})}{C_c(\boldsymbol{h})} + \log\left(\frac{1}{C_c(\mathbf{0})}\frac{C_c(\boldsymbol{h})}{C_c(\boldsymbol{h}) + C_0(\boldsymbol{h})}\right), \qquad \boldsymbol{h} \in \mathbb{R}^d, \end{aligned} \tag{6}$$

holds where γ_c is continuous and γ_0 is constant almost everywhere. The following result, which is an immediate consequence of Theorem 5.3.6 of Sasvári (1994), shows that both γ_c and γ_0 are variograms.

Theorem 2. *If γ is a measurable variogram, the decomposition (6) holds where γ_c is a continuous variogram. The function γ_0 is also a variogram and Lebesgue-almost everywhere constant.*

The theorem justifies restricting our attention to continuous variograms, as we do from now on. Any practically relevant discontinuous variogram is the sum of a continuous variogram and a nugget effect.

In analogy to Bochner's theorem for covariance functions, continuous variograms have a well-known spectral characterization (Cressie (1993, pp. 84, 87), Chilès and Delfiner (1999, pp. 64, 66–67)).

Theorem 3. *Let γ be a real continuous function on $\mathbb{R}^d$ with $\gamma(\mathbf{0}) = 0$.*

(a) *The function $\gamma(\cdot)$ is a variogram if and only if the representation*

$$\gamma(\boldsymbol{h}) = Q(\boldsymbol{h}) + \int \frac{1 - \cos(\boldsymbol{u}^\top \boldsymbol{h})}{|\boldsymbol{u}|^2}\,\mathrm{d}F(\boldsymbol{u}), \qquad \boldsymbol{h} \in \mathbb{R}^d,$$

holds, where Q is a nonnegative quadratic form and F is a nonnegative measure on $\mathbb{R}^d$ with no point mass at the origin and satisfying $\int (1 + |\boldsymbol{u}|^2)^{-1}\,\mathrm{d}F(\boldsymbol{u}) < \infty$.

(b) *The function $\gamma(\cdot)$ is a centered variogram if and only if it is a noncentered variogram and the quadratic form Q in the spectral representation vanishes.*

Any variogram γ satisfies an inequality of the form $\gamma(\boldsymbol{h}) \le a|\boldsymbol{h}|^2 + b$ for convenient constants $a, b \ge 0$. Furthermore, $\gamma(\boldsymbol{h})/|\boldsymbol{h}|^2 \to 0$ as $|\boldsymbol{h}| \to \infty$ if and only if γ is a centered variogram. See, for example, Matheron (1973) or Chilès and Delfiner (1999, p. 260).

2.3. Isotropic functions

Here we give sharper results under the assumption that γ is a spherically symmetric or *isotropic* function, that is, $\gamma(\boldsymbol{h}_1) = \gamma(\boldsymbol{h}_2)$ whenever $|\boldsymbol{h}_1| = |\boldsymbol{h}_2|$. This is the type of variogram model most often fitted in geostatistical practice. The spectral representation then reduces to a well-known Bessel integral for which we refer the reader to Cressie (1993, p. 88).

First, we strengthen Theorem 2. For isotropic variograms in $\mathbb{R}^d$, $d \ge 2$, the discontinuous part in the decomposition (6) is necessarily a nugget effect. The result follows readily from the analogous property for covariance functions (for example, Gneiting and Sasvári (1999)) and the equivalence of (a) and (c) in Theorem 1.

Theorem 4. *If γ is a measurable isotropic variogram in $\mathbb{R}^d$, $d \geq 2$, the decomposition $\gamma = \gamma_c + \gamma_0$ holds where γ_c is a continuous variogram and γ_0 is a nugget effect.*

The next theorem follows analogously from the corresponding result for covariance functions (Gneiting (1999b)). We denote by $\lfloor r \rfloor$ the integer part of a real number r and omit the straightforward proof.

Theorem 5. *Let γ be an isotropic variogram in $\mathbb{R}^d$, and let k be a nonnegative integer. If γ is differentiable of order $2k$ at $\mathbf{0}$, then γ is differentiable of order $2k + \lfloor d - 1/2 \rfloor$ on $\mathbb{R}^d \setminus \{\mathbf{0}\}$.*

In spatial data analysis, the approach of Sampson and Guttorp (1992) deforms the geographic coordinate space so that stationary and isotropic variogram models can be fitted to very general classes of random functions. Perrin and Meiring (1999) discuss identifiability questions in this context. Theorem 5 shows that their assumption (B2) is redundant if $d \geq 3$.

