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Polynomial covariance functions on intervals

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A characterization is presented of the class of stationary processes that have polynomial covariance functions of degree less than or equal to 4 on an interval. The results extend to isotropic random fields and have applications in spatial statistics.

Keywords: accelerant; correlation function; covariance matrix; Krein–Langer theory; locally polynomial; positive definite; turning bands

1. Introduction

Stationary Gaussian processes are characterized by their covariance function, and a plethora of statistical tools in time series analysis and spatial statistics are based on second-order properties. In this paper, we consider the class of stationary processes $Z(u)$, $0 \leqslant u \leqslant 1$, whose covariance function $C(t)$ is a polynomial, that is,

$$\operatorname{cov}(Z(u),\, Z(u+t)) = C(t), \qquad (0 \leqslant u \leqslant 1;\, 0 \leqslant u+t \leqslant 1),$$

where

$$C(t) = \sum_{i=0}^{k} b_i |t|^i \qquad (|t| \leqslant 1). \tag{1}$$

Covariance models of polynomial form have been fitted to geostatistical data in various applications, and we provide examples below. The statistical analysis of deterministic simulation experiments is another field where covariance models defined on intervals are of interest; see Mitchell *et al*. (1990) and the references therein. However, it is far from evident which conditions on the coefficients of the polynomial are to be imposed so that a stationary process $Z(u)$, $0 \leqslant u \leqslant 1$, with covariance function (1) exists. Clearly, such a process exists if and only if $C(t)$ is a positive definite function, and the associated analytical theory is detailed in Chapter 4 of Sasvári (1994).

The problem has a natural and practically relevant analogue for isotropic random fields defined on Euclidean balls in $\mathbb{R}^d$. These are of interest in geostatistics, where isotropic

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covariance functions are fitted to spatial data observed at scattered sites in d-dimensional Euclidean space $\mathbb{R}^d$; see, for example, Cressie (1993) or Chilès and Delfiner (1999). We may then assume that all spatial locations of interest are contained in a Euclidean ball of diameter δ in $\mathbb{R}^d$, and it suffices to consider covariance models defined for distances less than or equal to δ. Stol (1981) provides a list of references in the hydrological literature in which polynomial models of the form

$$C(x) = \sum_{i=0}^{k} b_i^{(d)} \|x\|^i \qquad (x \in \mathbb{R}^d;\ \|x\| \leqslant \delta) \tag{2}$$

are fitted to observed covariances between rainfall amounts measured in gauges at interstation distance $\|x\|$. Wiencek and Stoyan (1993) fit a polynomial covariance model of degree 4 to data from a simulation study for the Stienen model, a stationary and isotropic system of non-overlapping spheres in three-dimensional Euclidean space. We return to this example in Section 5.3 below. Further examples of the use of polynomial covariance models of the form (2) in spatial statistics are discussed by Gneiting (1999). The fitted polynomial model, then, is a valid covariance function if and only if it is positive definite, a property that in general is very difficult to check. Fortunately, Matheron's (1973) turning bands operator provides a way to reduce checks for positive definiteness in the general case (2) to checks for positive definiteness on the real line. If we put

$$b_i = \frac{\sqrt{\pi}\,\Gamma((d+i)/2)}{\Gamma(d/2)\Gamma((i+1)/2)} \delta^i b_i^{(d)} \qquad (i = 0, 1, \ldots, k), \tag{3}$$

then equation (4.1) of Matheron (1973), Theorem 3 of Gneiting (1999) and a straightforward scaling argument show that (2) is a covariance function in $\mathbb{R}^d$ if and only if (1) is a covariance function in $\mathbb{R}$. It is for this reason that we restrict our analytical discussion to covariance functions defined on intervals, even though the spatial case is of more immediate practical interest.

Matheron (1974) and Gneiting *et al.* (2001) characterized polynomial covariance functions of degree $k \leqslant 3$. Mitchell *et al.* (1990) considered the quintic case with vanishing linear and cubic terms. Our key result here is the characterization of covariance functions of the form

$$C(t) = r - \frac{1}{2}|t| + a_2 t^2 + \varepsilon \frac{a_3^2}{12}|t|^3 + \frac{a_4}{24} t^4 \qquad (|t| \leqslant 1), \tag{4}$$

where ε is either 1 or -1. This covers the quartic case except when the linear term vanishes. The characterization relies on functional analytic tools developed by Krein and Langer (1985) which we review in Section 2. The computations in Sections 3 and 4 establish the characterization, and Section 5 provides examples. At present we do not know of methods that give similar, comparably simple analytical results for higher polynomial orders, except for the aforementioned special case in Mitchell *et al.* (1990). Numerical checks of positive definiteness provide an alternative, and the paper concludes with a discussion of such an approach in Section 6.

