Chapter 2
Construction of Covariance Functions and Unconditional Simulation of Random Fields

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Abstract Covariance functions and variograms are the most important ingredients in the classical approaches to geostatistics. We give an overview over the approaches how models can be obtained. Variant types of scale mixtures turn out to be the most important way of construction. Some of the approaches are closely related to simulation methods of unconditional Gaussian random field, for instance the turning bands and the random coins. We discuss these methods and complement them by an overview over further methods.

2.1 Introduction

Random fields are used to model regionalized variables [65] such as temperature, humidity, soil moisture, wave heights or metal concentrations of reservoirs, to mention a few. A random field, Z say, can be seen as a random real function on $\mathbb{R}^d$, or as a bundle of dependent random variables $Z(x)$, indexed by $x \in \mathbb{R}^d$. Assuming that the variances exist, such a random field can be characterized by its expectation and its covariance function

$$C(x, y) = \operatorname{cov}(Z(x), Z(y)), \qquad x, y \in \mathbb{R}^d.$$

These two characteristics determine the random field uniquely if the field is Gaussian, i.e. if $(Z(x_1), \ldots, Z(x_n))$ has a multivariate Gaussian distribution for any $x_i \in \mathbb{R}^d$ and $n \in \mathbb{N}$. Considering the variances of linear combinations $\sum_{k=1}^{n} a_k Z(x_k)$ with $a_k \in \mathbb{R}$ and $x_k \in \mathbb{R}^d$, we get that

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E. Porcu et al. (eds.), *Advances and Challenges in Space-time Modelling of Natural Events*, Lecture Notes in Statistics 207, DOI 10.1007/978-3-642-17086-7_2,

$$\sum_{k=1}^{n} \sum_{j=1}^{n} a_k \, C(x_k, x_j) \, a_j \geq 0 \qquad \text{for all } x_k \in \mathbb{R}^d, \, a_k \in \mathbb{R}, \text{ and for all } n \in \mathbb{N}. \tag{2.1}$$

Hence, $C(x, y)$ cannot be any arbitrary function. On the other hand, Kolmogorov's existence theorem (cf. [9], for instance) shows that if a symmetric, real-valued function C satisfies (2.1) then at least a Gaussian random field exists that has C as covariance function. Note that not all covariance functions are compatible with a given marginal distribution. For instance, a log-Gaussian process on the real axis cannot have the cosine as covariance function [1, 68].

Beyond characterizing (Gaussian) random fields from both a practical and a theoretical point of view, covariance functions are the key elements to determine likelihoods, to perform simulations and to spatially interpolate data (kriging).

In this chapter, we concentrate on the construction of covariance functions. In Sect. 2.2, we give methods that are as elementary as important. Sections 2.3–2.5 introduce the spectral approach, the convolutions, and the power series. The approaches in Sects. 2.2–2.4 are closely related to simulation methods for unconditional Gaussian random fields. Hence, they are presented on the way. Unconditional simulations are the key ingredients for conditional simulations [55] and are used for simulation studies. Scale mixtures, discussed in Sect. 2.6, allow for an elegant way to construct models. In particular, scale mixtures of the "Gaussian" covariance model, $C(x, y) = \exp(-\|x - y\|)^2)$, play an exceptional role. The turning bands method, presented in Sect. 2.7, is primarily a simulation method, but also defines a way to construct covariance models. In Sect. 2.8, the *montée* is presented. Section 2.9 gives an overview over simulation methods that are not related to the construction of covariance functions. Sections 2.10 and 2.11 deal with the advanced topics of space-time covariance functions and multivariate covariance models. Some excercises are given in section 2.12.

Henceforth, we will always assume that the expectation of the random field is zero. Translation invariant covariance functions, i.e. covariance functions C with $C(x, y) = \varphi(x - y)$ for some function $\varphi : \mathbb{R}^d \to \mathbb{R}$, play a dominant role when modelling spatial data. In this case, the function φ is called a positive definite function. A corresponding random field is called (weakly) stationary. If, furthermore, the covariance function is motion invariant, i.e. $C(x, y) = \tilde{\varphi}(\|x - y\|)$ for some function $\tilde{\varphi} : [0, \infty) \to \mathbb{R}$, then the corresponding random field is called (weakly) stationary and isotropic. Henceforth, $\|\cdot\|$ will always denote the Eucledian distance.

If $Z(x + h) - Z(x)$ is weakly stationary for all $h \in \mathbb{R}^d$, then the random field Z is called intrinsically stationary and the (uncentred) (semi-)variogram γ is used to characterize the random field:

$$\gamma(h) = \frac{1}{2} \, \mathbb{E}(Z(h) - Z(0))^2.$$

Matheron [66] shows that a function $\gamma : \mathbb{R}^d \to [0, \infty)$ is a variogram if and only if $\gamma(0) = 0$ and γ is conditionally negative definite, i.e., γ is symmetric and

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j \gamma(x_i - x_j) \le 0 \quad \text{for all } x_i \in \mathbb{R}^d, a_i \in \mathbb{R} \text{ with } \sum_{i=1}^{n} a_i = 0, n \in \mathbb{N}. \tag{2.2}$$

If Z is even weakly stationary then $\gamma(h) = \varphi(0) - \varphi(h)$.

For theoretical considerations, we will also consider complex valued random fields and hence complex-valued covariance functions C, i.e., functions that satisfy

$$\sum_{k=1}^{n}\sum_{j=1}^{n} a_k\, C(x_k, x_j)\, \overline{a_j} \ge 0 \qquad \text{for all } x_k \in \mathbb{R}^d, a_k \in \mathbb{C}, \text{and for all } n \in \mathbb{N}. \tag{2.3}$$

[78] shows that any complex valued function satisfying (2.3) is Hermitian.

Complementaries and applications are given, for instance, in the books of [15], [18], and [55]. Related review papers are given by [36] and [60], for example. See also the technical report by [84].

Most of the models, many construction principles and nearly all simulation methods given here are available within the R package RandomFields of [87].

2.2 Basic Constructions of Positive Definite Functions

A simple, but also important example of a covariance function is the scalar product $C(x, y) = \langle x, y\rangle$. Most generally, let $H : \mathbb{R}^d \to \mathscr{H}$ be a mapping into a Hilbert space $\mathscr{H}$. Then

$$C(x, y) = \langle H(x), H(y)\rangle_{\mathscr{H}} \tag{2.4}$$

is a covariance function. This representation of covariance functions is used particularly in machine learning, see [27] and [95], for instance. As a consequence, the function

$$C(x, y) = e^{i\langle t, x-y\rangle} \tag{2.5}$$

is a covariance function for any fixed $t \in \mathbb{R}^d$. Here, i is the imaginary number.

Further, if C is a covariance function on $\mathbb{R}^d$ and A is a linear mapping from $\mathbb{R}^m$ into $\mathbb{R}^d$, then $C(A\cdot, A\cdot)$ is a covariance function on $\mathbb{R}^m$. In particular, rescaling $C(s\cdot, s\cdot)$, $s > 0$, does not change the property (2.1).

Remark 2.1. If A has full rank then the corresponding random field is called geometrically anisotropic, otherwise zonally anisotropic. Such kind of anisotropies are frequently assumed due to preferential directions of underlying processes. Note that the zonal anisotropy implies that if $\tilde{\varphi}(\|\cdot\|)$ is a positive definite function in $\mathbb{R}^d$ so is $\tilde{\varphi}(\|\cdot\|)$ in $\mathbb{R}^k$ with $k < d$.

Also sums and products of covariance functions are again covariance functions [15, 18]. This can easily be seen by considering sums and products of respective independent random fields. In particular, vC is a covariance function for any constant $v \geq 0$ since a non-negative constant function is positive definite.

Assume C_n is a sequence of covariance functions that converges pointwise to some function C,

$$C(x, y) = \lim_{n \to \infty} C_n(x, y), \qquad x, y \in \mathbb{R}^d. \tag{2.6}$$

Then, it can be easily seen that condition (2.1) holds also for C if $C(x, x)$ is finite for all $x \in \mathbb{R}^d$.

These basic construction principles for covariance functions already allow us to create many classes of covariance functions.

2.3 Spectral Representation

Equations (2.5) and (2.6), or (2.4) with a suitably defined scalar product, yield that

$$\varphi(h) = \int_{\mathbb{R}^d} e^{i\langle \omega, h \rangle} \mu(d\omega) \tag{2.7}$$

is a positive definite, complex valued function for any finite, non-negative measure μ on $\mathbb{R}^d$. For real-valued random fields we have

$$\varphi(h) = \int_{\mathbb{R}^d} \cos(\langle \omega, h \rangle) \mu(d\omega).$$

It is easy to see that φ is uniformly continuous. Bochner's celebrated theorem [10, 11] gives the reverse statement, namely that all continuous positive definite functions have a unique representation (2.7).