3. Locally equivalent stationary covariances

In this section, we explore the relationships between variograms and covariance functions through the correspondences (3) and (4). Our findings can be expressed equivalently in terms of locally stationary representations of intrinsic processes, as introduced by Matheron (1973), (1974) and recently reviewed by Chilès and Delfiner (1999, pp. 267–270). Other notions of local stationarity exist, in particular in the time series literature, and we note recent work by Mallat *et al.* (1998) and Keich (2000). Perrin and Senoussi (1999), (2000) discuss relationships between nonstationary and stationary processes in the aforementioned deformation approach of Sampson and Guttorp (1992).

3.1. Motivation

To begin with, we recall from (1) and (2) that if C is a covariance function in $\mathbb{R}^d$, then

$$\gamma(\boldsymbol{h}) = C(\mathbf{0}) - C(\boldsymbol{h}), \qquad \boldsymbol{h} \in \mathbb{R}^d, \tag{7}$$

is a centered variogram. Conversely, if γ is a bounded variogram, then it is of the form (7) for some covariance function C (Matheron (1973), Chilès and Delfiner (1999, p. 32)). However, (7) determines the covariance function only up to an additive constant. It is therefore not clear in general which values $C(\mathbf{0})$ the covariance function may attain at the origin. In Matheron's (1973), (1974) terminology, the smallest possible value for the variance of a stationary representation remains to be determined. The following theorem provides a simple necessary and sufficient condition on the variance.

Theorem 6. *The function C in the representation (7) for a bounded variogram γ in $\mathbb{R}^d$ is a covariance function if and only if*

$$C(\mathbf{0}) \geq \lim_{u\to\infty} (2u)^{-d} \int_{[-u,u]^d} \gamma(\boldsymbol{h})\, \mathrm{d}\boldsymbol{h}.$$

Proof. We already know that the representation (7) holds if $C(\mathbf{0})$ is sufficiently large. By Bochner's theorem, $C(\boldsymbol{h}) = C(\mathbf{0}) - \gamma(\boldsymbol{h})$ then admits a spectral measure in $\mathbb{R}^d$, F say, and by Theorem 1.3.7 of Bisgaard and Sasvári (2000), F has point mass

$$F(\{\mathbf{0}\}) = C(\mathbf{0}) - \lim_{u\to\infty} (2u)^{-d} \int_{[-u,u]^d} \gamma(\boldsymbol{h})\, \mathrm{d}\boldsymbol{h}$$

at the origin, which also shows the existence of the right-hand side. This quantity must be nonnegative, and the assertion of the theorem follows.

We note that Theorem 1.3.7 of Bisgaard and Sasvári (2000) concerns the case $d = 1$. The generalization to spectral measures in $\mathbb{R}^d$, $d \geq 1$, is straightforward.

3.2. Locally equivalent stationary covariances

If γ is unbounded, a relationship of the form (7) with a covariance function C cannot hold. However, a covariance function C might exist such that the correspondence holds locally,

$$\gamma(\boldsymbol{h}) = C(\boldsymbol{0}) - C(\boldsymbol{h}), \qquad \boldsymbol{h} \in \mathbb{R}^d, \ |\boldsymbol{h}| \leq r,$$

for some positive r. Then C is said to be a *locally equivalent stationary covariance*. Locally equivalent covariances have both theoretical and computational interest, because they allow for optimal prediction with genuinely positive definite matrices. We refer the reader to Section 6 of Matheron (1973), a technical report by Matheron (1974), and Section 4.6.2 of Chilès and Delfiner (1999, pp. 267–270) for a discussion of the associated random functions, that is, the *locally stationary representations* of intrinsic processes.