2. Krein–Langer theory

Here we review our key tools, which are due to Krein and Langer (1985). An even continuous function C defined on $[-1, 1]$ is said to have an accelerant H if: (i) $H(t) = -C''(t)$ exists for $t \neq 0$; (ii) $H(t)$ is absolutely integrable over $[-1, 1]$; and (iii) $C'(0+) < 0$. As Heinz Langer pointed out to us, the term refers to the second derivative and its physical interpretation of acceleration. With the accelerant H we associate the operator $\mathbf{H}$ in $L^2[0, 1]$, defined by

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

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 $(\cdot, \cdot)_{L^2[0,1]}$ stands for the inner product in $L^2[0, 1]$. See also Section 3.4 of Gneiting *et al*. (2001).

Theorem 1 (Krein and Langer). *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) $C(0) \geqslant ((\mathbf{I} + \mathbf{H})^{-1} C', C')_{L^2[0,1]}$.

The inner product in condition (ii) can be computed as follows. First we determine the resolvent kernel Γ corresponding to H, that is, the unique solution to the integral equation

$$\Gamma(t, s) + \int_0^1 H(t-u)\Gamma(u, s)\mathrm{d}u = H(t-s) \qquad (0 < s, t < 1). \tag{5}$$

Under the conditions of the theorem, the resolvent kernel is real. To see this, consider the difference between (5) and its conjugate complex. If H is real then $\Gamma - \overline{\Gamma}$ must be zero, since otherwise it would be an eigenfunction with eigenvalue -1 of the operator $\mathbf{H}$. With Γ we associate the operator $\mathbf{\Gamma}$ in $L^2[0, 1]$, defined by

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

Then

$$((\mathbf{I} + \mathbf{H})^{-1} C', C')_{L^2[0,1]} = ((\mathbf{I} - \mathbf{\Gamma})C', C')_{L^2[0,1]}. \tag{6}$$

In the following we apply these results to quartic polynomials of the form (4). Section 3 characterizes the eigenvalues of the operator $\mathbf{I} + \mathbf{H}$, and Section 4 shows how to compute the inner product (6). The accelerant associated with the polynomial $C(t)$ in (4) is

$$H(t) = -2a_2 - \varepsilon \frac{a_3^2}{2}|t| - \frac{a_4}{2}t^2 \qquad (t \neq 0), \tag{7}$$

and we note that both $C'(t)$ and $H(t) = -C''(t)$ do not exist at $t = 0$.

3. Computing the eigenvalues

Condition (i) of the Krein–Langer theorem suggests that we characterize the eigenvalues of the operator $\mathbf{I}+\mathbf{H}$ when C and H are given by (4) and (7), respectively. To this end, let $-\mu^2$ be a negative eigenvalue of the operator $\mathbf{H}$. Then there exists an eigenfunction V such that

$$-\mu^2 V(t) = \int_0^1 H(t-u)V(u)\mathrm{d}u \qquad (0<t<1), \tag{8}$$

which implies that V is three (and in fact infinitely many) times differentiable on the open unit interval. Differentiating (8) with respect to t yields

$$\mu^2 V'(t) + \int_0^1 H'(t-u)V(u)\mathrm{d}u = 0. \tag{9}$$

Next we divide the integral on the left-hand side of (9) into two parts, the first from 0 to t and the second from t to 1. Differentiating a second time and plugging in the specific form of $H'(t)$ gives

$$\mu^2 V''(t) - a_4\int_0^1 V(u)\mathrm{d}u - \varepsilon a_3^2 V(t) = 0. \tag{10}$$

Differentiating yet another time yields

$$\mu^2 V'''(t) - \varepsilon a_3^2 V'(t) = 0 \qquad (0<t<1). \tag{11}$$

We assume now that a_3 is strictly positive and defer the case $a_3=0$ to Section 5.2. If $\varepsilon=1$, the general solution of the differential equation (11) is

$$V(t) = c_1 + c_2\mathrm{e}^{a_3 t/\mu} + c_3\mathrm{e}^{-a_3 t/\mu} \qquad (0<t<1). \tag{12}$$