The representation (2.7) allows for an immediate simulation procedure. Let $Z(x) = \sqrt{\mu(\mathbb{R}^d)} e^{i(\langle R, x \rangle + \Phi)}$ or $Z(x) = \sqrt{\mu(\mathbb{R}^d)} \cos(\langle R, x \rangle + \Phi)$ where $\Phi \sim U[0, 2\pi)$ and $R \sim \mu / \mu(\mathbb{R}^d)$ are independent. Then Z is (strongly) stationary, i.e., the finite dimensional distributions of $(Z(x))_{x \in \mathbb{R}^d}$ and $(Z(x+h))_{x \in \mathbb{R}^d}$ are the same for any $h \in \mathbb{R}^d$. The marginal distributions are not multivariate Gaussian. However, an approximation Z' to a Gaussian random field is obtained if Z_i, $i = 1, \ldots, n$, are independent and identically distributed according to Z and $Z' = n^{-1/2} \sum_{i=1}^n Z_i$ for some n large enough.

Example 2.1. The important Whittle-Matérn model [44, 62, 90],

$$W_\nu(h) = 2^{1-\nu} (\Gamma(\nu))^{-1} \|h\|^\nu K_\nu(\|h\|), \qquad \nu > 0, \tag{2.8}$$

has spectral density

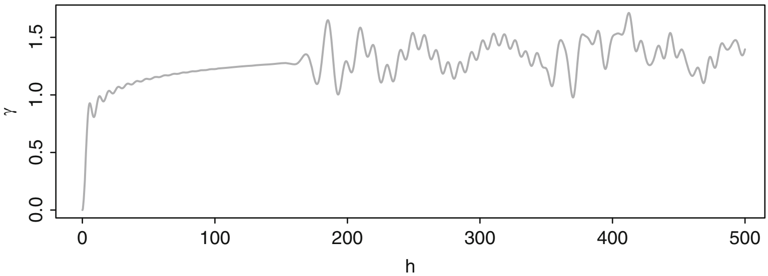

Fig. 2.1 A variogram in $\mathbb{R}$ constructed by an infinite sum over cosine functions, see example 2.2

$$\frac{d\mu(\omega)}{d\omega} = \frac{\Gamma(\nu + d/2)}{\Gamma(\nu)\pi^{d/2}(1 + \|\omega\|^2)^{\nu+d/2}}.$$

Here, Γ is the Gamma function and K_ν is a modified Bessel function of the second kind.

Example 2.2. Variograms with exceptional properties can be obtained by sums of cosine functions. However, they do not have any practical relevance. Let

$$\gamma(h) = \sum_{k=1}^{\infty} a_k(1 - \cos(h/b_k)).$$

If $a_k = 1$ and $b_k = k!$ then $\liminf_{h\to\infty} \gamma(h) = 0$ and $\limsup_{h\to\infty} \gamma(h) = \infty$ [4]. Independently, [50] showed that these two properties hold also for $b_k = 2^k$. Figure 2.1 illustrates γ for $a_k = 10^{-3} \cdot k^{1.1}$ and $b_k = 1.1^{1.1^k}$.

2.3.1 *Spectral Turning Bands*

An important special case appears when μ is rotation invariant and thus can be represented by spherical coordinates α and a radial coordinate r, i.e.,

$$\mu(d\omega) = s_{d-1}^{-1} d\alpha F(dr) \tag{2.9}$$

for some finite non-negative measure F on $[0, \infty)$. Here, s_d denotes the surface area of the d-dimensional sphere. Integrating over α in (2.7) we get

$$\tilde{\varphi}(r) = \int_{[0,\infty)} B_{(d-2)/2}(rs)F(ds) \quad \text{for all } r \in [0, \infty), \tag{2.10}$$

where

$$B_\nu(r) = \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(\nu+1)}{k!\Gamma(\nu+k+1)} \left(\frac{r}{2}\right)^{2k} = \Gamma(\nu+1)\left(\frac{2}{r}\right)^{\nu} J_\nu(r), \quad \nu > -\frac{1}{2}, \quad (2.11)$$

and J_ν is the Bessel function. Hence, the function $\varphi(h) = B_{(d-2)/2}(\|h\|)$ is *the* elementary rotation invariant, continuous positive definite function in $\mathbb{R}^d$. For $d = 1, 2$, and 3, the function $J_{(d-2)/2}(h)$ equals

$$\sqrt{2}\cos(h)/\sqrt{\pi h}, \qquad 2\pi^{-1}\int_0^\infty \sin(h\cosh t)dt, \quad \text{and} \quad \sqrt{2}\sin(h)/\sqrt{\pi h},$$

respectively [46]. In analogy to Bochner's theorem, [88] stated that a rotation invariant function $h \mapsto \tilde{\varphi}(\|h\|)$, $h \in \mathbb{R}^d$, is real, continuous and positive definite if and only if $\tilde{\varphi}$ is the Hankel transform (2.10) of a non-negative finite measure F on the half-line $[0, \infty)$. Note that equation 6.567.1 in [42] ensures that $B_\nu(\|h\|)$ is a positive definite function on $\mathbb{R}^d$ for any $\nu \geq (d-2)/2$.

Remark 2.2. In three dimensions we have

$$\tilde{\varphi}(r) = \int_{[0,\infty)} \frac{\sin rs}{rs} F(ds),$$

i.e., the elementary rotation invariant positive definite function in $\mathbb{R}^3$ is $\varphi(h) = \sin(\|h\|)/\|h\|$, the so-called *hole effect model*.

Example 2.3. Equations 6.649.2, 6.618.1, and 6.623.3 in [42] consider functions $\tilde{\varphi}$ of the form (2.10), and hence yield that $\tilde{\varphi}(\|h\|)$ is a positive definite function on $\mathbb{R}^d$ if

1. $\nu \geq (d-2)/4$ and $\tilde{\varphi}(r) = 2\nu I_\nu(r)K_\nu(r)$,
2. $\nu \geq (d-2)/4$ and $\tilde{\varphi}(r) = \begin{cases} 2^\nu \Gamma(\nu+1) r^{-2\nu} e^{-r^2} I_\nu(r^2), & r \neq 0 \\ 1, & r = 0 \end{cases}$,
3. $\nu \geq \max\{0, (d-2)/2\}$ and $\tilde{\varphi}(r) = \begin{cases} \frac{2^\nu\left(\sqrt{1+r^2}-1\right)^\nu}{r^{2\nu}}, & r > 0 \\ 1, & r = 0 \end{cases}$,

respectively. Here, I_ν denotes the Bessel I-function. For instance, the first model is $\lfloor \nu \rfloor$ times differentiable where $\lfloor \nu \rfloor$ denotes the largest integer less than or equal to ν; it decays at rate h^{-1} to infinity.

Remark 2.3. The function $B_\nu(2\sqrt{\nu}r)$ converges to the function $r \mapsto \exp(-r^2)$ as $\nu \to \infty$. Since $B_\nu(\|\cdot\|)$ is a positive definite function in $\mathbb{R}^d$ for $d < 2\nu + 2$, the "Gaussian" covariance function $C(x, y) = \exp(-\|x - y\|^2)$ is the candidate for a fundamental motion invariant covariance function that is valid in all dimensions d. This is indeed true, see Sect. 2.6.2.

The simulation method that uses decomposition (2.9) is called spectral turning bands method in geostatistics, see [61]. A random field Z with a motion invariant covariance function $C(x,y) = \tilde{\varphi}(\|x-y\|)$ is obtained if

$$Z(x) = \sqrt{2F([0,\infty))}\cos(R\langle S, x\rangle + \Phi)$$

and $R \sim F/F([0,\infty))$ is given by (2.9), $\Phi \sim U[0,2\pi)$, and $S \sim U\mathscr{S}_{d-1}$ is uniformly distributed on the $(d-1)$-dimensional sphere $\mathscr{S}_{d-1}$. All random variables are independent. Again, $Z' = n^{-1/2}\sum_{i=1}^{n} Z_i$ yields an approximation to a Gaussian random field for Z_i, $i = 1,\ldots,n$, that are independent and identically distributed according to Z. The value of n should be of order 500 to get good results. Figure 2.2 shows the performances of the method for the "Gaussian" covariance function.