As Matheron (1973, p. 466) and Chilès and Delfiner (1999, p. 291) point out, there exist variograms which do not admit locally equivalent stationary covariances. For instance, $\gamma(h) = h^2$ is a noncentered variogram on $\mathbb{R}$, but there is no real number $C(0)$ such that $C(h) = C(0) - \gamma(h)$ is a covariance function defined on a neighborhood of $h = 0$. Indeed, C is an analytic function, and any analytic covariance function defined on a neighborhood of the origin admits a unique extension to an analytic covariance function defined in $\mathbb{R}$ (Bisgaard and Sasvári (2000, Section 1.13)). However, the unique analytic extension of C is unbounded and therefore not a covariance function. In particular, the locally quadratic decay model proposed by Worsley *et al.* (1991) is not a permissible covariance model.

To give an explicit example of a centered variogram which does not admit a locally equivalent stationary covariance, we first prove a result of independent interest.

Theorem 7. *Let γ be a real even, twice continuously differentiable function in $\mathbb{R}$ with $\gamma(0) = 0$. Then γ is a variogram if and only if γ'' is a covariance function.*

Proof. If γ is a variogram, Exercise 6.1.7 of Sasvári (1994) implies that γ'' is a covariance function (see also Equation (4.22) of Chilès and Delfiner (1999)). Conversely, if γ'' is a covariance function, then Bochner's theorem applies. The arguments in the proof of Theorem 6 show that we can write

$$\gamma''(s) = 2c + \int_{-\infty}^{\infty} \cos(us)\, \mathrm{d}F(u), \qquad s \in \mathbb{R},$$

with a constant $c \geq 0$ and a finite nonnegative measure F on $\mathbb{R}$ with no point mass at the origin. Since $\gamma(0) = 0$, we have, for $h \in \mathbb{R}$,

$$\begin{aligned}\gamma(h) &= ch^2 + \int_0^h (h-s)\gamma''(s)\,\mathrm{d}s = ch^2 + \int_0^h (h-s)\int_{-\infty}^{\infty} \cos(us)\,\mathrm{d}F(u)\,\mathrm{d}s \\ &= ch^2 + \int_{-\infty}^{\infty}\int_0^h (h-s)\cos(us)\,\mathrm{d}s\,\mathrm{d}F(u) = ch^2 + \int_{-\infty}^{\infty} \frac{1-\cos(uh)}{u^2}\,\mathrm{d}F(u).\end{aligned}$$

By Theorem 3(a), γ is a variogram.

Consider the function

$$\gamma(h) = \tfrac{1}{2} \sum_{j=0}^{\infty} \frac{(-1)^j h^{2j+2}}{(j+1)(2j+1)j!}, \qquad h \in \mathbb{R},$$

for which $\gamma(0) = 0$ and $\gamma''(h) = \exp(-h^2)$ is a continuous covariance. Theorem 7 applies, and we note that γ is an analytic, unbounded variogram. Since $\gamma(h) = \mathcal{O}(h)$ as $h \to \infty$, the remarks at the end of Section 2.2 show that γ is a centered variogram. The argument in the example prior to the theorem (see also Chilès and Delfiner (1999, p. 291)) then implies that there is no real number $C(0)$ such that $C(h) = C(0) - \gamma(h)$ is a covariance function defined in a neighborhood of $h = 0$.

In this light, two key questions emerge: when does a locally equivalent stationary covariance exist; and if it does, what is the smallest attainable value at zero? As in the case of globally stationary representations, the second problem corresponds to the question for locally stationary representations with minimal variance. Hereinafter, we present a number of criteria which address these problems. We focus on the one-dimensional case and then without loss of generality on continuous functions $C(t)$ defined for $t \in [-1, 1]$. Then C is said to be a *covariance function* if it can be extended to a covariance function in $\mathbb{R}$ (compare Gneiting and Sasvári (1999) and the references therein). The turning bands operator allows for analogous results for isotropic functions defined on balls in $\mathbb{R}^d$ (see Gneiting (1999a)).

3.3. Criteria of Pólya type

It is almost immediate from Pólya's theorem (Cressie (1993, p. 86), Chilès and Delfiner (1999, p. 68)) that a variogram γ in $\mathbb{R}$ admits a locally equivalent stationary covariance if γ is concave on $[0, 1]$. The following criterion gives a sharper result.

