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Multivariate versions of dimension walks and Schoenberg measures

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Abstract. This paper considers multivariate Gaussian fields with their associated matrix valued covariance functions. In particular, we characterize the class of stationary-isotropic matrix valued covariance functions on *d*-dimensional Euclidean spaces, as being the scale mixture of the characteristic function of a *d* dimensional random vector being uniformly distributed on the spherical shell of \mathbb{R}^d , with a uniquely determined matrix valued and signed measure. This result is the analogue of celebrated Schoenberg theorem, which characterizes stationary and isotropic covariance functions associated to an univariate Gaussian fields.

The elements **C**, being matrix valued, radially symmetric and positive definite on \mathbb{R}^d , have a matrix valued generator φ such that $\mathbf{C}(\tau) = \varphi(||\tau||)$, $\forall \tau \in \mathbb{R}^d$, and where $|| \cdot ||$ is the Euclidean norm. This fact is the crux, together with our analogue of Schoenberg's theorem, to show the existence of operators that, applied to the generators φ of a matrix valued mapping **C** being positive definite on \mathbb{R}^d , allow to obtain generators associated to other matrix valued mappings, say $\tilde{\mathbf{C}}$, being positive definite on Euclidean spaces of different dimensions.

1 Introduction

The use of matrix valued covariances for modeling multivariate data indexed by spatial coordinates has become ubiquitous, for instance, in environmental and climate sciences monitors collect information on multiple variables such as temperature, pressure, wind speed and particulate matter. The recent survey in Genton and Kleiber (2015) puts emphasis on the output of climate models, and on physical models in computer experiments, which often involve multiple processes that are indexed by not only space and time, but also parameter settings. It is very common to model these multivariate spatial (or space-time) data as being the realization from a multivariate Gaussian field, with the clear implication that the first two moments become the crux of accurate inference and prediction. For a vector valued weakly stationary Gaussian field { $Z_1(\mathbf{x}), \ldots, Z_m(\mathbf{x})$ }, $\mathbf{x} \in \mathbb{R}^d$, the covariance

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function, denoted $\mathbf{C}(\cdot) = [C_{ij}(\cdot)]$ hereafter, is a matrix valued mapping, so that $C_{ij}(\tau) = \text{Cov}(Z_i(\mathbf{x}), Z_j(\mathbf{x} + \tau))$ is called cross covariance for $i \neq j$, and for i = j we have the autocovariances of the scalar processes Z_i .

There is a fertile literature in the last five years on this kind of mappings, and we refer the reader to Alonso-Malaver, Porcu and Giraldo (2015), Apanasovich and Genton (2010), Apanasovich, Genton and Sun (2011), Daley, Porcu and Bevilacqua (2015), Gneiting, Kleiber and Schlather (2010), Hristopoulos and Porcu (2014), Kleiber and Porcu (2015), Porcu et al. (2013) and Ruiz-Medina and Porcu (2015), as well as to the survey in Genton and Kleiber (2015) with the references therein.

In this paper, we use Φ_d^m to denote the class of matrix valued functions $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^m$, with $\varphi_{ij} : [0, \infty) \to \mathbb{R}$ being continuous, $\varphi_{ii}(0) = 1$, and such that there exists a stationary Gaussian *m*-variate random field {**Z**(**x**) = $(Z_1(\mathbf{x}), Z_2(\mathbf{x}), \dots, Z_m(\mathbf{x}))$ } with matrix valued covariance

$$\mathbf{C}(\boldsymbol{\tau}) = \left[C_{ij}(\boldsymbol{\tau})\right]_{i,j=1}^{m} = \operatorname{Cov}(\mathbf{Z}(\mathbf{x}), \mathbf{Z}(\mathbf{x}+\boldsymbol{\tau}))$$

= diag{ $\boldsymbol{\sigma}$ }[$\boldsymbol{\varphi}(\|\boldsymbol{\tau}\|)$]_{i,j=1}^{m} diag{ $\boldsymbol{\sigma}$ }, $\mathbf{x}, \boldsymbol{\tau} \in \mathbb{R}^{d}$ (1.1)

with $\|\cdot\|$ being the Euclidean norm and diag{ σ } a $m \times m$ diagonal matrix with $0 < \sigma_j < \infty$, j = 1, ..., m. We call φ the generator of **C** and, conversely, we call **C** the radial version of φ . Also, Φ_d shall be short notation for the class of functions Φ_d^1 , being the celebrated Schoenberg class as used in Daley and Porcu (2014), Gneiting (1999a) and Gneiting (1999b), which has a long history in probability and statistics [Schoenberg (1938)], Random Fields (RFs for short) theory [Yaglom (1987)] and numerical analysis [e.g. Fasshauer (1995), Wendland (1995) and Wendland (2005)].

Starting from Bochner–Khintchine representation of a stationary covariance function on \mathbb{R}^d —see Bochner (1933) and Khintchine (1934)—the class Φ_d has been characterized by Schoenberg (1938) as being the class of scale mixtures of the characteristic function of a random vector being uniformly distributed on the spherical shell of radius one in \mathbb{R}^d , with a probability measure on the positive real line (see subsequent Theorem A). A characterization of the class Φ_d^m remained elusive when m > 1 and the first part of the paper is devoted to show that a Schoenberg type representation can be extended to the matrix covariance case, but this time the probability measure in the scale mixture will be shown to be a matrix valued, with positive definite realizations.

This new result will offer then the arguments to show the existence of operators that allow for arbitrary walks through dimensions. Rephrased, this paper proposes operators that, applied to generators φ in the class Φ_d^m , allow to obtain new generators belonging to the classes $\Phi_{d'}^m$, for $d \neq d'$. The case m = 1 was originally proposed in Wendland (1995) (and rephrased in Gneiting (2002)), on the basis of Matheron (1965)'s tour de force. The importance of these operators relies in the following facts:

(a) By well-known results, the differentiability at the origin of the covariance function is crucial to determine the properties in terms of differentiability (in the mean square sense) of the associated Gaussian field, as well as in terms of fractal dimension. This fact extends *mutatis mutandis* to vector valued fields. A matrix valued and isotropic matrix valued mapping inherits the properties of its associated generator in terms of differentiability at the origin, seen as even extension, since generators are defined on the positive real line only. The operators proposed in this paper allow to modify the differentiability at the origin of the generator, at the expense of some walk through dimensions, exactly in the same way as obtained, for the case m = 1, by Wendland (1995).