We first put $c_3=0$ and check for the associated eigenvalues $-\mu^2$. Substituting (12) with $c_3=0$ into (10) with $t=1$, we are led to an expression for c_1 in terms of c_2. Then we substitute (12) with $c_3=0$ into (9) with $t=1$. Combining the two equations, we see that $-\mu^2$ is an eigenfunction for $\mathbf{H}$ if and only if

$$a_3(a_3^2+a_4)\coth\left(\frac{a_3}{2\mu}\right) + 2a_4\mu = 0, \tag{13}$$

where

$$\coth\left(\frac{a_3}{2\mu}\right) = \frac{\mathrm{e}^{a_3/(2\mu)}+\mathrm{e}^{-a_3/(2\mu)}}{\mathrm{e}^{a_3/(2\mu)}-\mathrm{e}^{-a_3/(2\mu)}} = \frac{1+\mathrm{e}^{-a_3/\mu}}{1-\mathrm{e}^{-a_3/\mu}}.$$

Putting $c_1=0$ or $c_2=0$ in (12) yields the same conclusion. Next we consider general coefficients in (12). Substituting (12) into (10) with $t=1$, we obtain

$$c_1 = -\frac{a_4\mu(c_2\mathrm{e}^{a_3/\mu} - c_2 + c_3 - c_3\mathrm{e}^{-a_3/\mu})}{a_3(a_3^2+a_4)}. \tag{14}$$

Then we substitute (12) and (14) into (9) with $t = 1$ to obtain

$$c_2 = c_3 \mathrm{e}^{-a_3/\mu} \tag{15}$$

and

$$c_1 = 2\frac{a_4 \mu c_3 (\mathrm{e}^{-a_3/\mu} - 1)}{a_3(a_3^2 + a_4)}. \tag{16}$$

Thus, we have expressed both c_1 and c_2 in terms of c_3. Finally, we substitute (12), (16) and (15) into (8) with $t = 1$ and simplify. This gives

$$6\mu a_3(a_3^2 + a_4)^2 \coth\left(\frac{a_3}{2\mu}\right) - 24\mu^2 a_3^2 a_4 - 12\mu^2 a_4^2 - 24 a_2 a_3^4 - 3a_3^6 - a_3^2 a_4^2 - 3a_3^4 a_4 = 0. \tag{17}$$

We conclude that the operator $\mathbf{I} + \mathbf{H}$ has no negative eigenvalues if and only if (13) and (17) do not admit solutions $\mu > 1$. Furthermore, -1 is an eigenvalue of the operator $\mathbf{H}$ if and only if $\mu = 1$ is a solution to (13) or (17). The preceding arguments exclude the case $a_3^2 + a_4 = 0$, in which similar computations show that all eigenvalues of $\mathbf{I} + \mathbf{H}$ are positive.

If $\varepsilon = -1$ the general solution to the differential equation (11) is

$$V(t) = c_1 + c_2 \mathrm{e}^{\mathrm{i} a_3 t/\mu} + c_3 \mathrm{e}^{-\mathrm{i} a_3 t/\mu}. \tag{18}$$

Proceeding as in the case where $\varepsilon = 1$, we substitute (18) into (10), (9) and (8) with $t = 1$. Again, we first put $c_3 = 0$, $c_2 = 0$ and $c_1 = 0$, respectively, and then consider general coefficients. It follows that the operator $\mathbf{I} + \mathbf{H}$ does not have negative eigenvalues if and only if $a_3 \leqslant \pi$ and the two equations

$$a_3\left(a_3^2 - a_4\right) \cot\left(\frac{a_3}{2\mu}\right) + 2a_4\mu = 0 \tag{19}$$

and

$$6\mu a_3\left(a_3^2 - a_4\right)^2 \cot\left(\frac{a_3}{2\mu}\right) + 24\mu^2 a_3^2 a_4 - 12\mu^2 a_4^2 - 24 a_2 a_3^4 + 3a_3^6 + a_3^2 a_4^2 - 3a_3^4 a_4 = 0 \tag{20}$$

do not admit solutions $\mu > 1$. Finally, -1 is an eigenvalue of the operator $\mathbf{H}$ if and only if a_3 is a multiple of π or $\mu = 1$ is a solution to (19) or (20). The computations leading to these results require that $a_3^2 \neq a_4$. If $a_3^2 = a_4$ then $\mathbf{I} + \mathbf{H}$ does not have negative eigenvalues if and only if $a_3 \leqslant \pi$, and -1 is an eigenvalue of $\mathbf{H}$ if and only if a_3 is a multiple of π.