Theorem 8. *Let C be an even continuous function defined on* $[-1, 1]$. *If C is convex and decreasing on* $[0, 1]$ *and* $\int_0^1 C(t)\,\mathrm{d}t \geq 0$, *then C is a covariance function.*

To prove the criterion it suffices to note that the extension of C to a function of period 2 in $\mathbb{R}$ is a covariance function, by Theorem 1 of Gneiting (1998). It follows that if C is even, continuous, and locally convex at the origin, then there exists an $a > 0$ such that $C(t)$ is a covariance function on $[-a, a]$. We have not succeeded in verifying related claims by Romanov (1982). For instance, Romanov's criterion (1.7) with $l = 1$ implies that $C(t) = A - |t|$ is a covariance function on $[-1, 1]$ whenever $A \leq 1$, which is clearly not true. Gneiting (2001) gives criteria of Pólya type for isotropic functions in $\mathbb{R}^d$ which apply in the present context, too. See Section 4.2 for an example.

3.4. Criteria based on Krein–Langer theory

Here we present results which derive from the functional analytic work of Krein and Langer (1985).

Definition 2. An even continuous function C, defined on $[-1, 1]$, is said to have an *accelerant* H if

(i) $\mathrm{H}(t) = -C''(t)$ exists for $t \in [-1, 1]$, $t \neq 0$;

(ii) $\mathrm{H} \in L^1[-1, 1]$; and

(iii) $C'(0+) < 0$.

With the function H we associate the operator $\mathbf{H}$ in $L^2[0, 1]$, defined by

$$(\mathbf{H}\varphi)(t) = \int_0^1 \mathrm{H}(t-s)\varphi(s)\,\mathrm{d}s, \qquad 0 \le t \le 1. \tag{8}$$

Then $\mathbf{H}$ is a selfadjoint and compact operator, and

$$\|\mathbf{H}\|_{L^2[0,1]} \le 2\int_0^1 |\mathrm{H}(s)|\,\mathrm{d}s \tag{9}$$

by results in Section 1 of Krein and Langer (1985). The following theorem is an immediate consequence of (4°) in Section 2 of Krein and Langer (1985, p. 324). The symbol $\mathbf{I}$ denotes the identity operator and $(\cdot,\cdot)_{L^2[0,1]}$ the scalar product in $L^2[0, 1]$.

Theorem 9. *Let C be a real even function on $[-1, 1]$ with accelerant* H *and $C'(0+) = -\frac{1}{2}$. If -1 is not an eigenvalue of* $\mathbf{H}$*, then C is a covariance function if and only if*

(i) *the operator $\mathbf{I} + \mathbf{H}$ in $L^2[0, 1]$ has no negative eigenvalues, and*

(ii) $C(0) \ge ((\mathbf{I} + \mathbf{H})^{-1}C', C')_{L^2[0,1]}$.

The lower bound on the right-hand side of the inequality can be computed as follows. First we determine the resolvent kernel Γ corresponding to H, that is, the unique solution of the equation

$$\Gamma(t,s) + \int_0^1 \mathrm{H}(t-u)\Gamma(u,s)\,\mathrm{d}u = \mathrm{H}(t-s), \qquad 0 \le s, t \le 1. \tag{10}$$

With Γ we associate the operator $\mathbf{\Gamma}$ in $L^2[0, 1]$, defined by

$$(\mathbf{\Gamma}\varphi)(t) = \int_0^1 \Gamma(t,s)\varphi(s)\,\mathrm{d}s, \qquad 0 \le t \le 1. \tag{11}$$

Then

$$((\mathbf{I} + \mathbf{H})^{-1}C', C')_{L^2[0,1]} = ((\mathbf{I} - \mathbf{\Gamma})C', C')_{L^2[0,1]}. \tag{12}$$

We close the section with the following, very general criterion. Additional information related to our approach is found in Sections 1.4 and 2.3 of Krein and Langer (1985).

Theorem 10. *If a real even function C on $[-1, 1]$ has an accelerant and*

$$\int_0^1 |C''(t)|\,\mathrm{d}t < -C'(0+), \tag{13}$$

then $C + r$ is a covariance function whenever $r \in \mathbb{R}$ is sufficiently large.

Proof. Without loss of generality we may assume that $-C'(0+) = \frac{1}{2}$. Then $\|\mathbf{H}\|_{L^2[0,1]} < 1$ in view of (13) and (9). Hence, the operator $\mathbf{I} + \mathbf{H}$ is positive and the assertion follows from Theorem 9.