Remark 2.4. The spectral representation by Bochner and Schoenberg leaves the question open, which discontinuous positive definite functions exist and which are of practical interest. In practice, only one discontinuous model exists that is regularly used as a summand in additive covariance models, the so-called nugget effect $\varphi(h) = \mathbf{1}_{\{0\}}(h)$ ([15], for instance). Here, $\mathbf{1}_A$ denotes the indicator function for a set A, i.e. $\mathbf{1}_A(h)$ equals 1 if $h \in A$ and 0 otherwise. It is easily seen that

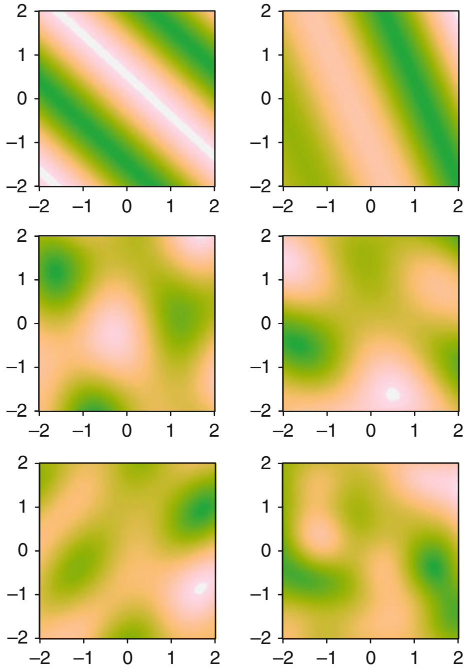

Fig. 2.2 Simulation of the spectral turning bands method with 1, 2, 3, 4, 10, and 1,000 lines (*top left to bottom right*); the random field has the "Gaussian" covariance function

the nugget effect is a positive definite function in any dimension. More generally, for any subgroup Q of $\mathbb{R}^d$, the validity of inequality (2.1) is readily checked for $C(x, y) = \mathbf{1}_Q(x - y)$.

Any measurable positive definite function φ is a sum of a continuous positive definite function and a positive definite function that vanishes almost everywhere [78]. If, additionally, φ is rotation invariant and $d \geq 2$, then φ must be the sum of a continuous positive definite function and a nugget effect [38]. However, covariance functions do not need to be measurable [78].

2.4 Convolutions and Random Coin Method

Another immediate consequence of equation (2.4) is that

$$\varphi(h) = \int_{\mathbb{R}^d} f(x) f(x + h) dx, \qquad h \in \mathbb{R}^d, \tag{2.12}$$

is a positive definite function for any real-valued L_2-function f on $\mathbb{R}^d$. The function φ is called a covariogram. If f is an indicator function, then φ is also called a set covariance function.

Whilst in $\mathbb{R}^1$ many functions f lead to analytic formulae for φ, the situations where the explicit calculation of φ is feasable are limited in higher dimensions. Examples are $f(x) = (\pi/4)^{d/4} \exp(-2\|x\|^2)$ leading to the "Gaussian" model $\varphi(h) = \exp(-\|h\|^2)$, and the indicator functions of the d-dimensional balls of radius $1/2$, up to a multiplicative constant, yielding covariance functions with finite range 1, i.e. compact support. Examples are the hat function $\varphi(h) = (1 - |h|)_+$ for $d = 1$, the circulant model $\varphi(h) = 1 - 2\pi^{-1}(\|h\|\sqrt{1 - \|h\|^2} + \arcsin(\|h\|))$, $\|h\| \leq 1$, in $\mathbb{R}^2$ and the spherical model $\varphi(h) = 1 - \frac{3}{2}\|h\| + \frac{1}{2}\|h\|^3$, $\|h\| \leq 1$, in $\mathbb{R}^3$. See [33] for further properties of these functions, and sufficient conditions for positive definiteness based on these properties.

A random field that corresponds to (2.12) can be defined as

$$Z(x) = \sum_{y \in \Pi} f(x - y)$$

where Π is a stationary Poisson point process on $\mathbb{R}^d$ with intensity $\lambda = 1$. The random field Z has a direct interpretation as the sum of effects of certain events $y \in \Pi$ and is therefore a convenient model for a non-Gaussian random field in many applications. It possesses a lot of names, for instance, dilution random field [15], random coin model, random token model [55], shot noise process [17, 69], moving average model [62], and trigger process [20]. Of course, an approximation to a Gaussian random field can be obtained through the central limit theorem.

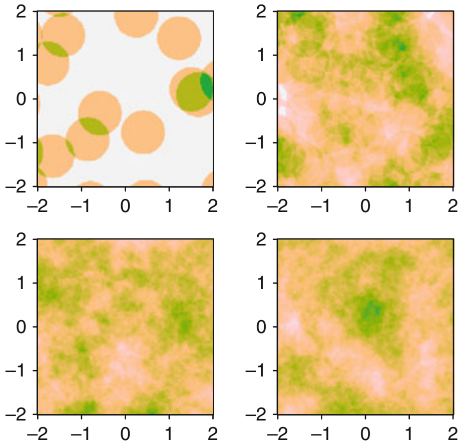

Fig. 2.3 Recentred and renormalised superpositions of 1, 10, 100, and 1,000 simulations of an additive Boolean model with radius $r = 1/2$ of the disks (*top left, top right, bottom left, bottom right*)

Figure 2.3 shows Z for $\lambda = 4/\pi$ and f the indicator function of a disk with radius 0.5, i.e., the covariance function of Z is the circulant model. A satisfying approximation to the Gaussian distribution is obtained if $n \approx 500$ independent realizations are superposed.

Remark 2.5. A related method to obtain positive definite functions and corresponding random fields replaces the product in the integrand of (2.12) by a maximum:

$$\psi(h) = \int_{\mathbb{R}^d} \max\{f(x), f(x+h)\}dx, \qquad h \in \mathbb{R}^d,$$

Here, f is a non-negative, integrable function. Then, ψ is a conditionally negative definite function and the function $\varphi(h) = 2\int f(x)dx - \psi(h)$ is positive definite. These functions appear in extreme value theory and are called extremal coefficient functions ψ or extremal correlation functions φ [25]. A random field that has $C(x, y) = \varphi(x - y)$ as its covariance function appears as a thresholded max-stable random field [85], a special class of Boolean random functions [47].

Both, the spectral representation and the convolution representation are special cases of the Karhunen orthogonal representation [52]. We refer here to the version of [8] who give a more rigorous proof and more general results.

Theorem 2.1. *Let Z be a second order random field on $V \subset \mathbb{R}^d$, i.e.* $\operatorname{Var} Z(x)$ *exists for all $x \in \mathbb{R}^d$. Assume that for some measurable space $(W, \mathscr{W})$, the covariance function C allows for a representation*

$$C(x, y) = \int_W g(x, s)\overline{g(y, s)}F(ds), \qquad x, y \in V,$$

where

1. *F is a positive, σ-finite measure on W;*
2. *L is the L_2 space of functions that are square integrable with respect to F;*
3. *$g : V \times W \to \mathbb{C}$ is such that $g(x,\cdot) \in L$ for all $x \in V$;*
4. $\dim(\operatorname{span}\{g(x,\cdot) : x \in V\}^{\perp}) \le \dim(\overline{\operatorname{span}}\{Z(x) : x \in V\})$ *where the complement is taken with respect to L.*

Then Z can be represented as

$$Z(x) = \int_W g(x,s)d\zeta(s), \qquad x \in V,$$

where ζ is a uniquely determined random orthogonal measure on $\mathscr{W}_0 = \{A \in \mathscr{W} : F(A) < \infty\}$ with $\zeta(A \cup B) = \zeta(A) + \zeta(B)$ for all disjoint $A, B \in \mathscr{W}_0$ and $\mathbb{E}\,\zeta(A)\zeta(B) = F(A \cap B)$ for any $A, B \in \mathscr{W}_0$.

This theorem complements Mercer's theorem [7] which implies that any continuous covariance function $C(x,y)$ on a compact set can be decomposed into eigenfunctions. In case the eigenvalues drop quickly towards zero, fast simulation algorithms for excellent approximations can be obtained by neglecting eigenfunctions that have small eigenvalues.

2.5 Power Series

Since products and pointwise limits of covariance functions are covariance functions, power series of covariance functions with summable, non-negative coefficients yield further models.

For instance, consider the Taylor development of $(1+x)^q$ ([42], formula 1.10), i.e.,

$$(1+x)^q = 1 + qx + \frac{q(q-1)}{2!}x^2 + \dots + \frac{q(q-1)\dots(q-k+1)}{k!}x^k + \dots$$

Then we get that

$$C_1(x,y) = (M - C(x,y))^q - M^q, \qquad q < 0, \quad M > \sup C, \tag{2.13}$$

$$C_2(x,y) = \sum_{j=0}^{2k+1} \frac{q(q-1)\dots(q-j+1)}{j!}[-C(h)]^j M^{q-j} - (M - C(h))^q,$$
$$q \in (2k, 2k+1), \quad k \in \mathbb{N}_0, \quad M \ge \sup C,$$

and

$$C_3(x,y) = (M - C(h))^q - \sum_{j=0}^{2k} \frac{q(q-1)\dots(q-j+1)}{j!}[-C(h)]^j M^{q-j}, \quad (2.14)$$

$$q \in (2k-1, 2k), \quad k \in \mathbb{N}_0, \quad M \geq \sup C,$$

are covariance functions for any covariance function C. In particular,

$$\varphi(0)^q - (\varphi(0) - \varphi(\cdot))^q, \quad (2.15)$$

is a positive definite function for $q \in (0,1]$ and any positive definite function φ. The function $1 - \frac{1}{\sqrt{2}}(1-\rho)^{1/2}$ has the form (2.15) up to an additive constant, and appears as the covariance function of a thresholded extremal Gaussian random field [85].