(b) These operators are then crucial in order to simulate Gaussian fields through turning bands techniques, being well understood in the case m = 1, but almost unexplored for the case m > 1.

It is necessary to notice that the representation given in equation (3.1)-Theorem 3.1—is relating about the isotropic matrix correlations functions which are Lebesgue integrable, and since all the results developed is this paper are based on this representation—Theorems 4.1, 4.2 and 5.1—it is straight to deduce that all the paper is restricted to the class of Lebesgue integrable isotropic matrix correlations functions.

The remainder of this paper is organized as follow: Section 2 introduces the background and notation, the analogue of Schoenberg theorem to the class Φ_d^m is presented in Section 3, Section 4 is dedicated to introduce the multivariate versions of Montée and Descente with special attention to show this operators as dimensional walks. At the end, Section 5, some dimensional operators are shown which are the analogues of the Turning Bands equations introduced by Matheron—see Matheron (1965, 1972, 1973)—result which opens a line to research in the simulation of vector valued Gaussian fields.

2 Background and notation

Let M_m be the set of $m \times m$ -dimensional complex-matrices. A mapping $\mathbf{K} = [K_{ij}]_{i,j=1}^m : \mathbb{R}^d \times \mathbb{R}^d \to M_m$ is positive definite if for any finite dimensional collection of points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of \mathbb{R}^d and the same number of *m*-dimensional vectors $\mathbf{c}_1, \ldots, \mathbf{c}_n \in \mathbb{C}^m$, $\mathbf{c}_i = (c_{i1}, \ldots, c_{im})'$, the following inequality holds:

$$\sum_{j,k}^{n} \sum_{i,l}^{m} c_{ji} \overline{c}_{kl} K_{il}(\mathbf{x}_j, \mathbf{x}_k) \ge 0.$$
(2.1)

Kolmogorov's existence theorem—see Billingsley (1995), Theorems 36.1–36.2 implies that, for any positive definite mapping **K** as defined above, there exists a Gaussian vector valued field $\mathbf{Z}(\mathbf{x}) = (Z_1(\mathbf{x}), \dots, Z_m(\mathbf{x}))'$ on \mathbb{R}^d such that

$$\operatorname{Cov}(Z(\mathbf{x}), Z(\mathbf{y})) = \mathbf{K}(\mathbf{x}, \mathbf{y}) = [K_{ij}(\mathbf{x}, \mathbf{y})]_{i,j=1}^{m}, \qquad \mathbf{x}, \mathbf{y} \in \mathbb{R}^{d}$$

Under the additional assumption of stationarity, there exists a matrix function C, such that K(x, y) = C(x - y).

As stated in the Introduction, the present paper deals with the class Φ_d^m of generators $\varphi : [0, \infty) \to M_m$ associated to positive definite, stationary and isotropic matrix valued mappings $\mathbf{C} : \mathbb{R}^d \to M_m$ in a way that $\mathbf{C}(\tau) = \text{diag}\{\sigma\}\varphi(\|\tau\|) \text{diag}\{\sigma\}, \tau \in \mathbb{R}^d$, where σ_j is the variance of the field $Z_j, j = 1, ..., m$.

We shall equivalently use $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^m$ or $\varphi_d(\cdot) = [\varphi_{dij}(\cdot)]_{i,j=1}^m$ in order to denote an element of the class Φ_d^m as it will be apparent from the context. The notation φ_{dij} will be especially important when dealing with projection operators as those illustrated in Section 5.

Matheron (1965) proposed the terms Montée and Descente to describe operators that, applied to generators $\varphi \in \Phi_d$, offer respectively members of Φ_{d-2} (for $d \ge 3$) and Φ_{d+2} . We present their multivariate analogues and show that similar results yield for the case m > 1 within the classes Φ_d^m . In particular, we call these operators *m*-Montée and the *m*-Descente. Wendland (2005) adopts the illustrative name walk through dimension for the case m = 1 and we make use of this even for the *m*-variate case.

The class Φ_d^m is non-increasing in d, and the following inclusion relations

$$\Phi_1^m \supset \Phi_2^m \supset \cdots \supset \Phi_\infty^m$$

are strict. To show this, consider the following example. In the univariate case (m = 1), Schaback (1995) defined Euclid's hat function $h_d(\cdot)$, as the self-convolution of the indicator function of the *d*-dimensional ball of radius one in \mathbb{R}^d , and Gneiting (1999c) showed that the function $h_d(\cdot)$ belongs to the class of functions Φ_d but is not in $\Phi_{d'}$ for any integer d' > d. From this univariate example, we can define the *m*-variate matrix covariance function $\mathbf{H}(\tau) := \text{diag}\{h_d(||\tau||), \ldots, h_d(||\tau||)\}_{m \times m}$, with $\tau \in \mathbb{R}^d$, which belongs to the class of functions Φ_d^m and the results in Gneiting (1999c) allow us to show that it does not belong to Φ_d^m for any positive integer d' > d.

Closing this section, we present two celebrated results which are the starting point of all developments, we report them for the sake of a self-contained exposition. The former is the Cramer's generalization of the Bochner–Khintchine's theorem from univariate RF's to multivariate RF's, and the latter one is the Schoenberg's integral representation of an isotropic correlation function.

Theorem A (Cramer, 1940). Let $\mathbf{X}(t) = (X_1(t), X_2(t), \dots, X_m(t))$ be a complex continuous¹ stationary process, then the matrix covariance function of $\mathbf{X}(t)$, are for all real t given by the Fourier–Stieltjes integral of the form

$$\mathbf{C}(t) = \operatorname{Cov}(\mathbf{X}(t+h), \mathbf{X}(h)) = [C_{ij}(t)]_{i,j=1}^{m}$$

$$= \left[\int_{-\infty}^{\infty} e^{itx} F_{ij}(\mathrm{d}x)\right]_{i,j=1}^{m} =: \int_{-\infty}^{\infty} e^{itx} \mathbf{F}(\mathrm{d}x),$$
(2.2)

¹Continuity in mean square sense.

where the F_{ij} are functions of bounded variation in $(-\infty, \infty)$, which we may assume to be everywhere continuous to the right. And given $a, b \in \mathbb{R}$ with $a \leq b$, $\mathbf{F}(b) - \mathbf{F}(a) = [F_{ij}(b) - F_{ij}(a)]$ is a positive definite matrix.