4. Examples and applications

In this final section, we illustrate our findings with examples and applications. The first two examples are concerned with exponential variogram models and fractional Brownian motion, respectively. Then we turn to isotropic covariance functions of locally polynomial type, $C(\boldsymbol{h}) = \sum_{k=0}^{n} a_k |\boldsymbol{h}|^k$ for $\boldsymbol{h} \in \mathbb{R}^d$, $|\boldsymbol{h}| \leq 1$. Covariance models of this form have been fitted frequently; see Mitchell *et al.* (1990), Currin *et al.* (1991), Wiencek and Stoyan (1993), Onn *et al.* (1994), and the references in Gneiting (1999a). Section 4.3 discusses the quadratic case, and Section 4.4 characterizes locally cubic covariances. Our results complement previous work by Matheron (1974) and Mitchell *et al.* (1990).

4.1. Exponential variogram model

Perhaps the most often used variogram in geostatistics is the exponential model,

$$\gamma(\boldsymbol{h}) = \sigma^2(1 - \mathrm{e}^{-\lambda|\boldsymbol{h}|}), \qquad \boldsymbol{h} \in \mathbb{R}^d,$$

where σ^2 and λ are positive parameters. It is well known that $\mathrm{e}^{-\lambda|\boldsymbol{h}|}$ is a covariance function for $\boldsymbol{h} \in \mathbb{R}^d$. Thus,

$$C(t) = \sigma^2(\mathrm{e}^{-\lambda|t|} + r), \qquad -1 \leq t \leq 1, \tag{14}$$

is a covariance function whenever $r \geq 0$. We proceed to find the locally equivalent stationary covariance with the smallest attainable value of r. From Theorem 8 it is immediate that (14) is a covariance function whenever

$$r \geq p_\lambda = -\frac{1 - \mathrm{e}^{-\lambda}}{\lambda}.$$

To apply Theorem 9, we put $\sigma^2 = (2\lambda)^{-1}$ such that $\mathrm{H}(t) = -(\lambda/2)\,\mathrm{e}^{-\lambda|t|}$ for $t \neq 0$ and $C'(0+) = -\frac{1}{2}$. The unique solution of the integral equation (10) for the resolvent kernel Γ is

$$\Gamma(s,t) = -\frac{\lambda}{\lambda+2}(1 + \lambda \min(s,t))(1 + \lambda(1 - \max(s,t))), \qquad 0 \leq s,t \leq 1.$$

The covariance model (14) satisfies the inequality (13) and therefore condition (i) of Theorem 9. Using (12) and condition (ii), we find that (14) is a covariance function if and only if

$$r \geq r_\lambda = -\frac{2}{\lambda+2}.$$

It is interesting to observe that p_λ/r_λ is a decreasing function of $\lambda > 0$, with $p_\lambda/r_\lambda \to 1$ as $\lambda \downarrow 0$ and $p_\lambda/r_\lambda \to \frac{1}{2}$ as $\lambda \to \infty$.

4.2. Locally stationary representations of fractional Brownian motion

Fractional Brownian motion with index $\alpha \in (0,2)$ is the intrinsic Gaussian random function $Z(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^d$, with centered variogram

$$\gamma(\boldsymbol{h}) = |\boldsymbol{h}|^\alpha, \qquad \boldsymbol{h} \in \mathbb{R}^d.$$

Matheron (1974) studied the locally stationary representations of fractional Brownian motion. In a *tour de force*, he proved that

$$C(t) = A - |t|^\alpha, \qquad -1 \leq t \leq 1, \tag{15}$$

is a covariance function if and only if

$$A \geq \frac{1}{2^{\alpha}\pi^{1/2}}\Gamma\left(\frac{1+\alpha}{2}\right)\Gamma\left(1-\frac{\alpha}{2}\right). \tag{16}$$