4. Computing the inner product

The second condition in Theorem 2 leads us to the calculation of the inner product on the left-hand side of (6). Let C and H be given by (4) and (7), respectively. We first find the resolvent kernel Γ, that is, the unique solution to (5). Plugging in the accelerant (7) and partitioning the integral on the left-hand side of (5) yields

$$\Gamma(t, s) + \int_0^t \left(-2a_2 - \varepsilon\frac{a_3^2}{2}(t-u) - \frac{a_4}{2}(t-u)^2\right)\Gamma(u, s)\mathrm{d}u \tag{21}$$

$$+ \int_t^1 \left(-2a_2 - \varepsilon\frac{a_3^2}{2}(u-t) - \frac{a_4}{2}(t-u)^2\right)\Gamma(u, s)\mathrm{d}u = -2a_2 - \varepsilon\frac{a_3^2}{2}|t-s| - \frac{a_4}{2}(t-s)^2,$$

thereby showing that $\Gamma(t, s)$ is smooth and differentiable infinitely often away from $t = s$. Differentiating three times with respect to t, we obtain

$$\frac{\partial^3}{\partial t^3}\Gamma(t, s) - \varepsilon a_3^2 \frac{\partial}{\partial t}\Gamma(t, s) = 0 \qquad (0 < s,\ t < 1;\ s \neq t). \tag{22}$$

Indeed, if $s > t$, differentiating both sides of (21) with respect to t yields

$$\frac{\partial}{\partial t}\Gamma(t, s) - \varepsilon\frac{a_3^2}{2}\int_0^t \Gamma(u, s)\mathrm{d}u + \varepsilon\frac{a_3^2}{2}\int_t^s \Gamma(u, s)\mathrm{d}u + \varepsilon\frac{a_3^2}{2}\int_s^1 \Gamma(u, s)\mathrm{d}u \tag{23}$$

$$-a_4\int_0^t (t-u)\Gamma(u, s)\mathrm{d}u - a_4\int_t^s (t-u)\Gamma(u, s)\mathrm{d}u - a_4\int_s^1 (t-u)\Gamma(u, s)\mathrm{d}u = \varepsilon\frac{a_3^2}{2} - a_4(t-s),$$

where we partition the third integral on the left-hand side of (21). Differentiating once more with respect to t gives

$$\frac{\partial^2}{\partial t^2}\Gamma(t, s) - \varepsilon a_3^2 \Gamma(t, s) - a_4\int_0^s \Gamma(u, s)\mathrm{d}u - a_4\int_s^1 \Gamma(u, s)\mathrm{d}u + a_4 = 0, \tag{24}$$

and differentiating yet another time leads to (22). If $s < t$, we obtain analogously

$$\frac{\partial}{\partial t}\Gamma(t, s) - \varepsilon\frac{a_3^2}{2}\int_0^s \Gamma(u, s)\mathrm{d}u - \varepsilon\frac{a_3^2}{2}\int_s^t \Gamma(u, s)\mathrm{d}u + \varepsilon\frac{a_3^2}{2}\int_t^1 \Gamma(u, s)\mathrm{d}u \tag{25}$$

$$-a_4\int_0^s (t-u)\Gamma(u, s)\mathrm{d}u - a_4\int_s^t (t-u)\Gamma(u, s)\mathrm{d}u - a_4\int_t^1 (t-u)\Gamma(u, s)\mathrm{d}u = -\varepsilon\frac{a_3^2}{2} - a_4(t-s),$$

once again leading to (24) and (22).