In the previous result, the functions F_{jj} are probability measures in \mathbb{R} and, for $i \neq j$, F_{ij} are in general signed measures in \mathbb{R} .

Theorem B (Schoenberg, 1938). For every positive integer $d \ge 1$, $\varphi \in \Phi_d$ if and only if there exists a probability measure λ_d on $[0, \infty)$, such that

$$\varphi(t) = \int_0^\infty \Omega_d(rt) \lambda_d(\mathrm{d}r), \qquad (2.3)$$

where $\Omega_d(t) = E(\exp^{it(\mathbf{e}_1, \boldsymbol{\eta})})$ for $t \ge 0$, \mathbf{e}_1 is a unit vector in \mathbb{R}^d , and $\boldsymbol{\eta}$ is a random vector uniformly distributed on the unit spherical shell $\mathbb{S}^{d-1} \subset \mathbb{R}^d$.

3 Multivariate version of Schoenberg's theorem

In this section, we extend the Schoenberg's Theorem B, to the *m*-variate case $(m \ge 2)$.

Theorem 3.1 (Extension of Schoenberg's representation to the class Φ_d^m). Let *m* and *d* be positive integers. A matrix valued function $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^m$: $[0, \infty) \to M_m$ with φ_{ij} continuous, *i*, *j* = 1, ..., *m*, and $\varphi_{ii}(0) = 1$, belongs to the class Φ_d^m if and only if it can be written as

$$\boldsymbol{\varphi}(t) = \left[\varphi_{ij}(t)\right]_{i,j=1}^{m} = \left[\int_{0}^{\infty} \Omega_d(rt)\lambda_{ij}(\mathrm{d}r)\right]_{i,j=1}^{m} =: \int_{0}^{\infty} \Omega_d(rt)\mathbf{\Lambda}_d(\mathrm{d}r), \quad (3.1)$$

where $\lambda_{ij}(\cdot)$ are functions of bounded variation on $[0, \infty)$, and given $a, b \in [0, \infty)$ with $0 \le a \le b$, $\Lambda_d(b) - \Lambda_d(a) = [\lambda_{ij}(b) - \lambda_{ij}(a)]_{i,j=1}^m$ is a positive definite matrix, that is, the function

$$H(c_1, c_2, \dots, c_m) = \sum_{i,j=1}^m c_i \overline{c}_j [\lambda_{ij}(b) - \lambda_{ij}(a)], \qquad (3.2)$$

is non-negative for all $c_1, c_2, \ldots, c_m \in \mathbb{C}$.

Proof. Without lost of generality, we give a constructive proof assuming $\sigma_1 = \cdots = \sigma_m = 1$ —see equation (1.1)—that is, we shall work inside the class of matrix valued correlation functions.

The proof is based on the following arguments: (i) first, we show that every matrix valued function $\varphi \in \Phi_d^m$ can be represented in the form (3.1) and the restriction (3.2) is satisfied, then (ii) we show the converse, that is, if a matrix valued function φ can be written in the form (3.1) and the restriction (3.2) is fulfilled then

 $\boldsymbol{\varphi}$ belongs to Φ_d^m (i.e., $\mathbf{C}(\mathbf{x}) = \boldsymbol{\varphi}(\|\mathbf{x}\|)$ is a positive definite matrix valued function on \mathbb{R}^d), and finally (iii) we show that the functions $\lambda_{ij}(\cdot)$ are functions of bounded variation on $[0, \infty)$.

(i) Let $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^m$ be a member of Φ_d^m . Following Schoenberg (1938), we define $\omega(d\xi)$ as the area of an element of the spherical shell $\mathbb{S}^{d-1} = \{\xi \in \mathbb{R}^d : \|\xi\| = 1\}$, and ω_d the total area of \mathbb{S}^{d-1} . The mean value of $e^{i\tau \cdot \xi}$ over \mathbb{S}^{d-1} is invariant with respect to rotations in \mathbb{R}^d about the origin and can be written as

$$\Omega_d(\|\boldsymbol{\tau}\|) = \frac{1}{\boldsymbol{\omega}_d} \int_{\mathbb{S}^{d-1}} e^{i\boldsymbol{\tau}\cdot\boldsymbol{\xi}} \omega(\mathrm{d}\boldsymbol{\xi}), \qquad \boldsymbol{\tau} \in \mathbb{R}^d.$$
(3.3)

By assumption the matrix valued function $C(\tau)$ is rotation invariant, then we can write

$$\boldsymbol{\varphi}(\|\boldsymbol{\tau}\|) = \frac{1}{\omega_d} \int_{\mathbb{S}^{d-1}} \mathbf{C}(\|\boldsymbol{\tau}\|\boldsymbol{\xi}) \omega(\mathrm{d}\boldsymbol{\xi}).$$
(3.4)

Using Cramer's representation of $C(\cdot)$ —see equation (2.2)—equation (3.4) becomes

$$\mathbf{C}(\boldsymbol{\tau}) = \int_{\mathbb{R}^d} \left[\frac{1}{\boldsymbol{\omega}_d} \int_{\mathbb{S}^{d-1}} e^{i \|\boldsymbol{\tau}\| \boldsymbol{\xi} \cdot \boldsymbol{\alpha}} \boldsymbol{\omega}(\mathrm{d}\boldsymbol{\xi}) \right] \mathbf{F}(\mathrm{d}\boldsymbol{\alpha})$$
$$= \int_{\mathbb{R}^d} \Omega_d (\|\boldsymbol{\tau}\| \|\boldsymbol{\alpha}\|) \mathbf{F}(\mathrm{d}\boldsymbol{\alpha}), \quad \boldsymbol{\alpha} \in \mathbb{R}^d.$$
(3.5)

Now, the components of the matrix \mathbf{F} can be seen as signed measures, so that it is well defined

$$\mathbf{\Lambda}_{d}(u) = \int_{\|\boldsymbol{\alpha}\| \le u, \boldsymbol{\alpha} \in \mathbb{R}^{d}} \mathbf{F}(\mathrm{d}\boldsymbol{\alpha}) = \mathbf{F}(\|\boldsymbol{\alpha}\| \le u), \qquad u \in \mathbb{R},$$
(3.6)

and equation (3.5) turns into equation (3.1) after a direct inspection.