Theorem 8 shows that if $\alpha \in (0, 1]$ then (15) is a covariance function whenever $A \geq (1+\alpha)^{-1}$. Taking $k = 0$ and $l = 1$ in Theorem 1.1 of Gneiting (2001), we see that if $\alpha \in (0, 2)$ then

$$C(t) = \begin{cases} \dfrac{(3-\alpha)(4-\alpha)}{3(2-\alpha)^2} - |t|^{\alpha}, & |t| \leq 1, \\ \dfrac{\alpha(2-\alpha)^2}{48}\left(\dfrac{4-\alpha}{2-\alpha} + 3|t|\right)\left(\dfrac{4-\alpha}{2-\alpha} - |t|\right)^3, & 1 \leq |t| \leq \dfrac{4-\alpha}{2-\alpha}, \\ 0, & |t| \geq \dfrac{4-\alpha}{2-\alpha}, \end{cases}$$

is a covariance function in $\mathbb{R}$. Thus locally stationary representations of fractional Brownian motion exist, and (15) is a covariance function if

$$A \geq \frac{(3-\alpha)(4-\alpha)}{3(2-\alpha)^2}.$$

While our approach does not yield Matheron's necessary and sufficient condition (16), it provides straightforward existence proofs for locally equivalent stationary covariances. As mentioned before, the turning bands operator allows for an immediate generalization to d-variate fractional Brownian motion. We refer the reader to Section 2 of Gneiting (2000) for further discussion.

4.3. Locally quadratic covariance functions

As a prelude to the following example, we consider the quadratic function

$$C(t) = \sigma^2(1 - b_1|t| + b_2t^2), \qquad -1 \leq t \leq 1. \tag{17}$$

In view of our discussion in Section 3.2 we may assume that $b_1 > 0$, and in order to apply Theorem 9 we put $\sigma^2 = (2b_1)^{-1}$. The associated accelerant is $\mathrm{H}(t) = -b_2/b_1$ for $t \neq 0$, and the unique eigenvalue of $\mathbf{H}$ is $-b_2/b_1$. It follows from condition (i) of the theorem that $b_2 \leq b_1$ is a necessary condition on (17) to be a covariance. Finally, for $b_2 < b_1$ the resolvent Γ is constant, equal to $b_2/(b_2 - b_1)$. Using (12), we find from condition (ii) and a continuity argument that (17) is a covariance function on $[-1, 1]$ if and only if

$$\tfrac{3}{2}b_1 - \tfrac{1}{2}(3b_1(8-b_1))^{1/2} \leq b_2 \leq b_1. \tag{18}$$

This recovers condition (3–1) of Matheron (1974) which is quoted by Chilès and Delfiner (1999, p. 268). Figure 1 illustrates the permissible region for the parameter values in the (b_1, b_2) plane.

4.4. Locally cubic covariance functions

We turn to the more general case of the cubic function

$$C(t) = r - \tfrac{1}{2}|t| + a_2t^2 + \varepsilon\frac{a_3^2}{12}|t|^3, \qquad -1 \leq t \leq 1, \tag{19}$$

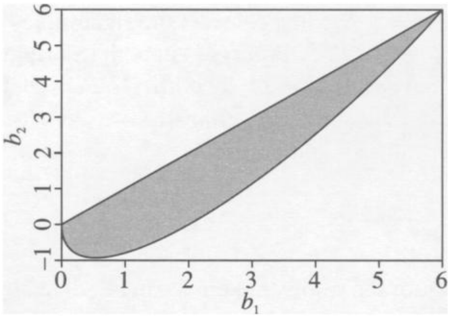

FIGURE 1: The admissible region (18) for the locally quadratic model (17).

where $a_3 \geq 0$ and ε is either 1 or -1. Using Theorem 9, we characterize covariance functions of the form (19). This leads to the differential equations solved below, and to conditions (25) and (30) for $\varepsilon = 1$ and (31) and (32) for $\varepsilon = -1$, respectively. In view of the turning bands operator, the result generalizes immediately to isotropic functions defined on balls in $\mathbb{R}^d$. See Matheron (1973), Section 7.4.2 of Chilès and Delfiner (1999) and Gneiting (1999a) for details.

The characterization of locally cubic covariance functions is also one of the main topics in the aforementioned report of Matheron (1974). The techniques used there differ from ours.