Further examples of functions that have power series with non-negative coefficients are exp, sinh and cosh. Hence, if C is a covariance function, so are $\exp(C)$, $\sinh C$ and $\cosh C$. See also [86].

2.5.1 *Application to Variograms*

If γ is a variogram then

$$C(x,y) = \gamma(x) + \gamma(y) - \gamma(x-y)$$

is a covariance function [66]. This is readily seen if an intrinsically stationary random field Y with variogram γ is considered and the covariance function of $Z(x) = Y(x) - Y(0)$ is calculated. As $e^{-s(\gamma(x)+\gamma(y))}$ is a covariance function by (2.4), cf. [66], it follows that

$$h \mapsto \exp(-s\gamma(h)) \quad (2.16)$$

is a positive definite function for all $s > 0$ and any conditionally negative definite function γ. Since $\gamma(h) = \lim_{s\to 0} s^{-1}(1 - e^{-s\gamma(h)})$, the reverse holds as well, i.e., if the function given by (2.16) is positive definite for all $s > 0$, then γ is a conditionally negative definite function.

Remark 2.6. Equations (2.16) and (2.15) yield that for any conditionally negative definite function γ and any $q \in (0,1]$ the function

$$\gamma_q(h) = \lim_{s\to 0}(s^{-1}(1 - e^{-s\gamma(h)}))^q = \gamma^q(h) \quad (2.17)$$

is non-negative and conditionally negative definite. As additing a constant does not change the property of a function being conditionally negative definite, $(\gamma + a)^q - a^q$ is a variogram for any variogram γ and $a \geq 0$.

Note that for $q > 1$, the function γ^q may not be a variogram anymore. In general, products of variograms are not variograms. See [100] for a discussion and classes of examples. In contrast, any convex combination of variograms is a variogram.

Example 2.4. It is immediately seen from inequality (2.2) that $\gamma(h) = \langle h, h \rangle$ is a variogram for any scalar product $\langle \cdot, \cdot \rangle$. Equation (2.17) yields that $h \mapsto \|h\|^\alpha$, $\alpha \in (0, 2]$ is a variogram model for any dimension d. If $d = 1$, the corresponding random field is called fractional Brownian motion, and Brownian motion if $\alpha = 1$. Equation (2.13) yields that $(1 + \gamma)^{-\beta} = \lim_{s \to 0}(1 + s^{-1} - s^{-1}\exp(-s\gamma))^{-\beta}$ is a positive definite function for any variogram γ and $\beta > 0$. Hence, the generalized Cauchy model [28],

$$\varphi(h) = (1 + \|h\|^\alpha)^{-\beta/\alpha} \tag{2.18}$$

and, by (2.16), the powered exponential model $\varphi(h) = \exp(-\|h\|^\alpha)$ are positive definite functions on $\mathbb{R}^d$ for any $d \in \mathbb{N}$, $\beta > 0$ and $\alpha \in (0, 2]$.

Although power series are useful for constructing covariance functions, they have not been of direct use for simulating random fields.

2.6 Mixtures

Equation (2.6) yields that $C = \int C_\nu \mu(d\nu)$ is a covariance function if μ is a non-negative finite measure and C_ν are covariance functions such that C is finite everywhere. In this case, C is called a mixture of the models C_ν.

Example 2.5. Integrating (2.16) over the interval [0, 1] with respect to s yields that

$$\varphi(h) = \begin{cases} \dfrac{1 - e^{-\gamma(h)}}{\gamma(h)}, & \gamma(h) \neq 0 \\ 1, & \gamma(h) = 0 \end{cases}$$

is a positive definite function for any variogram γ.

2.6.1 Scale Mixtures

The most important class of mixtures are the scale mixtures. Let φ and φ_0 be complex-valued functions on $\mathbb{R}^d$. The function φ is called a *scale mixture* of φ_0 if there exists a non-negative measure F on $[0, \infty)$, such that

$$\varphi(h) = \int_{[0,\infty)} \varphi_0(sh) F(ds) \qquad \text{for all } h \in \mathbb{R}^d \tag{2.19}$$

or, more generally,

$$C((x_1,\dots,x_d),(y_1,\dots,y_d)) = \int_{[0,\infty)^d} C_0((s_1x_1,\dots,s_dx_d),(s_1y_1,\dots,s_dy_d))\,F(d(s_1,\dots,s_d)), \qquad x_i, y_i \in \mathbb{R},$$

for some non-negative measure F on $[0,\infty)^d$. For instance, all continuous, isotropic covariance functions are scale mixtures of Bessel functions, see Sect. 2.3.1.

Example 2.6. The scale mixture of the "Gaussian" model with mixing density

$$f(s) = \frac{(\kappa/\delta)^\lambda}{2K_\lambda(\delta\kappa)} s^{\lambda-1} \exp\big(-(\kappa^2 s + \delta^2/s)/2\big)$$

yields the generalized hyperbolic model [3, 28, 89],

$$\tilde{\varphi}(r) = \frac{\delta^{-\lambda}}{K_\lambda(\kappa\delta)}(\delta^2+r^2)^{\lambda/2} K_\lambda(\kappa(\delta^2+r^2)^{1/2}), \qquad r \ge 0.$$

Here, the parameters λ, κ, and δ satisfy:

$$\delta \ge 0,\ \kappa > 0 \text{ for } \lambda > 0,$$
$$\delta > 0,\ \kappa > 0 \text{ for } \lambda = 0,$$
$$\delta > 0,\ \kappa \ge 0 \text{ for } \lambda < 0.$$

It includes, as special cases, the Cauchy model (2.18) with $\alpha = 2$ and the Whittle-Matérn model in example 2.1.

2.6.2 Completely Monotone Functions

A continuous function ψ on $[0,\infty)$ with $\psi(0) \in \mathbb{R} \cup \{\infty\}$ is called completely monotone function if it is infinitely often differentiable and $(-1)^n \psi^{(n)}(r) \ge 0$ for any $r \in (0,\infty)$ and $n \in \mathbb{N}$. It is well-known [98] that ψ is completely montone if and only if it is a scale mixture of the exponential function, i.e.,

$$\psi(r) = \int_0^\infty e^{-sr} F(ds), \qquad r > 0, \tag{2.20}$$

for some non-negative measure F such that ψ is finite on $(0,\infty)$. A function ψ is called absolutely monotone if all derivatives are positive.

Since $\exp(-s\gamma)$ is a positive definite function for any $s > 0$ and any variogram γ, the function $\psi(\gamma)$ is positive definite on $\mathbb{R}^d$ for any bounded, completely monotone function ψ and any variogram γ on $\mathbb{R}^d$. As $h \mapsto \|h\|^2$ is variogram for any dimension d, we get that $\psi(\|h\|^2)$ is a covariance function for any dimension d and any bounded, completely monotone function ψ. [88] proved that the reverse also holds. Namely, if $\psi(\|h\|^2)$, $h \in \mathbb{R}^d$, is a continuous and isotropic positive definite function in all dimensions $d \in \mathbb{N}$, then ψ is a bounded, completely monotone function.

Since $1 - e^{-s\gamma} = s \int_0^\gamma e^{-ts} dt$ is a variogram for any variogram γ we get that $\int_0^\gamma \psi(u) du$ is a variogram for any completely monotone, integrable function ψ. A non-negative function on $(0, \infty)$ that is infinitely often differentiable and whose first derivative is completely monotone is called a Bernstein function. For particular properties and a considerable amount of examples, see [74] and [83].

Example 2.7. The conditional negative definiteness of γ^α, $\alpha \in (0, 1)$, see equation (2.17), also follows immediately from the fact that $r \mapsto r^\alpha$ is a Bernstein function.

Example 2.8. A completely monotone function is $r \mapsto (1 + r)^{-1}$, cf. (2.18), which implies that

$$h \mapsto \log(\gamma(h) + 1)$$

is a variogram for any variogram γ. If $\gamma(h) = \|h\|^\alpha$, $\alpha \in (0, 2]$, then the model $h \mapsto \log(\|h\|^\alpha + 1)$ is called de Wijsian model [96].