As in Section 3, we assume that $a_3 > 0$ and defer the case $a_3 = 0$ to Section 5.2. If $\varepsilon = 1$, the general solution to the differential equation (22) is

$$\Gamma(t, s) = c_0(s) + c_+(s)\mathrm{e}^{a_3 t} + c_-(s)\mathrm{e}^{-a_3 t} \qquad (0 < s,\ t < 1;\ s \neq t).$$

To determine the constants, we put $s = 0$ and find $\Gamma(t, 0)$ first. Then (22) takes the form

$$\frac{\mathrm{d}^3}{\mathrm{d}t^3}\Gamma(t, 0) - a_3^2\frac{\mathrm{d}}{\mathrm{d}t}\Gamma(t, 0) = 0 \qquad (0 < t < 1),$$

the general solution to which is

$$\Gamma(t, 0) = c_0 + c_+\mathrm{e}^{a_3 t} + c_-\mathrm{e}^{-a_3 t}. \tag{26}$$

We substitute (26) into (25), (24) and (21) with $t = 1$ and simplify. Putting $f_0(a_3, a_4) = a_3(a_3^2 + a_4)\coth(a_3/2) - 2a_4$,

$$f_1(a_2, a_3, a_4) = 6a_3\left(a_3^2 + a_4\right)^2 \coth\left(\frac{a_3}{2}\right) - 24a_3^2a_4 - 12a_4^2 - 24a_2a_3^4 - 3a_3^6 - a_3^2a_4^2 - 3a_3^4a_4,$$

and

$$f_2(a_2, a_3, a_4) = -\frac{a_3^2}{f_0(a_3, a_4)f_1(a_2, a_3, a_4)(1 - e^{a_3})^2}$$
$$\times \left[6a_4\left((a_3^2 + a_4)^2 + 2a_3a_4 + 4a_2a_3^3\right)(1 - e^{a_3}) + a_3\left(3a_3^6 + 6a_3^4a_4 + 6a_3^2a_4^2 + 2a_4^3\right)(1 + e^{a_3})\right.$$
$$+ a_3^2a_4^3 + 2a_3a_4^3 + 4a_3^4a_4^2 + 6a_3^3a_4^2 + 12a_3^2a_4^2 + 6a_3^6a_4 + 6a_3^5a_4 + 12a_3^4a_4 + 24a_2a_3^4a_4$$
$$\left.+ 3a_3^8 + 24a_2a_3^6\right],$$

we find that the coefficients in (26) are

$$c_0 = 6a_4\frac{f_0(a_3, a_4)}{f_1(a_2, a_3, a_4)}, \qquad c_+ = f_2(a_2, a_3, a_4), \qquad c_- = f_2(a_2, -a_3, a_4).$$

Notice that $f_0(a_3, a_4) = 0$ if and only if $\mu = 1$ is a solution to (13), and $f_1(a_2, a_3, a_4) = 0$ if and only if $\mu = 1$ is a root of (17). In other words, our expressions are well-defined unless -1 is an eigenvector of $\mathbf{H}$ and Theorem 1 does not apply. Finally, we put

$$g(t, s) = \Gamma(1 - t, 0)\Gamma(1 - s, 0) - \Gamma(t, 0)\Gamma(s, 0) \tag{27}$$

and obtain $\Gamma(t, s)$ from $\Gamma(t, 0)$. Under the conditions of Theorem 1, Corollary 1.1 of Krein and Langer (1985) implies that

$$\Gamma(t, s) = \Gamma(|t - s|, 0) + \int_0^{\min(s,t)} g(t - r, s - r)\mathrm{d}r \qquad (0 < s,\ t < 1). \tag{28}$$

If $\varepsilon = -1$, we may replace a_3 by $\mathrm{i}a_3$ in the solution for the case $\varepsilon = 1$. Specifically, the solution $\Gamma(t, 0)$ to the differential equation

$$\frac{\mathrm{d}^3}{\mathrm{d}t^3}\Gamma(t, 0) + a_3^2\frac{\mathrm{d}}{\mathrm{d}t}\Gamma(t, 0) = 0 \qquad (0 < t < 1)$$

is of the general form $\Gamma(t, 0) = c_0 + c_+e^{\mathrm{i}a_3t} + c_-e^{-\mathrm{i}a_3t}$, and substitution into (25), (24) and (21) with $t = 1$ shows that

$$c_0 = 6a_4\frac{f_0(\mathrm{i}a_3, a_4)}{f_1(a_2, \mathrm{i}a_3, a_4)}, \qquad c_+ = f_2(a_2, \mathrm{i}a_3, a_4), \qquad c_- = f_2(a_2, -\mathrm{i}a_3, a_4).$$

Using (27) and (28) and the trigonometric form of the resolvent kernel,

$$\Gamma(t, 0) = c_0 + 2\,\mathrm{Re}(c_+)\cos(a_3t) - 2\,\mathrm{Im}(c_+)\sin(a_3t),$$

we find the solution $\Gamma(t, s)$ to the integral equation (5) and subsequently the inner product on the right-hand side of (6).