4.4.1. *Differential equations.* In view of Theorem 9 and (12), C is a covariance function if and only if the operator $\mathbf{I} + \mathbf{H}$ has no negative eigenvalues and

$$r \geq ((\mathbf{I} - \boldsymbol{\Gamma})C', C')_{L^2[0,1]}, \tag{20}$$

where $\mathbf{H}$ and $\boldsymbol{\Gamma}$ are defined by (8) and (11), respectively. If $-\mu^2$ is a negative eigenvalue of $\mathbf{H}$, then there exists an eigenfunction V such that

$$\mu^2 V(t) + \int_0^1 \mathrm{H}(t-u)V(u)\,\mathrm{d}u = 0, \qquad 0 \leq t \leq 1. \tag{21}$$

The equation implies that V is twice differentiable on [0, 1] and

$$\mu^2 V''(t) - \varepsilon a_3^2 V(t) = 0, \qquad 0 \leq t \leq 1. \tag{22}$$

To compute the right-hand side of (20) we determine the resolvent kernel $\Gamma(t, s)$, that is, the solution of the integral equation (10). The latter can be rewritten as

$$\Gamma(t,s) + \int_0^t \left(-2a_2 - \varepsilon\frac{a_3^2}{2}(t-u)\right)\Gamma(u,s)\,\mathrm{d}u + \int_t^1 \left(-2a_2 - \varepsilon\frac{a_3^2}{2}(u-t)\right)\Gamma(u,s)\,\mathrm{d}u + 2a_2 + \varepsilon\frac{a_3^2}{2}|t-s| = 0. \tag{23}$$

If $t \neq s$ then $\Gamma(t, s)$ is twice differentiable and

$$\frac{\partial^2\Gamma(t,s)}{\partial t^2} - \varepsilon a_3^2\Gamma(t,s) = 0. \tag{24}$$

4.4.2. *Characterization for* $\varepsilon = 1$. We first consider the eigenvalues of **H**. The general solution of (22) is $V(t) = c_1\,\mathrm{e}^{-a_3 t/\mu} + c_2\,\mathrm{e}^{a_3 t/\mu}$. From (21) in both its original and differentiated form, we find that $c_1 = c_2\,\mathrm{e}^{a_3/\mu}$ and $8a_2 + a_3^2 - 2a_3\mu\coth(a_3/2\mu) = 0$. Thus, **H** has eigenvalue -1 if and only if $a_2 = -\frac{1}{8}a_3^2 + \frac{1}{4}a_3\coth(a_3/2)$. Since $\nu \to \nu\coth(\nu^{-1})$ is isotone, the operator $\mathbf{I} + \mathbf{H}$ has no negative eigenvalues if and only if

$$a_2 \le -\tfrac{1}{8}a_3^2 + \tfrac{1}{4}a_3\coth\left(\frac{a_3}{2}\right). \tag{25}$$

The equations (23) and (24) for the resolvent kernel can be solved by standard techniques. We find that

$$\Gamma(t,s) = f(a_2,a_3)(\Gamma_1(t,s) + \Gamma_2(t,s)), \qquad 0 \le s,t \le 1, \tag{26}$$

where

$$\Gamma_1(t,s) = (8a_2 + a_3^2)(\cosh(a_3(1 - |s-t|)) + \cosh(a_3(1-s-t))), \tag{27}$$

$$\Gamma_2(t,s) + 2a_3(\sinh(a_3(|s-t|-1)) + \sinh(a_3|s-t|)), \tag{28}$$

and

$$\frac{a_3}{2}\frac{1}{f(a_2,a_3)} = (8a_2 + a_3^2)\sinh a_3 - 4a_3\cosh^2\frac{a_3}{2}. \tag{29}$$

The inequality (20) then yields

$$r \ge \tfrac{1}{4} + \tfrac{1}{2}a_2 + 4\frac{a_2^2}{a_3^2} + \tfrac{1}{48}a_3^2 - \frac{(a_3^2 + 8a_2)^2}{8a_3^3}\tanh\left(\frac{a_3}{2}\right). \tag{30}$$

We summarize that if $\varepsilon = 1$ then (19) is a covariance function if and only if (25) and (30) hold. This result is due to Matheron (1974) whose condition (3–3) is equivalent to (25) and (30). Note that Theorem 9 does not apply when equality holds in (25). However, in this case the sufficiency of (30) is obvious, because limits of covariance functions are covariance functions. The necessity of the condition follows from the fact that the class of covariance functions forms a convex cone.