Example 2.9. The concatenation of two Bernstein functions is a Bernstein function [5]. This is a consequence of the product rule for the nth derivative, which implies that the product of two completely monotone functions is completely monotone. Hence,

$$r \mapsto \int_0^{f(r)} g(f^{\leftarrow}(s)) ds$$

is a Bernstein function for any completely monotone function g and any Bernstein function f. For instance, choosing $g(r) = \exp(-r)$ and $f(r) = r^{1/2}$ shows that $\mathrm{erfc}(\sqrt{\gamma})$ is a covariance function for any variogram γ. The latter function appears as the covariance function of a thresholded Brown-Resnick process [51].

Remark 2.7. If ψ is a bounded and absolutely monotone function and C is a covariance function then $\psi(C)$ is a covariance function, see Sect. 2.5. Let $0 < M < \pi/2$, $\alpha \in (0, 1)$ and ρ be a covariance function with $|\rho| \le 1$. Then the following functions are also covariance functions

$$\rho/(1-e^{-4M\rho}), \quad \arcsin\rho, \quad \tan M\rho, \quad \mathrm{cossec}(\rho)-\rho^{-1}, \quad (2M\rho)^{-1}-\cot(2M\rho),$$

$$\sec\rho, \quad -\log(1-\alpha\rho), \quad \log|\rho/\sin\rho|, \quad -\log\cos(M\rho), \quad \log|\tan(M\rho)/(M\rho)|.$$

The function $\arcsin\rho$ appears as the covariance function of a thresholded Gaussian random field, see [2] for instance.

Remark 2.8. If ψ is a bounded, absolutely monotone function, the function $\psi(\cdot) - \psi(0)$ is also absolutely monotone and should be considered preferentially, since the covariance function $\psi(C)$ with $\psi(0) \neq 0$ always refers to a non-ergodic random field.

2.6.3 More Mixture Models

Mixtures of $\exp(-\lambda\gamma)$ yield several mappings from the set of variograms to the set of positive definite functions.

For instance, equation 6.521.3 in [42] and equation (2.8) yield that

$$\varphi(h) = \begin{cases} \dfrac{\gamma_1^\nu(h) - \gamma_2^\nu(h)}{\gamma_1(h) - \gamma_2(h)}, & \gamma_1(h) \neq \gamma_2(h) \\ \nu\gamma_1^{\nu-1}(h), & \text{otherwise} \end{cases},$$

is a positive definite function for $\nu \in (0, 1]$ and any two non-negative, conditionally negative definite functions γ_1 and γ_2 where at least one of them is strictly positive. Equation 9.111 in [42] and example 2.4 yield that

$$F(\alpha; \beta; \delta; -\gamma) \tag{2.21}$$

is a positive definite function for $\alpha > 0$, $\delta > \beta > 0$ and any variogram γ. Here, F is the hypergeometric function, see Sect. 9.1 in [42]. Similarly, $F(\alpha; \beta; \delta; C(x, y))$ is a covariance function for any covariance function C with $C(x, y) < 1$ for all $x, y \in \mathbb{R}^d$, if $(\alpha + k)(\beta + k)/(\delta + k) \geq 0$ for all $k \in \mathbb{N}$.

Furthermore,

$$\varphi(h) = \begin{cases} \dfrac{f(\gamma(h))}{\gamma(h)}, & \gamma(h) \neq 0 \\ 1 & \text{otherwise} \end{cases}$$

is a positive definite function for $f(z) = \log(1+z)$, $f(z) = \arctan(z)$, $f = \log(z + \sqrt{z^2 + 1})$ and any variogram γ, see equations 9.121.6, 9.121.27 and 9.121.28 in [42], respectively. See also example 2.5.

One more example is

$$\varphi(h) = \int_0^\infty e^{-s^2\gamma_1(h)} e^{-\gamma_2(h)/s^2} e^{-\beta s^2} ds = \frac{\sqrt{\pi}}{2\sqrt{\beta + \gamma_1(h)}} \exp\{-2\sqrt{(\beta + \gamma_1(h))\gamma_2(h)}\},$$

where γ_1 and γ_2 are variograms and $\beta > 0$, cf. equation 3.325 in [42] and [22]. Hence,

$$\varphi(h) = (\beta + \gamma_1(h))^{-1/2} \tilde{\varphi}\left(\sqrt{(\beta + \gamma_1(h))\gamma_2(h)}\right)$$

is a positive definite function for any bounded, completely monotone function $\tilde{\varphi}$.

2.7 Turning Bands Operator

The turning bands method, introduced by [67], see also [49], allows for the simulation of a stationary random field using a projection technique onto one-dimensional spaces. In almost all applications, the field is assumed to be isotropic and the dimension d is less than or equal to 3.

The turning bands method is based on the following idea. Let s be an arbitrary fixed orientation in $\mathbb{R}^d$ and Z_s a random field in $\mathbb{R}^d$ that is constant on hyperplanes perpendicular to s. Assume that the random process Y along direction s is stationary. Then Z_s is stationary, but not isotropic, except for the trivial case that Y is constant for any realization. An isotropic random field is obtained if we replace s by a random unit vector S that is uniformly distributed on the $(n-1)$-dimensional sphere $\mathscr{S}_{n-1}$ and that is independent of Y,

$$Z_S(x) = Y(\langle x, S\rangle), \qquad h \in \mathbb{R}^d.$$

Let $C_1(x,y) = \varphi_1(x-y)$ be the covariance function of Y. Then, the covariance function $C(x,y) = \varphi(x-y)$ of Z_S is given by

$$\varphi(h) = \mathbb{E}\,\varphi_1(\langle h, S\rangle) = \int_{\mathscr{S}_{n-1}} \varphi_1(\langle h, s\rangle)\pi(ds) = \int_{\mathscr{S}_{n-1}} \varphi_1(\|h\|\langle e, s\rangle)\pi(ds)$$

where π is the uniform probability measure on $\mathscr{S}_{n-1}$ and $e \in \mathbb{R}^d$ denotes any fixed unit vector. Hence, C is rotation invariant, i.e., $C(x,y) = \tilde{\varphi}(\|x-y\|)$ for some function $\tilde{\varphi} : [0,\infty) \to \mathbb{R}$. [67] showed the following relation between $\tilde{\varphi}$ and φ_1:

$$\varphi_1(r) = \begin{cases} \dfrac{d}{dr}[r\tilde{\varphi}(r)], & d = 3 \\ \dfrac{d}{dr}\displaystyle\int_0^r \frac{s\tilde{\varphi}(s)}{\sqrt{r^2-s^2}}ds, & d = 2 \end{cases}, \qquad r > 0. \tag{2.22}$$

In fact, relation (2.22) holds reversely for any continuous positive definite function $\tilde{\varphi}(\|\cdot\|)$ on $\mathbb{R}^d$, $d = 2$ and 3, respectively [32]. The mapping which assigns $\tilde{\varphi}_1$ to $\tilde{\varphi}$ is called the *turning bands operator*. See Fig. 2.4 for an illustration of the turning bands method. In Sect. 7.4.2 of [15] the case of a general dimension $d \in \mathbb{N}$ is considered.

Note that the continuity assumption is equivalent to the assumption that C has no nugget effect [38] and that C is at least m times differentiable away from the origin for m the largest integer less than or equal to $(d-1)/2$ [32].

An approximation to a Gaussian random field is again obtained through the central limit theorem:

$$Z(x) = n^{-1/2}\sum_{i=1}^{n} Y_i(\langle x, S_i\rangle).$$

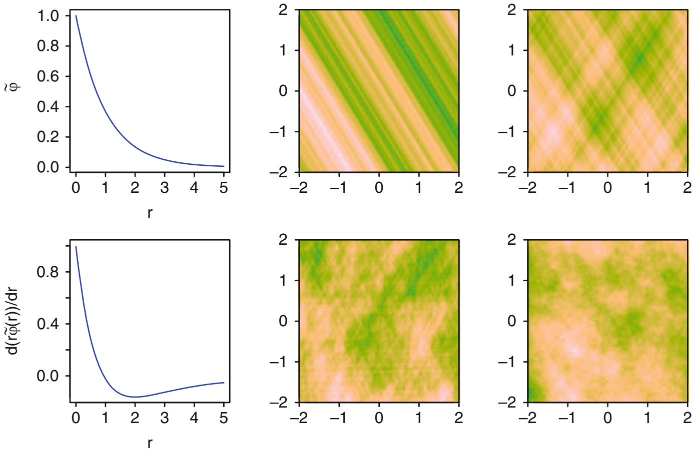

Fig. 2.4 Recentred and renormalised superpositions of 1, 10, 100, and 1000 simulations of an additive Boolean model with radius $r = 1/2$ of the disks (top left, top right, bottom left, bottom right)

Here, $Y_i \sim Y$, $i = 1, \ldots, n$, and $S_i \sim S$, $i = 1, \ldots, n$, are all independent. The number of independent copies k that are needed is about 60 for $d = 2$ and 500 for $d = 3$ [30], see also [55]. The simulation of the random field Y is performed on a grid for example by methods described in Sect. 2.9, and the closest grid point to the left, say, is taken as an approximation for $\langle x, S \rangle$.