In order to verify that the function H in equation (3.2) is non-negative for all $0 \le a \le b$, we define a *m*-variate stationary-isotropic field $Z(\mathbf{x}) = (Z_1(\mathbf{x}), \ldots, Z_m(\mathbf{x}))^T$, $\mathbf{x} \in \mathbb{R}^d$, with matrix valued covariance function $\mathbf{C}(\tau) = \boldsymbol{\varphi}(\|\boldsymbol{\tau}\|) = [\varphi_{ij}(\|\boldsymbol{\tau}\|)]_{i,j=1}^m$, $\tau \in \mathbb{R}^d$. Let

$$L(\mathbf{x}) := \sum_{i=1}^{m} c_i Z_i(\mathbf{x})$$

be a univariate field with $c_1, c_2, \ldots, c_m \in \mathbb{C}$. The covariance function of $L(\cdot)$ is

$$C_L(\boldsymbol{\tau}) = \sum_{i,j=1}^m c_i \overline{c}_j \varphi_{ij} (\|\boldsymbol{\tau}\|),$$

that is, C_L is a stationary-isotropic univariate covariance function on \mathbb{R}^d , and by equation (2.3) in Theorem B, it can be written as

$$C_L(t) = \int_{[0,\infty)} \Omega_d(rt) \lambda_L(\mathrm{d}r), \qquad (3.7)$$

where $\lambda_L(r)$ is a bounded and non-decreasing function for $r \ge 0$. The relation in (3.7) is one-to-one, so that the function $\lambda_L(\cdot)$ is unique and

$$0 \le \lambda_L(b) - \lambda_L(a) = \sum_{i,j=1}^m c_i \overline{c}_j [\lambda_{ij}(b) - \lambda_{ij}(a)],$$

for any $a, b \in [0, \infty)$ with $0 \le a \le b$.

(ii) For the converse, we need to prove that, given the form

$$Q(\mathbf{t}, \mathbf{c}) = \sum_{i,j}^{n} \sum_{k,l}^{m} c_{ik} \overline{c}_{jl} \varphi_{kl}(t_{ij})$$

with $\varphi_{kl}(t_{ij})$ as in equation (3.1), and the set of functions λ_{ij} 's obeying the property (3.2), $Q(\mathbf{t}, \mathbf{c})$ is a positive definitive form for all $n \in \mathbb{N}$, for all $c_{ik} \in \mathbb{C}$ (i = 1, 2, ..., n; k = 1, 2, ..., m), and all $t_{ij} \in (0, \infty)$ (i, j = 1, 2, ..., n).

We suppose *n* locations $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n$ on \mathbb{R}^d such that, $\|\mathbf{x}_i - \mathbf{x}_j\| = t_{ij}$. By equation (3.1), we have

$$Q(\mathbf{t}, \mathbf{c}) = \int_{[0,\infty)} \sum_{i,j}^{n} \sum_{k,l}^{m} c_{ik} \overline{c}_{jl} \Omega_d (\|\mathbf{x}_i - \mathbf{x}_j\| u) \lambda_{kl} (\mathrm{d}u), \qquad (3.8)$$

so that using the analytic expansion of $\Omega_d(\cdot)$ as in equation (3.3), we have

$$Q(\mathbf{t}, \mathbf{c}) = \frac{1}{\boldsymbol{\omega}_d} \int_{S^{d-1}} \left[\int_{[0,\infty)} \sum_{k,l}^m \sum_{i,j}^n c_{ik} \overline{c}_{jl} e^{iu(\mathbf{x}_i - \mathbf{x}_j) \cdot \boldsymbol{\xi}} \lambda_{kl}(\mathrm{d}u) \right] \omega(\mathrm{d}\boldsymbol{\xi})$$

$$= \frac{1}{\boldsymbol{\omega}_d} \int_{S^{d-1}} \left[\int_{[0,\infty)} \sum_{k,l}^m z_k \overline{z}_l \lambda_{kl}(\mathrm{d}u) \right] \omega(\mathrm{d}\boldsymbol{\xi}),$$
(3.9)

where $z_k = \sum_{i}^{n} c_{ik} e^{iu\mathbf{x}_i \cdot \boldsymbol{\xi}}$. By property (3.2), the inner integral in (3.9) is positive. The proof is completed.

(iii) To verify that the function $\lambda_{ij}(t)$ is a function of bounded variation in $[0, \infty)$, from equation (3.6), it is enough to write

$$\left| \int_{[0,\infty)} \lambda_{ij}(\mathrm{d}t) \right| = \left| \int_{\mathbb{R}^d} F_{ij}(\mathrm{d}\alpha) \right| = \left| C_{ij}(\mathbf{0}) \right| \le \left[C_{ii}(\mathbf{0}) C_{jj}(\mathbf{0}) \right]^{1/2}.$$
(3.10)

Under the assumption $\varphi(\cdot) \in L_1([0, \infty))$, component-wise, we can represent φ in equation (3.1) as an ordinary Fourier integral, see Yaglom (1987, pages 311–312).

Corollary 3.1.1 (*m*-variate version of Schoenberg's Lemma 4). Let $\varphi(\cdot) \in \Phi_d^m$, then $\varphi(\cdot)$ is $\lfloor \frac{d-1}{2} \rfloor$ -differentiable, that is the function $\varphi^{(v)}(t) = [\varphi_{ij}^{(v)}(t)]_{i,j=1}^m$ is well defined on $(0, \infty)$, for $v \leq \lfloor \frac{d-1}{2} \rfloor$, where [x] is the greatest integer less than or equal to x.

Proof. For proving this result, it is enough to recall $\frac{\partial^v}{\partial t^v}\Omega_d(t) = \Omega_d^{(v)}(t) = \mathcal{O}(t^{-(d-1)/2})$ and hence $\Omega_d^{(v)}(tr) = \mathcal{O}(r^{v-(d-1)/2})$ —see Schoenberg (1938)—so that $\Omega_d^{(v)}(tr)$ converges absolutely, in r, for $v \leq \lfloor \frac{d-1}{2} \rfloor$.

4 Montée and Descente for the class Φ_d^m

This section extends the results in Matheron (1965), and subsequent results in Gneiting (2002), Daley and Porcu (2014), Schaback (1995) and Wendland (1995) to the class Φ_d^m , for m > 1. Some definitions are needed, for a neater exposition.