5. Examples and special cases

Given numerical values of a_2, a_3 and a_4, the previous two sections show us how to check whether or not the polynomial (4) is a covariance function. In the case where $\varepsilon = 1$, we find the roots of (13) and (17), respectively. If roots $\mu > 1$ exist, then (4) is not a covariance function. If all roots are smaller than 1, we proceed to compute the inner product (6) as detailed in the preceding section. By the Krein–Langer theorem, the polynomial $C(t)$ in (4) is a covariance function if and only if $C(0)$ is greater than or equal to the value of the inner product (6). This procedure works unless (17) or (20) respectively admits the exact root $\mu = 1$, a case which seems irrelevant in practice and can usually be dealt with by a continuity argument. If $\varepsilon = -1$ in (4), we proceed analogously. Ready-to-use Maple worksheets are available from Tilmann Gneiting.

In the following, we give three examples. The first concerns the case where $a_4 = 0$ vanishes and recovers the key result of Gneiting *et al*. (2001). The second discusses the case $a_3 = 0$, which was omitted in the previous two sections. Our third and final example turns to applications in spatial statistics.

5.1. Vanishing quartic term

Here we consider the cubic polynomial

$$C(t) = r - \frac{1}{2}|t| + a_2 t^2 + \varepsilon \frac{a_3^2}{12}|t|^3 \qquad (|t| \leqslant 1), \tag{29}$$

that is, the case where $a_4 = 0$ and $a_3 > 0$ in (4). If $\varepsilon = 1$, (13) does not have positive roots and (17) simplifies to

$$6\mu a_3^5 \coth\left(\frac{a_3}{2\mu}\right) - 24 a_2 a_3^4 - 3a_3^6 = 0. \tag{30}$$

Notice that $\mu = 1$ is a solution to (30) if

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

Furthermore, the left-hand side of (30) is an increasing function of μ. Thus, (30) does not admit solutions $\mu > 1$ if and only if

$$a_2 \leqslant -\frac{1}{8}a_3^2 + \frac{1}{4}a_3 \coth\left(\frac{a_3}{2}\right). \tag{31}$$

The calculations in Section 4 simplify and eventually imply that (29) is a covariance function if and only if (31) holds and

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

The case $\varepsilon = -1$ is analogous, and we recover the results in Section 4.4 of Gneiting *et al.* (2001).

5.2. Vanishing cubic term

Here we consider the case $a_3 = 0$ which we skipped in Sections 3 and 4. For functions of the form

$$C(t) = r - \frac{1}{2}|t| + a_2 t^2 + \frac{a_4}{24} t^4 \qquad (|t| \leqslant 1), \tag{32}$$

the differential equation (11) for an eigenfunction V with eigenvalue $-\mu^2$ for the operator $\mathbf{H}$ reduces to

$$\mu^2 V'''(t) = 0 \qquad (0 < t < 1),$$

the general solution to which is

$$V(t) = c_0 + c_1 t + \frac{c_2}{2} t^2 \qquad (0 < t < 1).$$

We proceed as in Section 3. First we put $c_2 = 0$ and find that $V(t) = 1 - 2t$ is an eigenfunction to the operator $\mathbf{H}$ with eigenvalue $a_4/12$. Thus, we require that $a_4 \geqslant -12$. Putting $c_1 = 0$ or $c_0 = 0$, respectively, does not yield additional constraints. Then we consider general coefficients, express c_0 and c_1 in terms of c_2, and substitute into (8) with $t = 1$. We conclude that $-\mu^2$ is an eigenvalue for $\mathbf{H}$ if and only if

$$720\mu^4 - 1440 a_2 \mu^2 - 60 a_4 \mu^2 - a_4^2 = 0.$$

It follows that the operator $\mathbf{I} + \mathbf{H}$ does not have negative eigenvalues if and only if $a_4 \geqslant -12$ and

$$a_2 \leqslant \frac{1}{2} - \frac{1}{24} a_4 - \frac{1}{1440} a_4^2. \tag{33}$$