Remark 2.9. Closed solutions for the Abel integral (2.22) in the case $d = 2$ are rare [29]. Hence, the covariance function on the line must be evaluated numerically, using the following more convenient form if $r\tilde{\varphi}(r)$ is differentiable:

$$\tilde{\varphi}_1(r) = \frac{d}{dr} \int_0^1 r\tilde{\varphi}(r\sqrt{1-s^2})ds = \int_0^1 \frac{d}{dr} r\tilde{\varphi}(r\sqrt{1-s^2})ds. \tag{2.23}$$

Alternatively, if $\tilde{\varphi}(\|\cdot\|)$ is a positive definite function also in $\mathbb{R}^3$, the space $\mathbb{R}^2$ can be considered as a hyperplane in $\mathbb{R}^3$ and the simulation is performed in $\mathbb{R}^3$.

Remark 2.10. In practice, one should not use random directions S_i in the two-dimensional turning bands method. Instead, equal angles between the lines should be taken. By choosing the direction of the very first line purely random, isotropy is still guaranteed from a theoretical point of view.

In dimension 3 or higher, a deterministic point pattern of equally spaced locations does not exist for an arbitrary number of points. Therefore, the directions are usually chosen randomly. A random direction S in $\mathbb{R}^3$ is obtained by

$$(\sqrt{1-V^2}\cos U, \sqrt{1-V^2}\sin U, V),$$

where $U \sim U[0, 2\pi]$ is independent of $V \sim U[0, 1]$, see [26], for instance.

Remark 2.11. [32] generalizes the turning bands operator in the following way. Let $\tilde{\varphi}(\|\cdot\|)$ be a positive definite function on $\mathbb{R}^d$ and

$$\tilde{\varphi}_{d-2}(r) = \tilde{\varphi}(r) - \frac{r}{d-2}\tilde{\varphi}'(r), \qquad d-2 \geq 1.$$

Then $\tilde{\varphi}_{d-2}(\|\cdot\|)$ is a positive definite function in $\mathbb{R}^{d-2}$, and vice versa.

2.8 *Montée*

Apart from the turning bands operator, further operators transform between sets of positive definite functions by means of derivations or integrals.

For instance, the ith second partial derivative $\partial^2\varphi(h)/(\partial h_i)^2$ of a positive definite function φ is positive definite, provided it exists (e.g., [81]). This is proved by considering the covariance function of the ith partial derivative of a random field corresponding to φ.

[71] show that, if $\varphi(h) = \tilde{\varphi}(\|h\|)$ is a positive definite function in $\mathbb{R}^d$, then $\varphi_1(h) = \tilde{\varphi}_1(\|h\|)$ with $\tilde{\varphi}_1(r) = d\tilde{\varphi}(\sqrt{r})/dr$ is a positive definite function in $\mathbb{R}^{d-2}$.

Here, the *montée*, and its inverse, the *descente*, are considered. See [101] for a unified approach to the turning bands operator and the *montée*.

Let $Z(x_1, x_2)$ be a random field on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ with covariance function C and $C((x_1, x_2), (y_1, y_2)) = C((x_1, x_2 - y_2), (y_1, 0))$. Let

$$Y_M(x_1) = \frac{1}{(2M)^{d_2/2}} \int_{[-M,M]^{d_2}} Z(x_1, x_2)dx_2, \qquad x_1 \in \mathbb{R}^{d_1}.$$

Then, the covariance function C_M of the random field Y_M yields

$$\begin{aligned} C_M(x_1, y_1) &= \frac{1}{(2M)^{d_2}} \int_{[-M,M]^{d_2}} \int_{[-M,M]^{d_2}} C((x_1, x_2), (y_1, y_2))dx_2dy_2 \\ &\to \int_{\mathbb{R}^{d_2}} C((x_1, h), (y_1, 0))dh \qquad (M \to \infty). \end{aligned}$$

This transformation of the covariance functions is called *montée* [64]. If $C(x, y) = \tilde{\varphi}(\|x - y\|)$ is motion invariant, then $C_M(x, y) \to \tilde{\varphi}_{d_1}(\|x - y\|)$ with

$$\tilde{\varphi}_{d_1}(r) = \begin{cases} 2\displaystyle\int_0^\infty \tilde{\varphi}(\sqrt{r^2 + s^2})ds, & d_2 = 1 \\ 2\pi \displaystyle\int_r^\infty s\tilde{\varphi}(s)ds, & d_2 = 2 \end{cases}.$$

That is, $\tilde{\varphi}_{d_1}(\|x-y\|)$ is a positive definite function in $\mathbb{R}^{d_1}$. Reversely, let $\varphi(h) = \tilde{\varphi}(\|h\|)$ be a positive definite function in $\mathbb{R}^d$ and assume that $\tilde{\varphi}''(0)$ exists. Then the *descente* is given by

$$D\tilde{\varphi}(r) = \begin{cases} 1, & r = 0 \\ \tilde{\varphi}'(r)/(r\tilde{\varphi}''(0)), & r > 0 \end{cases},$$

and $\varphi(h) = D\tilde{\varphi}(\|h\|)$ is a positive definite function in $\mathbb{R}^{d+2}$ [34].

[31], see also [97] and [12], uses the *montée* to construct classes of differentiable covariance functions with compact support from the function

$$\tilde{\varphi}(r) = (1-r^b)^a 1_{[0,1]}(r).$$

If $b = 1$, then the function $\tilde{\varphi}(\|h\|)$ is positive definite if and only if $a \geq (d+1)/2$ [40]. For instance, $\varphi(h) = \tilde{\varphi}(\|h\|)$ is a positive definite function in $\mathbb{R}^d$ for

$$\tilde{\varphi}(r) = (1 + (\nu+2)r + 3^{-1}[(\nu+2)^2 - 1]r^2)(1-r)^{\nu+2} 1_{[0,1]}(r)$$

and $\nu \geq (d+5)/2$.

[80] and [79] extend the *montée* by considering integrations of real-valued order. See [45] for a further extension of the Wendland-Gneiting functions. [70] derive vector-valued covariance functions with comport support.

2.9 General Simulation Methods

In the following, widely used simulation methods are presented that are not immediately related to construction methods of covariance functions and variograms.

2.9.1 Simulation of a Multivariate Gaussian Vector

Let Y be an n-vector of independent Gaussian random variables with zero expectation and unit variance, and $D = D_0 D_0^\top$ be any positive semi-definite $n \times n$-matrix. Let

$$X \sim D_0 Y. \tag{2.24}$$

Then X has a multivariate, centred Gaussian distribution with covariance matrix D. Of course, this basic fact can also be used to simulate from stationary or non-stationary random fields, defining $D = (C(x_i, x_j))_{i,j=1,\ldots,n}$. The method has its numerical limitation at about $n = 10^4$ for general matrices.

2.9.2 Circulant Embedding

The circulant embedding method allows to simulate a stationary random field on a grid which is equally spaced in each direction. The idea is to expand the covariance matrix to a circulant matrix, i.e. to simulate from a torus. If this is feasible, the square root of the expanded matrix can be calculated using the Fast Fourier Transform. This approach was independently published by [23] and [13, 99]. [99] show that such an expansion is always possible if the covariance function has compact support. The algorithm is then exact in principle. In case negative eigenvalues appear in the expanded matrix, [99] suggest an approximation by putting them to zero. However, this can lead to deficient simulation results.

If n is the number of grid points and d the dimension, the number of flops is of order $2^d n \log(2^d n)$, hence the simulation method is very fast unless the dimension d is high.

Extensions to conditional simulation, to arbitrary locations [24], and to multivariate random fields [14] exist.

Further extensions are the intrinsic circulant embedding and the cut-off circulant embedding [39, 91]. The idea is to replace a given covariance function by a covariance function that equals or essentially equals the required covariance on the given finite grid, but has finite range.

2.9.3 Approximations Through Markovian Fields

In a space-time setup, a field might be simulated on a few spatial points at arbitrary locations, but at many instances in time on a grid. Instead of simulating all variables at once, (approximating) Markov fields can be used in the temporal direction, using a temporal neighbourhood of k instances. Namely, for each instance, Gaussian variables are simulated simultaneously for all locations, conditioned on the previous k instances and all locations.