Definition 4.1. Let $\mathbf{f}(t) = [f_{ij}(t)]_{i,j=1}^m : [0,\infty) \to M_m$, with $f_{ij} : [0,\infty) \to \mathbb{R}$. We define the *m*-Montée and *m*-Descente operators as, respectively,

$$\tilde{I}_m \mathbf{f}(t) := \left[\frac{\int_t^\infty u f_{ij}(u) \, \mathrm{d}u}{\alpha_i \alpha_j} \right]_{i,j=1}^m, \qquad t \ge 0,$$
(4.1)

where $\alpha_j = (\int_0^\infty u f_{jj}(u) \, du)^{1/2}, \ j = 1, ..., m$, and

$$\tilde{D}_m \mathbf{f}(t) := \left[\frac{-f'_{ij}(t)}{t\beta_i \beta_j} \right]_{i,j=1}^m, \qquad t > 0.$$
(4.2)

where $\beta_j = (-\lim_{t \downarrow 0} \frac{f'_{jj}(t)}{t})^{1/2}, j = 1, ..., m.$

The *m*-Montée operator can be written as

$$\tilde{I}_m \mathbf{f}(t) = \operatorname{diag}\{\boldsymbol{\alpha}\} I_m \mathbf{f}(t) \operatorname{diag}\{\boldsymbol{\alpha}\}, \qquad (4.3)$$

with diag{ α } a $m \times m$ diagonal matrix, where the *m*-vector $\alpha = (\alpha_1^{-1}, \dots, \alpha_m^{-1})$ and

$$I_m \mathbf{f}(t) = \left[\int_t^\infty u f_{ij}(u) \, \mathrm{d}u \right]_{i,j=1}^m$$

can be thought as the non-standardized version of the m-Montée operator. Analogously, for the m-Descente, we have

$$\hat{D}_m \mathbf{f}(t) = \operatorname{diag}\{\boldsymbol{\beta}\} D_m \mathbf{f}(t) \operatorname{diag}\{\boldsymbol{\beta}\}, \qquad (4.4)$$

with diag{ $\boldsymbol{\beta}$ } a $m \times m$ diagonal matrix where $\boldsymbol{\beta} = (\beta_1^{-1}, \dots, \beta_m^{-1})$, and

$$D_m \mathbf{f}(t) = \left[\frac{-f_{ij}'(t)}{t}\right]_{i,j=1}^m$$

is the non-standardized version of the *m*-Descente operator.

The arguments in Gneiting (1999b, page 89) and direct inspection show that if the matrix valued function f(t) in (4.1) is componentwise 2k-times differentiable at zero, k = 0, 1, 2, ..., then $\tilde{I}_m \mathbf{f}(t)$ has 2k + 2 derivatives at zero. To show the result, note that

$$(\tilde{I}_m \mathbf{f})^{(v+2)}(t) = -(v+1)\mathbf{f}^{(v)}(t) - t\mathbf{f}^{(v+1)}(t), \qquad v = 0, 1, \dots, 2k,$$
(4.5)

where $\mathbf{f}^{(v)}(t) = \begin{bmatrix} \frac{\partial J_{ij}(t)}{\partial t^v} \end{bmatrix}_{i,j=1}^m$. Here, by derivative at zero we mean the even extension of the function \mathbf{f} , because these functions are supported on the positive real line.

In the next two theorems, we summarize two of the most important findings in this paper. In the first one, we show that \tilde{I}_m is a descending dimensional walk, from Φ_d^m to Φ_{d-2}^m $(d \ge 3)$, and the second one says \tilde{D}_m is an ascending dimensional walk, from Φ_d^m to Φ_{d+2}^m . These two results are well known in the univariate case, see Matheron (1965, 1972).

Theorem 4.1. Let *m* and *d* be positive integers. If $\varphi(\cdot) = [\varphi_{ij}(\cdot)]_{i,j=1}^{m}$ belongs to the class Φ_d^m and $\int_{[0,\infty)} t\varphi_{ij}(t) dt$ is finite (i, j = 1, ..., m), then for $d \ge 3$ the function $\boldsymbol{\varrho}(t) := \tilde{I}_m \boldsymbol{\varphi}(t)$ belongs to Φ_{d-2}^m , and

$$\boldsymbol{\varrho}(t) = \left[\int_{[0,\infty)} \Omega_{d-2}(tu)\eta_{ij}(\mathrm{d}u)\right]_{i,j=1}^m = \int_{[0,\infty)} \Omega_{d-2}(tu) \boldsymbol{\Lambda}_{\boldsymbol{\varrho}}(\mathrm{d}u), \qquad (4.6)$$

where

$$\Lambda_{\boldsymbol{\varrho}}(\mathrm{d}\boldsymbol{u}) = \left[\eta_{ij}(\mathrm{d}\boldsymbol{u})\right]_{i,j=1}^{m} = \left[\frac{(d-2)\lambda_{ij}(\mathrm{d}\boldsymbol{u})}{\alpha_{i}\alpha_{j}\boldsymbol{u}^{2}}\right]_{i,j=1}^{m},\tag{4.7}$$

with $\lambda_{ij}(\cdot)$ given in equations (3.1) and (3.2) $(i, j = 1, 2, ..., m), \alpha_j =$ $(\int_{[0,\infty)} u\varphi_{jj}(u) du)^{1/2}, j = 1, \dots, m, and given a, b \in [0,\infty), a \le b$ the function

$$K_1(c_1, c_2, \dots, c_m) = \sum_{i,j=1}^m c_i \overline{c}_j [\eta_{ij}(b) - \eta_{ij}(a)],$$
(4.8)

is non-negative for all $c_1, c_2, \ldots, c_m \in \mathbb{C}$.

In order to prove the assertion, we need to prove that given an element φ of the class of functions Φ_d^m , we have that $\boldsymbol{\varrho}(\cdot) = I_m \boldsymbol{\varphi}(\cdot)$ satisfies the equations (4.6) to (4.8), and $\int_{[0,\infty)} u\varphi_{jj}(u) du \ge 0$ so the standardization constants α_j are well defined (j = 1, ..., m). The rest of the proof will come from Theorem 3.1.