4.4.3. *Characterization for* $\varepsilon = -1$. The general solution of the differential equation (22) is now $V(t) = c_1\sin(a_3 t/\mu) + c_2\cos(a_3 t/\mu)$. Arguments as before show that -1 is an eigenvalue of **H** unless $a_3 < \pi$ and $a_2 < \frac{1}{8}a_3^2 + \frac{1}{4}a_3\cot(a_3/2)$. We conclude that $\mathbf{I} + \mathbf{H}$ has no negative eigenvalues if and only if $a_3 \le \pi$ and

$$a_2 \le \tfrac{1}{8}a_3^2 + \tfrac{1}{4}a_3\cot\left(\frac{a_3}{2}\right). \tag{31}$$

It is then not difficult to check that the solution Γ to (23) and (24) is obtained from (26)–(29) if we replace each occurrence of a_3 by $\mathrm{i}a_3$. Similarly, the condition on r for $\varepsilon = -1$,

$$r \ge \tfrac{1}{4} + \tfrac{1}{2}a_2 - 4\frac{a_2^2}{a_3^2} - \tfrac{1}{48}a_3^2 + \frac{(a_3^2 - 8a_2)^2}{8a_3^3}\tan\left(\frac{a_3}{2}\right), \tag{32}$$

is obtained from (30) if we replace a_3 by $\mathrm{i}a_3$. The characterization is valid when equality holds in (31).

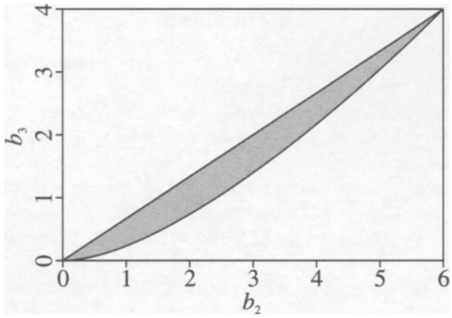

FIGURE 2: The admissible region (34) for the differentiable locally cubic model (33).

We note a discrepancy to Matheron's (1974) condition (3–6) which may result from a sign error in his report. To give an explicit example,

$$\begin{aligned} C(t) &= \tfrac{1}{4} - \tfrac{5}{384}\pi^2 - \tfrac{1}{2}|t| + \frac{\pi^2}{16}t^2 - \frac{\pi^2}{48}|t|^3 \\ &= \frac{\pi^2}{384}(1-2|t|)\left(\frac{5+c}{2} - 2|t|\right)\left(\frac{5-c}{2} - 2|t|\right), \qquad -1 \le t \le 1, \end{aligned}$$

where $c^2 = (45\pi^2 - 384)/\pi^2$, is obviously a covariance function because it is a product of three covariance functions. The parameter values satisfy (31) and (32) but not Matheron's condition (3–6).

4.4.4. *Differentiable, locally cubic covariance functions.* Theorem 9 does not apply to functions C which are differentiable at zero. However, if we return to the case $\varepsilon = 1$ in (19) and adopt Matheron's parameterization, $\alpha = a_3 > 0$, $A = 2r/a_3^2$ and $B = 4a_2/a_3^2$, we obtain differentiable functions in the limit as $\alpha \to \infty$. In terms of a more natural parameterization,

$$C(t) = \sigma^2(1 - b_2t^2 + b_3|t|^3), \qquad -1 \le t \le 1, \tag{33}$$

we find that (33) is a covariance function if

$$2 + b_2 - \tfrac{1}{3}(36 + 36b_2 - 3b_2^2)^{1/2} \le b_3 \le \tfrac{2}{3}b_2. \tag{34}$$

The associated region in the (b_2, b_3) plane is illustrated in Figure 2. Furthermore, it is easy to see that the upper bound is sharp, because $-C''(t) = 2b_2 - 6b_3|t|$ must be a covariance on $[-1, 1]$ too. In fact, (3–2) of Matheron (1974) shows that (34) characterizes covariance functions of the form (33). Mitchell *et al.* (1990) discuss differentiable, locally cubic covariances too, but omit the upper bound in the characterization. The condition cited in a subsequent paper (Currin *et al.* (1991)) is equivalent to (34) and complete.

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