Similarly, the differential equation (22) for the resolvent kernel $\Gamma(t, s)$ reduces to

$$\frac{\partial^3}{\partial t^3} \Gamma(t, s) = 0 \qquad (0 < s,\ t < 1;\ s \neq t).$$

Proceeding as in Section 4, we find that

$$\Gamma(t, 0) = c_0 + c_1 t + \frac{1}{2} c_2 t^2 \qquad (0 < t < 1), \tag{34}$$

where

$$c_0 = \frac{-9\,(1920a_2 + 640a_2a_4 + 48a_4^2 + a_4^3)}{(12 + a_4)(720 - 1440a_2 - 60a_4 - a_4^2)},$$

$$c_1 = \frac{36a_4(240a_2 + 30a_4 + a_4^2)}{(12 + a_4)(720 - 1440a_2 - 60a_4 - a_4^2)},$$

$$c_2 = \frac{-60a_4(12 + a_4)}{720 - 1440a_2 - 60a_4 - a_4^2};$$

and the general expression for $\Gamma(t, s)$ follows readily from (27) and (28). Computing the scalar product (6) yields

$$r \geqslant \frac{1}{100\,800}\,\frac{302\,400 - 604\,800a_2 + 403\,200a_2^2 + 10\,080a_2a_4 + 180a_4^2 + a_4^3}{12 + a_4}. \tag{35}$$

Specifically, if $a_4 = 0$ then (32) is a covariance function if and only $a_2 \leqslant \frac{1}{2}$ and

$$r \geqslant \frac{1}{4} + \frac{1}{3}a_2^2 - \frac{1}{2}a_2,$$

which recovers the result in Section 4.3 of Gneiting *et al*. (2001). If $a_2 = 0$ then (32) is a covariance function if and only if $-12 < a_4 \leqslant -30 + 18\sqrt{5}$ and

$$r \geqslant \frac{1}{100\,800}\,\frac{302\,400 + 180a_4^2 + a_4^3}{12 + a_4}.$$

We return to this latter case in Section 6.

5.3. A spatial example

Wiencek and Stoyan (1993) fit a polynomial covariance function to data from a simulation study for the Stienen model, a stationary and isotropic system of non-overlapping spheres in three-dimensional Euclidean space. Their covariance model reads

$$C(x) = 0.125 - 1.828\|x\| + 1.642\|x\|^2 + 98.247\|x\|^3 - 400.320\|x\|^4 \quad (x \in \mathbb{R}^3;\ \|x\| \leqslant 0.12). \tag{36}$$

Here and in the following the reported numerical values are truncated, even though we used 500-digit precision in the computations. The turning bands equation (3) reduces to $b_i = (i + 1)\delta^i b_i^{(3)}$ if $d = 3$. Thus, the fitted model (36) is a covariance function in three-dimensional space if and only if

$$C(t) = 0.142 - \frac{1}{2}\,|t| + 0.0808\,t^2 + 0.774\,|t|^3 - 0.473\,t^4 \quad (|t| \leqslant 1) \tag{37}$$

is a covariance function on the real line. Returning to the notation in (4), we put

$$a_2 = 0.080\,84, \qquad a_3 = 3.047\,49, \qquad a_4 = -11.352\,61, \tag{38}$$

and find the values of $r > 0$ for which

$$C(t) = r - \frac{1}{2}|t| + a_2 t^2 + \frac{a_3^2}{12}|t|^3 + \frac{a_4}{24}t^4 \qquad (|t| \leqslant 1) \tag{39}$$

is a covariance function. This corresponds to the $\varepsilon = 1$ case, and it is straightforward to check that (13) and (17) do not admit roots $\mu \geqslant 1$. From equations (28) and (6) and condition (ii) of Theorem 1 we conclude that (39) with the numerical values in (38) is a covariance function if and only if $r \geqslant 0.110\,94$. This confirms the validity of the covariance model (37) and thereby the permissibility of the three-dimensional model (36) fitted by Wiencek and Stoyan (1993).

6. Discussion

In the preceding sections we have characterized covariance functions that are polynomials of degree less than or equal to 4 on intervals. Our results cover the quartic case except when the linear term vanishes. The technical difficulties in characterizing polynomial covariance functions of higher orders are considerable with our approach. At present we do not know of methods that give similar, comparably simple analytical results for higher orders, except for the quintic case with vanishing linear and cubic terms which was settled by Mitchell *et al*. (1990). Related results are given in Lasinger (1993).