Proof. We make use of the next properties (see Daley and Porcu (2014)): (i) $1 = \Omega_d(0) > |\Omega_d(x)|$ for all x > 0, (ii) $\lim_{x \to \infty} \Omega_d(x) = 0$ and (iii). $\Omega'_d(x) = 0$ $\frac{-x}{d}\Omega_{d+2}(x)$, for $d \ge 1$, and this derivative is uniformly bounded for all $x \ge 0$. For short, these properties will be recalled as P-(i), P-(ii) and P-(iii), respectively.

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Mimicking Daley and Porcu (2014), we have

$$\int_{0}^{t} z \boldsymbol{\varphi}(z) \, \mathrm{d}z = \int_{0}^{t} z \left[\int_{[0,\infty)} \Omega_{d}(zu) \mathbf{\Lambda}_{d}(\mathrm{d}u) \right] \mathrm{d}z \qquad \text{by (3.1)}$$

$$= \int_{[0,\infty)} \left[\int_{0}^{t} z \Omega_{d}(zu) \, \mathrm{d}z \right] \mathbf{\Lambda}_{d}(\mathrm{d}u) \qquad \text{by Fubini's theorem.}$$

$$(4.9)$$

Here, we have to recall $\Lambda_d(\cdot)$ is a matrix valued function of bounded variation componentwise—so we can write $\Lambda_d(\cdot) = \mathbf{G}(\cdot) - \mathbf{H}(\cdot)$, with **G** and **H** matrices componentwise non-decreasing functions,² and use Fubini's theorem over the double integral of the difference $\mathbf{G} - \mathbf{H}$.

By *P*-(iii), equation (4.9) becomes

$$\int_{0}^{t} z \boldsymbol{\varphi}(z) \, \mathrm{d}z = \int_{[0,\infty)} u^{-2} \Big[\int_{0}^{tu} -(d-2) \Omega'_{d-2}(v) \mathrm{d}v \Big] \mathbf{\Lambda}_{d}(\mathrm{d}u) = \int_{[0,\infty)} (d-2) u^{-2} \big[\Omega_{d-2}(0) - \Omega_{d-2}(tu) \big] \mathbf{\Lambda}_{d}(\mathrm{d}u).$$
(4.10)

Since $\int_{[0,\infty)} t\varphi(t) dt$ is finite by assumption, we have that $u^{-2}\Lambda_d(du)$ is a function of bounded variation on \mathbb{R}_+ . By *P*-(ii), we can bound the difference $\Omega_{d-2}(0) - \Omega_{d-2}(tu)$ in (4.10) and writing $\Lambda_d(du) = \mathbf{G}(du) - \mathbf{H}(du)$, then we can use dominated convergence theorem to justify taking the limit $t \to \infty$ there. This provides that $\int_0^\infty z\varphi(z) dz = (d-2) \int_{[0,\infty)} u^{-2} \Lambda_d(du)$.

Then, by complement,

$$\tilde{I}_m \boldsymbol{\varphi}(z) = \left[\int_{[0,\infty)} \Omega_{d-2}(tu) \eta_{ij}(\mathrm{d}u) \right]_{i,j=1}^m$$

with $\eta_{ij}(du)$ as stated, therefore (4.6) and (4.7) are satisfied. To prove the property (4.8), given $0 \le a \le b$, we have

$$\eta_{ij}(b) - \eta_{ij}(a) = \int_a^b \eta_{ij}(\mathrm{d}u) = \frac{d-2}{\alpha_i \alpha_j} \int_a^b u^{-2} \lambda_{ij}(\mathrm{d}u),$$

then

$$K_{1}(c_{1},...,c_{m}) = \sum_{i,j=1}^{m} c_{i}\overline{c}_{j}[\eta_{ij}(b) - \eta_{ij}(a)]$$

$$= (d-2)\sum_{i,j=1}^{m} \frac{c_{i}\overline{c}_{j}}{\alpha_{i}\alpha_{j}} \Big[\int_{a}^{b} u^{-2}\lambda_{ij}(du) \Big]$$
(4.11)
$$= (d-2)\int_{a}^{b} u^{-2}\sum_{i,j=1}^{m} a_{i}\overline{a}_{j}\lambda_{ij}(du) \ge 0$$
by equation (3.2).

²In fact $\mathbf{G}(x) = V(\mathbf{\Lambda}_d, [0, x])$ and $\mathbf{H}(x) = \mathbf{G}(x) - \mathbf{\Lambda}_d(x)$, where V(f, [0, x]) denotes the total variation of the function f in the set [0, x]. We may alternatively suppose that $\mathbf{G}(\cdot)$ and $\mathbf{H}(\cdot)$ are strictly—component—increasing functions.

Here $a_i = c_i / \alpha_i$ (j = 1, ..., m).

Remark A. By the same arguments leading to equation (4.10) and by P-(i), we have

$$0 \le (d-2)E(U^{-2}) = (d-2)\int_{[0,\infty)} u^{-2}\lambda_{jj}(du) = \int_0^\infty z\varphi_{jj}(z) \, dz < \infty, \qquad j = 1, \dots, m,$$

where *U* is a random variable distributed on $[0, \infty)$ according the cumulative distribution function λ_{jj} , j = 1, ..., m.

Theorem 4.2. Let *m* and *d* be positive integers. If a matrix valued function $\varphi(t) = [\varphi_{ij}(t)]_{i,j=1}^m$ belongs to Φ_d^m with each φ_{ij} being differentiable (i, j = 1, ..., m), then the function $\mathbf{v}(t) = \tilde{D}_m \varphi(t)$ is well defined for $t \ge 0$, it belongs to Φ_{d+2}^m , and

$$\mathbf{v}(t) = \left[\int_{[0,\infty)} \Omega_{d+2}(tu) \kappa_{ij}(\mathrm{d}u)\right]_{i,j=1}^m = \int_{[0,\infty)} \Omega_{d+2}(tu) \mathbf{\Lambda}_{\mathbf{v}}(\mathrm{d}u), \qquad (4.12)$$

where

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$$\mathbf{\Lambda}_{\boldsymbol{\nu}}(\mathrm{d}\boldsymbol{u}) = \left[\kappa_{ij}(\mathrm{d}\boldsymbol{u})\right]_{i,j=1}^{m} = \left[\frac{u^{2}\lambda_{ij}(\mathrm{d}\boldsymbol{u})}{d\beta_{i}\beta_{j}}\right]_{i,j=1}^{m},\tag{4.13}$$

with $\lambda_{ij}(\cdot)$ as in equations (3.1) and (3.2) (i, j = 1, ..., m), $\beta_j =: (-\lim_{t\downarrow 0} \varphi_{jj}(t)/t)^{1/2}$ (j = 1, ..., m), and given $a, b \in [0, \infty)$, $a \leq b$ the function

$$K_{2}(c_{1}, c_{2}, \dots, c_{m}) = \sum_{i,j=1}^{m} c_{i} \overline{c}_{j} [\kappa_{ij}(b) - \kappa_{ij}(a)], \qquad (4.14)$$

is non-negative for all $c_1, c_2, \ldots, c_m \in \mathbb{C}$.