[77] rigorously suggest to approximate Gaussian random fields through Markov fields with a huge increase in speed for the simulations. In a recent paper, [56] relate the Markov random fields to partial differential equations.

2.10 Space-Time Models

A current, important task is to find covariance functions that are useful for modelling space-time data. In the following, let d be the dimension in space. Mathematically, the set of space-time covariance functions cannot be distinguished from the set of covariance functions in $\mathbb{R}^{d+1}$. However, the sets of those covariance functions that are of interest in practice differ. In the purely spatial context, an isotropic random field constitutes the standard model. In contrast, the temporal development of a process differs in most cases from the spatial development, leading to anisotropies between space and time. For example, geometrical anisotropy matrices A, see remark 2.1, that have the form

$$A = \begin{pmatrix} A_0 & -v \\ 0 & s \end{pmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}$$

connect space and time through the vector $v \in \mathbb{R}^d$. The latter can be interpreted, for instance, as wind speed in a meteorological context [43]. The matrix $A_0 \in \mathbb{R}^{d\times d}$ gives the purely spatial anisotropy and $s > 0$ is a scaling factor for the temporal axis.

To simulate space-time random fields, all the approaches presented in the previous sections can be used if they are appropriate. For example, circulant embedding will be useful if the space-time data lie on a grid. In the following, some additional, specific methods are presented.

2.10.1 Separable Models

The simplest class of anisotropic space-time models are separable models. By definition, a separable model has one of the following two forms

$$C((x,t),(y,s)) = C_S(x,y)+C_T(t,s) \quad \text{or} \quad C((x,t),(y,s)) = C_S(x,y)C_T(t,s),$$

where C_S is a covariance function in $\mathbb{R}^d$ and C_T is a covariance function in $\mathbb{R}$ [75]. All other models are called non-separable. It is easy to see from the results in Sect. 2.2 that separable models are covariance functions. A variogram is called separable if

$$\gamma(h,u) = \gamma_S(h) + \gamma_T(u)$$

for two variograms $\gamma_S(h)$ and $\gamma_T(u)$ in $\mathbb{R}^d$ and $\mathbb{R}$, respectively. Products of variograms should not be considered, cf. remark 2.6. Random fields with separable covariance function can easily be simulated. Namely, a spatial random field with covariance C_S that is constant in time is added (or multiplied, respectively) to a temporal random process with auto-covariance C_T that is independent of the former and is constant in space. The obtained field is not Gaussian and an approximation can be obtained through the central limit theorem. Although separable models are quite appealing, they have practical disadvantages [19, 54, 76] and theoretical disadvantages [92].

Many non-separable models given in the literature are based on separable models and general transformations of covariance functions and variograms as presented in the preceding sections. An example that refers to the models discussed in Sect. 2.5

is $\varphi(h,u) = (1 + |h|^\nu + |u|^\lambda)^{-\delta}$, cf. [21]. The function φ is positive definite on $\mathbb{R}^d \times \mathbb{R}^{d'}$ for any dimensions d and d', if $\nu, \lambda \in [0,2]$ and $\delta > 0$. Another example is $\varphi(h,u) = [1 - \varphi_S(h)\varphi_T(u)]^{-\alpha}$, where $\alpha > 0$ and $\varphi_S(0)\varphi_T(0) < 1$ [57].

Further models are obtained by means of scale mixtures of separable models. For instance,

$$C(h,u) = \int_0^\infty e^{-s\gamma(h)} \cos(s|u|)ds = \frac{\gamma(h)}{\gamma(h)^2 + |u|^2}$$

is a covariance model in $\mathbb{R}^d \times \mathbb{R}$ for any strictly positive, conditionally negative definite function γ on $\mathbb{R}^d$, cf. [22].

2.10.2 Gneiting's Class

[35] has introduced an important class of space-time covariance functions generalizing the findings in [19]. Let $\tilde{\varphi}_S(r)$, $r \geq 0$, be a bounded, completely monotone function and

$$\varphi(h,u) = \gamma(u)^{-d/2}\, \tilde{\varphi}_S\left(\|h\|^2/\gamma(u)\right), \qquad (h,u) \in \mathbb{R}^d \times \mathbb{R}.$$

[35] shows that φ is a positive definite function if $\gamma(u) = \psi(|u|^2)$ for some strictly positive Bernstein function ψ. [100] show that φ is a positive definite function if and only if γ is a strictly positive, conditionally negative definite function. Note that Gneiting's model is fully symmetric [35], i.e. $C((x,t),(y,s)) = C((x,-t),(y,-s))$, restricting its ability to model correlations between space and time.

[86] generalizes Gneiting's model towards models that are not fully symmetric, using the fact that $\exp(-u^2\gamma(h))$ is, for fixed u, a positive definite function in h, and, for fixed h, the spectral density of the "Gaussian" model.

Remark 2.12. The ambivalency that a function is a positive definite function in one argument and a spectral density in the other has been used previously by [94] considering the function $[c_1(a_1^2 + \|h\|^2)^{\alpha_1} + c_2(a_2^2 + \|u\|^2)^{\alpha_2}]^{-\nu}$. Here, $h \in \mathbb{R}^{d_1}$, $u \in \mathbb{R}^{d_2}$, $a_1^2 + a_2^2 > 0$ and $c_1, c_2, \nu_1, \nu_2, \alpha_1, \alpha_2 > 0$, such that $d_1/(\alpha_1\nu) + d_2/(\alpha_2\nu) < 2$. If $\alpha_1 = 1$, then the corresponding positive definite function is given by

$$\varphi(h,u) = \frac{\pi^{d_2/2} W_{\nu-d/2}(f(\|u\|^2)\|h\|)}{2^{\nu-d_2/2-1} c_2^\nu \Gamma(\nu) f(\|u\|^2)^{2\nu-d_2}}.$$

The function f equals $f(s) = (a_2^2 + c_1 c_2^{-1}(a_1^2 + s)^{\alpha_1})^{1/2}$, $s \geq 0$, and W_ν denotes the Whittle-Matérn model with parameter ν. See [58] and [94] for further, sophisticated models, and [93] for non-stationary covariance functions.

2.10.3 Turning Layers

Space-time data typically consist of longer, regularly measured time series given at several arbitrary locations in $\mathbb{R}^d$. The turning layers method respects this fact and is applicable for fully symmetric models that are isotropic in space. As for the turning bands method, a non-ergodic random field that is isotropic in space is obtained if a random field with translation invariant covariance function C_1 is simulated on a plane where one axis has a random direction in space and the other axis equals the time axis. The random field in $\mathbb{R}^d \times \mathbb{R}$ is constant in perpendicular direction to the plane, cf. [53]. Denote the covariance function of the latter by C. Similar to the derivation of the turning bands relation we obtain a reverse formula for $C_1((x_1, t), (y_1, s)) = \tilde{\varphi}_1(|x_1 - y_1|, |t - s|)$ given $C((x, t), (y, s)) = \tilde{\varphi}(\|x - y\|, |t - s|)$:

$$\tilde{\varphi}_1(r, t) = \begin{cases} \dfrac{\partial}{\partial r}[r\tilde{\varphi}(r, t)], & d = 3 \\ \dfrac{\partial}{\partial r}\displaystyle\int_0^r \frac{s\tilde{\varphi}(s, t)}{\sqrt{r^2 - s^2}} ds, & d = 2 \end{cases}. \tag{2.25}$$

An approximation to a Gaussian random field is obtained through the central limit theorem as in the case of the turning bands method. A realization on the plane might be obtained by using circulant embedding, see Sect. 2.9.2. The turning layers have the advantages of being an exact method in the temporal direction at any fixed location. However, it exhibits the usual approximation error of the turning bands method in space.

Remark 2.13. Assume that, for some functions $f, g : \mathbb{R} \to \mathbb{R}$ and $\tilde{\varphi}_S : [0, \infty) \to \mathbb{R}$, the function $\varphi(r, t)$ is of the form $g(t)\tilde{\varphi}_S(rf(t))$, as it is the case for the Gneiting class. Let $\tilde{\varphi}_{1,S}$ be the function obtained for $\tilde{\varphi}_S$ through (2.22) for $d = 2, 3$. Then we get

$$\tilde{\varphi}_1(r, t) = g(t)\varphi_{1,S}(rf(t)),$$

assuming that equality (2.23) holds if $d = 2$.

Naturally, the turning layers can be generalized to simulate random fields on $\mathbb{R}^d \times \mathbb{R}^n$, $n \geq 1$, that are isotropic in both components. Namely, the two-dimensional random field Y can be replaced by a higher dimensional one, or the turning bands principle can be applied also to the second component of Y.