Another approach to checking positive definiteness proceeds numerically, using the fact that if the function C on $[-1, 1]$ is a covariance function, then the $(n+1) \times (n+1)$ Toeplitz matrix

$$M_n(C) = \left(C\left(\frac{1}{n}(i-j)\right)\right)_{i,j=0}^{n} \tag{40}$$

is non-negative definite for $n = 1, 2, \ldots$. For a given function C defined on $[-1, 1]$, put

$$C_r(t) = C(t) - C(0) + r \qquad (|t| \leqslant 1)$$

such that $C_r(0) = r$. If C has an accelerant and regularity conditions hold, the Krein–Langer theorem implies that there exists a positive constant r_∞ such that C_r is a covariance function if and only if $r \geqslant r_\infty$, where

$$r_\infty = \inf\{r \in \mathbb{R} : C_r \text{ is a positive definite function}\}.$$

A straightforward heuristic approximation to r_∞ can be computed as follows. For $n = 1, 2, \ldots,$ define

$$r_n = \sup\{r \in \mathbb{R} : M_n(C_r) \text{ has a negative eigenvalue}\}.$$

We expect that $r_n \to r_\infty$ as $n \to \infty$; and if n is reasonably large we expect that r_n will be a good approximation to r_∞. The following theorem provides a rigorous result.

Theorem 2. *If C is a continuous function on $[-1, 1]$ and there exists a positive number r_∞ such that C_r is a covariance function if and only if $r \geqslant r_\infty$, then* $\lim_{n\to\infty} r_n = r_\infty$.

Proof. It suffices to prove that whenever $r < r_\infty$, the Toeplitz matrix $M_n(C_r)$ in (40) has at least one negative eigenvalue for sufficiently large n. To this end, let $r < r_\infty$. Since C_r is not a positive definite function, there exist a positive integer m and numbers $x_1, \ldots, x_m \in [0, 1]$ such that the matrix

$$(C_r(x_i - x_j))_{i,j=1}^m$$

has a negative eigenvalue. By continuity, there exists a positive number ϵ such that the matrix

$$(C_r(y_i - y_j))_{i,j=1}^m$$

has a negative eigenvalue whenever $y_1, \ldots, y_m \in [0, 1]$ satisfy $|y_i - x_i| < \epsilon$ for $i = 1, \ldots, m$. The initial assertion now follows from the fact that for sufficiently large n the set

$$\left\{\frac{k}{n} : k = -n, \ldots, n\right\} \cap (x_i - \epsilon, x_i + \epsilon)$$

is non-empty, for all $i = 1, \ldots, m$. The proof is complete. □

Tables 1 and 2 summarize the results of four numerical experiments performed by the authors. Table 1 gives the parameter values for the quartic polynomial (39). Evidently, cases (ii) and (iii) are associated with Section 5.2, and case (iv) returns us to the spatial example of Wiencek and Stoyan (1993) in Section 5.3. Table 2 compares the values of r_n for $n = 10$, 20, 30, 40 and 50 to the analytical lower bounds r_∞ which we obtained with the methods of Sections 4 and 5. In the entries for r_n the numerical values are truncated, but the last digit is sharp, and we performed the eigenvalue calculations with 500-digit

Table 1. Numerical values of the parameters in (39) used in four numerical experiments

Case	(i)	(ii)	(iii)	(iv)
a_2	0	0	0	0.080 84
a_3	1	0	0	3.047 49
a_4	−1	−10	10	−11.352 61

Table 2. The lower bounds r_n ad r_∞ as defined in the text

Case	(i)	(ii)	(iii)	(iv)
r_{10}	0.229 987	1.517 54	0.144 01	0.110 48
r_{20}	0.229 992	1.567 00	0.144 70	0.110 82
r_{30}	0.229 993	1.567 57	0.144 82	0.110 88
r_{40}	0.229 993	1.579 95	0.144 87	0.110 91
r_{50}	0.229 994	1.581 52	0.144 89	0.110 92
r_∞	$\frac{1}{1440}\,\frac{373\mathrm{e} - 1583}{\mathrm{e} - 1}$	$\frac{1597}{1008}$	$\frac{1607}{11\,088}$	0.110 94

precision. The results are quite encouraging, especially in view of the low values of n that we used. For polynomial functions of higher order, we expect numerical checks of this type to provide reasonably accurate lower bounds on r_∞, too.

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