Proof. Again, we need to prove that the equations (4.12)–(4.14) are satisfied for $v(\cdot) = \tilde{D}_m \varphi(\cdot)$. Then, we need show that $-\lim_{t\downarrow 0} \varphi_{jj}(t)/t \ge 0$, so that the constants β_j are well defined (j = 1, ..., m), and finally we can use Theorem 3.1 to prove the assertion.

We have $\tilde{D}_m \boldsymbol{\varphi}(t) = \left[\frac{-\varphi'_{ij}(t)}{t\beta_i\beta_j}\right]_{i,j=1}^m$. Then working componentwise,

$$\frac{-\varphi_{ij}'(t)}{t\beta_i\beta_j} = \frac{-1}{t\beta_i\beta_j} \int_{[0,\infty)} \frac{\partial\Omega_d(tu)}{\partial t} \lambda_{ij}(du)$$
$$= \frac{-1}{t\beta_i\beta_j} \int_{[0,\infty)} \frac{-tu^2}{d} \Omega_{d+2}(tu)\lambda_{ij}(du) \qquad \text{by } P\text{-(ii)} \qquad (4.15)$$
$$= \int_{[0,\infty)} \Omega_{d+2}(tu)\kappa_{ij}(du).$$

Here $\kappa_{ij}(du) = u^2 \lambda_{ij}(du)/d\beta_i \beta_j$. Given *m* and *d* positive integers, equation (4.15) implies that the definition of $\tilde{D}_m \mathbf{f}(\cdot)$ can be extended to t = 0 whenever $\boldsymbol{\varphi} \in \Phi_d^m$, understanding the differentiability of φ at zero as even extension of each component $\varphi_{ii}(\cdot), i, j = 1, \dots, m$.

Following the same arguments as in (4.11), we shall show that the form (4.14)is non-negative. For this, we have

$$\kappa_{ij}(b) - \kappa_{ij}(a) = \int_a^b \kappa_{ij}(\mathrm{d}u) = \frac{1}{d\beta_i\beta_j} \int_a^b u^2 \lambda_{ij}(\mathrm{d}u),$$

and

$$K_{2}(c_{1}, c_{2}, \dots, c_{m}) = \sum_{i,j=1}^{m} c_{i}\overline{c}_{j} [\kappa_{ij}(b) - \kappa_{ij}(a)]$$

$$= \frac{1}{d} \int_{a}^{b} u^{2} \sum_{i,j=1}^{m} b_{i}\overline{b}_{j}\lambda_{ij}(du) \ge 0, \quad \text{by equation (3.2).}$$

$$(4.16)$$

$$\text{tre } b_{i} = c_{i}/\beta_{i}, \ i = 1, \dots, m.$$

Here $b_i = c_i / \beta_i, j = 1, ..., m$.

Remark B. From arguments which lead us to equation (4.15) and by P-(i), we have

$$0 \le \frac{1}{d} E(U^2) = \frac{1}{d} \int_{[0,\infty)} u^2 \lambda_{jj}(\mathrm{d}u) = \lim_{t \downarrow 0} \frac{-\varphi'_{ij}(t)}{t}, \qquad j = 1, \dots, m,$$

where U is a random variable distributed on $[0, \infty)$ according the cumulative distribution function λ_{jj} , j = 1, ..., m.

Remark C. Let *d* and *m* be positive integers, suppose that $\boldsymbol{\varphi} = [\varphi_{ij}]_{i,j=1}^m \in \Phi_d^m$ is a matrix function differentiable (componentwise). Then by Theorem 4.2 $\boldsymbol{\eta} =$ $[\eta_{ij}]_{i,j=1}^m := \tilde{D}_m \varphi \in \Phi_{d+2}^m$ and it is well defined. Since $\eta = -[h_i h_j \frac{\varphi'_{ij}(t)}{t}]_{i,j=1}^m$ with h_j non-negative constants defined as Definition 4.1, $\int_t^\infty u \eta(u) \, du := [\int_t^\infty u \eta_{ij}(u) \, du] = [h_i h_j \varphi_{ij}(t)]$ and $\int_0^\infty u \eta_{jj}(u) \, du = h_j^2$ (i, j = 1, ..., m). So, the conditions of Theorem 4.1 are satisfied, and we have $\tilde{I}_m(\tilde{D}\varphi) = \varphi$. Analogously, given d and m positive integers, $\eta \in \Phi_{d+2}^m$ under conditions in Theorem 4.1, we can show that $\tilde{D}_m(\tilde{I}_m\eta) = \eta$, that is, \tilde{D}_m and \tilde{I}_m are inverse operators. This result is well known in univariate context, see Wendland (1995).

Remark D. As consequence of previous remark, we can generalize a well-known result in the univariate context. Let φ be a element of the class $\Phi_d^m - d \ge 3$ with 2k derivatives at zero—componentwise—k = 1, 2, ..., then $\eta(t) := \tilde{D}_m \varphi(t)$ is (2k - 2)-times differentiable at zero. For proving this assertion is enough to check equation (4.5) and the comment before it.

5 Projection operators and walks trough dimensions

Let d and d* be positive integers, $d \neq d^*$. We look for a potential one-to-one relation between the classes Φ_d^m and $\Phi_{d^*}^m$ through projection operators. This is parenthetical to the case of turning bands operators as proposed in Gneiting (1999b) and Mantoglou (1987) for scalar valued RFs. For the univariate case, Gneiting (1999a) and Gneiting (1999b) show dimension walks between the classes Φ_d and Φ_1 , as well as relations between Φ_d and Φ_{d-2} . In the subsequent section, we show analogues of such relations for the classes Φ_d^m and $\Phi_{d^*}^m$, m > 1.