2.10.4 Spectral Turning Layers

A variant of the turning layers that corresponds to the spectral turning bands is useful for covariance functions of the form

$$C(h, t) = \mathbb{E}\,\tilde{\varphi}(\|x - Vt\|^2). \tag{2.26}$$

Here, $\tilde{\varphi}$ is a bounded, completely monotone function and V is a d-dimensional random vector that might be interpreted as wind speed in a meteorological context [16]. A corresponding random field Z is obtained as

$$Z(x,t) = \sqrt{2F([0,\infty))}\cos(A\langle S, x - Vt\rangle + \Phi)$$

where $A \sim F/F([0,\infty))$, F is the radial spectral measure for $\tilde{\varphi}$ given by (2.9), $\Phi \sim U[0,2\pi)$, and $S \sim U\mathscr{S}_{d-1}$ is uniformly distributed on the $(d-1)$-dimensional sphere $\mathscr{S}_{d-1}$. All the random variables are independent. We call the method spectral turning layers.

Let $\tilde{\varphi}$ be a bounded, completely monotone function and $V \sim \mathscr{N}(\mu, M/2)$ for some covariance matrix M. [86] shows that C has a closed form,

$$C(h,t) = \frac{1}{\sqrt{\mathbf{1} + t^2 M}}\tilde{\varphi}\left((h - t\mu)^\top (\mathbf{1} + t^2 M)^{-1}(h - t\mu)\right)$$

which is fully symmetric if and only if $\mu = 0$.

2.10.5 Models Related to PDEs

A challenging problem is to find closed-form covariance models that refer to solutions of physical equations. Let B be the random orthogonal measure on $\mathbb{R}^2$ such that $B(I \times J) \sim \mathscr{N}(0, |I||J|)$ for any bounded intervals $I, J \subset \mathbb{R}$. [48] show that the solution of

$$\left(\frac{\partial^2}{\partial t^2} - a\frac{\partial}{\partial x} - b^2\right) Y(x,t)dx = B(d(x,t)), \qquad x,t \in \mathbb{R},$$

has covariance function

$$C(h,u) = \frac{1}{2}\left\{e^{-b|u|}\mathrm{erfc}\left(\frac{2b|h| - c|u|}{2\sqrt{c|h|}}\right) + e^{b|u|}\mathrm{erfc}\left(\frac{2b|h| + c|u|}{2\sqrt{c|h|}}\right)\right\}, \quad h,u \geq 0,$$

see also [53] and the references therein. [58] generalizes this covariance function by showing that $|h|$ on the right hand side can be replaced by $\sqrt{\gamma(h)}$ for any variogram γ.

2.11 Multivariate Models

A commonly used model for a multivariate process $Z = (Z_1, \ldots, Z_n)$ is the so-called linear model of coregionalization [41], where each component Z_j is a linear combination $\sum_{i=1}^{K} a_{ji} Y_i$ of independent, latent processes Y_i. Assume Y_i has covariance function C_i. Then the matrix valued covariance function of Z,

$$C_{ij}(x, y) = \text{cov}(Z_i(x), Z_j(y)), \qquad i, j = 1, \ldots, n, \quad x, y \in \mathbb{R}^d,$$

equals $ACA^\top$ with $A = (a_{ij})_{j=1,\ldots,n;i=1,\ldots,K}$ and $C = \text{diag}(C_1, \ldots, C_K)$.

Except for some further special constructions, see [96] and [86] for instance, parametrized classes have been rare.

Recently, [37] introduced an extension of the Whittle-Matérn model W_ν to the multivariate case. In the bivariate case, they show that $C_{ij}(h) = (b_{ij} W_{\nu_{ij}}(a_{ij} h))_{i,j=1,2}$ with $C_{ij} = C_{ji}$, $\nu_{ij} > 0$, $i, j = 1, 2$ and $b_{ii} \geq 0$, $i = 1, 2$, is a matrix-valued positiv definite function if and only if

$$b_{ij}^2 \leq b_{11} b_{22} \frac{\Gamma(\nu_{11} + \frac{d}{2}) \Gamma(\nu_{22} + \frac{d}{2}) \Gamma(\nu_{12})^2}{\Gamma(\nu_{11}) \Gamma(\nu_{22}) \Gamma(\nu_{12} + \frac{d}{2})^2} \frac{a_{11}^{2\nu_{11}} a_2^{2\nu_{22}}}{a_{12}^{4\nu_{12}}} \inf_{t \geq 0} \frac{(a_{12}^2 + t^2)^{2\nu_{12}+d}}{\prod_{i=1}^{2} (a_{ii}^2 + t^2)^{\nu_{ii}+d/2}}.$$

[70] derive multivariate models with compact support. [82] give both necessary and sufficient conditions such that a matrix-valued covariance function is divergence free or curl free. They also show that this property is inherited by the corresponding Gaussian random field.

[14] present a multivariate version of the circulant embedding method, Sect. 2.9.2. Nonetheless, further methods for simulating multivariate models need to be developed.

2.12 Exercises

In the following, we give examples of covariance functions given in the literature that can be derived from the assertions presented in Sects. 2.2–2.8.

Exercise 2.1. [72] show that certain quasi-arithmetic means of completely monotone functions lead to positive definite functions. They give three examples for classes of positive definite functions. Show the positive definiteness for two of their examples:

1. Gumbel-Hougard family

$$\varphi(h_1, h_2) = \exp(-(\|h_1\|^{\rho_1} + \|h_2\|^{\rho_2})^\beta)$$

for any $\beta \in [0, 1]$, $\rho_i \in [0, 2]$, $h_i \in \mathbb{R}^{d_i}$, $d_i \in \mathbb{N}$, $i = 1, 2$.

2. Clayton family

$$\varphi(h_1, h_2) = [(1 + \|h_1\|)^{\rho_1} + (1 + \|h_2\|)^{\rho_2}]^{-\beta}$$

for any $\beta > 0$, $\rho_i \in [0, 1]$, $h_i \in \mathbb{R}^{d_i}$, $d_i \in \mathbb{N}$, $i = 1, 2$.

Hint: show that γ^{-1} is a covariance function for any strictly positive, conditionally negative definite function γ, considering a suitable mixture of the functions $\exp(-s\gamma)$, $s \geq 0$.

Exercise 2.2. [73] introduce the Dagum family

$$\gamma(h) = (1 + \|h\|^{-\beta})^{-\alpha}$$

and show that γ is a variogram in $\mathbb{R}^3$ if $\beta < (7-\alpha)/(1+5\alpha)$ and $\alpha < 7$. [6] present conditions so that the function $r \mapsto (1 + r^{-\beta})^{-\alpha}$ is completely monotone. Show that the Dagum family yields a variogram on $\mathbb{R}^d$ for $d \in \mathbb{N}$, $\alpha \in (0,1]$ and $\beta \in (0,2]$.

Hint: show that

$$\frac{\psi(0) - \psi(h)}{1 + \psi(0) - \psi(h)}$$

is a variogram for any positive definite function ψ, and conclude that $\gamma_0/(1+\gamma_0)$ is a variogram for any variogram γ_0. See [63] for an alternative proof.

Exercise 2.3. Let Z be an intrinsically stationary random field on $\mathbb{R}^d$ with variogram γ and z be fixed. Show that the covariance function of Y with $Y(x) = Z(x+z) - Z(x)$ equals

$$C(x,y) = \gamma(x-y+z) + \gamma(x-y-z) - 2\gamma(x-y), \qquad x, y \in \mathbb{R}^d$$

and conclude that

1. $f(h,z) = 2\gamma(z) + 2\gamma(h) - \gamma(h+z) - \gamma(h-z)$ is a variogram for any fixed z. See, for instance, Lemma 17 in [74] and Lemma 1 in [59] for proofs given in the literature.

   Show further that, although $f(z,h) = f(h,z)$, the function f is not a variogram in (h,z), in general. To this end, consider $\gamma(h) = |h|$ on $\mathbb{R}^1$ and verify that (2.2) is not satisfied.
2. The function $\varphi(h) = 0.5(\|h+1\|^{\alpha} - 2\|h\|^{\alpha} + \|h-1\|^{\alpha})$ is positive definite for $\alpha \in (0,2]$. The corresponding random field is called fractional Gaussian noise if $d = 1$.

Acknowledgements The author is grateful to Sebastian Engelke, Alexander Malinowski, Marco Oesting, Robert Schaback, and Kirstin Strokorb for valuable hints and comments.

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http://www.springer.com/978-3-642-17085-0

Advances and Challenges in Space-time Modelling of Natural Events

Porcu, E.; Montero, J.; Schlather, M. (Eds.)

2012, XIV, 252 p. 29 illus., Softcover
ISBN: 978-3-642-17085-0