Throughout this section, we denote an element of the class Φ_d^m as $\varphi_d(\cdot) = [\varphi_{d^i j}(\cdot)]_{i,j=1}^m$ where the subindex *d* indicates the dimension of the space \mathbb{R}^d .

Theorem 5.1. Let *m* and *d* be positive integers. For any element $\varphi_d(\cdot) = [\varphi_{dij}(\cdot)]_{i,j=1}^m$ of the class Φ_d^m , the relation

$$\boldsymbol{\varphi}_{d}(t) = \frac{2\Gamma(d/2)}{\pi^{1/2}\Gamma((d-1)/2)} \frac{1}{t} \int_{0}^{t} \left(1 - \frac{u^{2}}{t^{2}}\right)^{(d-3)/2} \boldsymbol{\varphi}_{1}(u) \,\mathrm{d}u \tag{5.1}$$

defines a bijection from Φ_1^m into Φ_d^m .

Proof. Using the analytic expansion $\Omega_d(t) = \Gamma(\frac{d}{2})(\frac{2}{t})^{(d-2)/2}J_{(d-2)/2}(t)$ and well known facts, see Abramowitz and Stegun (1972), formula 9.1.20,

$$J_{\nu}(z) = \frac{2(1/2z)^{\nu}}{\pi^{1/2}\Gamma(\nu+1/2)} \int_0^1 (1-u^2)^{\nu-1/2} \cos(zu) \,\mathrm{d}u,$$

by Theorem 3.1, we have

(i) any element $\varphi_1 = [\varphi_{1ij}(t)]_{i,j=1}^m$ belonging to Φ_1^m admits, the integral representation

$$\varphi_1(t) = \left[\int_{[0,\infty)} \cos(tr)\lambda_{ij}(\mathrm{d}r)\right]_{i,j=1}^m =: \int_{[0,\infty)} \cos(tr)\mathbf{\Lambda}_1(\mathrm{d}r), \qquad (5.2)$$

with $\lambda_{ij}(\cdot)$ as in equations (3.1) and (3.2). For the univariate case, see Gneiting (1998).

(ii) And, given $\varphi_d = [\varphi_{dij}(t)]_{i,j=1}^m \in \Phi_d^m, \varphi_d$ can be represented as

$$\varphi_{d}(t) = \int_{[0,\infty)} \Omega_{d}(tr) \mathbf{\Lambda}_{d}(dr)$$

$$= \frac{2\Gamma(d/2)}{\pi^{1/2}\Gamma((d-1)/2)} \int_{[0,\infty)} \left(\int_{0}^{1} (1-z^{2})^{(d-3)/2} \cos(trz) \, \mathrm{d}z \right) \mathbf{\Lambda}_{d}(dr).$$
(5.3)

Here, we recall that $\Lambda_d(\cdot)$ is a matrix function of bounded variation—componentwise—then we can write $\Lambda_d(\cdot) = \mathbf{G}(\cdot) - \mathbf{H}(\cdot)$, for **G** and **H** $m \times m$ matrix componentwise non-decreasing functions. Using this decomposition, we can use Fubini's theorem and equation (5.3) becomes

$$\varphi_d(t) = \frac{2\Gamma(d/2)}{\pi^{1/2}\Gamma((d-1)/2)} \int_0^1 (1-z^2)^{(d-3)/2} \left(\int_{[0,\infty)} \cos(trz) \mathbf{\Lambda}_d(dr) \right) dz.$$
(5.4)

The inner integral in (5.4) is analogue to that in equation (5.2), so that, a change of variable—z = u/t—and direct computation leads to the result.

In addition, for $d \ge 3$, applying Leibniz rule for differentiation under the integral (5.1)—see Flanders (1973)—leads to the recursive formula

$$\boldsymbol{\varphi}_{d-2}(t) = \boldsymbol{\varphi}_d(t) + \frac{t}{d-2} \boldsymbol{\varphi}_d'(t), \qquad (5.5)$$

which allow us to map Φ_d^m into Φ_{d-2}^m .

A well-known interpretation of equation (5.1) is as follows—see Gneiting (1999a). Let $\mathbf{Z}(x) = (Z_1(x), \ldots, Z_m(x)), x \in \mathbb{R}$, be a *m*-variate stationary RF with matrix correlation function $\varphi_1(|\cdot|)$ on the real line. Let U be uniformly distributed on \mathbb{S}^{d-1} and independent of \mathbf{Z} . Then

$$\mathbf{Y}(\mathbf{x}) := \mathbf{Z}(\mathbf{x}^T \mathbf{U}),$$

 $\mathbf{x} \in \mathbb{R}^d$, defines a *m*-variate stationary-isotropic RF with matrix correlation function $\varphi_d(\|\cdot\|)$ on \mathbb{R}^d .

As illustration, when d = 2, 3, equation (5.1) reduces to

$$\varphi_2(t) = \frac{2}{\pi} \int_0^t \frac{\varphi_1(u)}{(t^2 - u^2)^{1/2}} \, \mathrm{d}u = \frac{1}{\pi} \int_0^{\pi/2} \varphi_1(t\sin\theta) \, \mathrm{d}\theta \tag{5.6}$$

and

$$\varphi_3(t) = \frac{1}{t} \int_0^t \varphi_1(u) \,\mathrm{d}u.$$
 (5.7)

The former is an Abel type integral equation—see Gorenflo and Vessella (1991, equation 3.a)—and the latter is an usual integral equation, which can be inverted for φ_1 by standard techniques as:

$$\varphi_1(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left[\int_0^t \frac{u\varphi_2(u)}{(t^2 - u^2)^{1/2}} \,\mathrm{d}u \right]$$
(5.8)

and

$$\varphi_1(t) = \frac{\mathrm{d}}{\mathrm{d}t} [t\varphi_3(t)]. \tag{5.9}$$

Equations (5.8) and (5.9), are essential in turning bands simulations of univariate Gaussian RFs in \mathbb{R}^2 and \mathbb{R}^3 respectively, and may lead to a multivariate version of the Turning Bands simulation process. The reader is deferred to Gneiting (1998), Journel and Huijbregts (2003), Mantoglou (1987), Mantoglou and Wilson (1982) and Matheron (1973) for the Turning Bands developments in the univariate case.

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