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# Compactly-supported isotropic covariances on spheres obtained from matrix-valued covariances in Euclidean spaces

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## Abstract

Our findings are summarized as follows. Let  $p, d$  be positive integers, with  $d$  odd. Let  $\phi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  be the isotropic part of a matrix-valued and isotropic covariance function (a positive semidefinite matrix-valued function) that is defined over the  $d$ -dimensional Euclidean space. If  $\phi$  is compactly supported over  $[0, \pi]$ , then we show that the restriction of  $\phi$  to  $[0, \pi]$  is the isotropic part of a matrix-valued covariance function defined on a  $d$ -dimensional sphere, where isotropy in this case means that the covariance function depends on the geodesic distance. Our result does not need any assumption of continuity for the mapping  $\phi$ . Further, we provide an analytical expression of the  $d$ -Schoenberg sequence associated with the compactly-supported covariance on the sphere, which only requires knowledge of the Fourier transform of its isotropic part, and illustrate with the Gauss hypergeometric covariance model, which encompasses the well-known spherical, cubic, Askey and generalized Wendland covariances, and with a hole effect covariance model. Special cases of the results presented in this paper have been earlier provided by [Gneiting \(2013\)](#), [Ma \(2016\)](#) and subsequently by [Nie and Ma \(2019\)](#).

Key words: Positive semidefinite functions; Spectral density; Schoenberg sequence; Direct and cross-covariances; Multiply monotone functions.

# 1 Introduction

There is a growing interest in developing random field models indexed by spherical coordinates, especially for applications in atmospheric sciences, geodesy, geophysics or astronomy, where one has to process remote sensing data or observatory data scattered over a large portion of the Earth or in the sky (Hofmann-Wellenhof and Moritz, 2006; Marinucci and Peccati, 2011; Fournier et al., 2011; Heaton et al., 2014). Other applications in the geosciences and natural resources engineering relate to the modeling of direction-dependent variables in structural geology and geotechnics (Sánchez et al., 2019, 2021).

In most of these applications, the available spherically-indexed data are often of a multivariate nature, which motivates the search for vector random field models rather than just scalar random fields. In particular, the spatial correlation structure of the data is represented by a matrix-valued covariance function consisting of direct or auto-covariances associated with each variable, and cross-covariances between each pair of variables. The fitting of a multivariate model is critical to address spatial prediction problems (Wackernagel, 2003). The simplest covariance models on the sphere are isotropic, i.e., the covariance between any two data only depends on the geodesic distance between both data. These models are still widely used in practice (Gneiting, 2013) and are the building block of more complex models, e.g., axially symmetric covariances obtained by longitudinal integration (Emery et al., 2019) or covariances with locally adaptive spectral representations (Emery and Alegría, 2020).

To date, a wealth of matrix-valued isotropic covariance models on spheres, together with analytical expressions of their spectral representations, have been proposed in the literature, see Porcu et al. (2016), Guella and Menegatto (2019), Alegría et al. (2019), Alegría et al. (2020), Bevilacqua et al. (2020), Emery et al. (2021) and references therein, but few examples exist of compactly-supported models. One approach is Yadrenko’s construction (Yadrenko, 1983), where a multivariate isotropic covariance on the  $d$ -dimensional sphere is obtained by restricting a multivariate isotropic covariance in the  $(d + 1)$ -dimensional Euclidean space, which provides compactly-supported models that are functions of the chordal distance on the sphere, but the spectral representation of such models is generally not expressible in an analytical form (Emery et al., 2022). A more straightforward approach is to consider an isotropic covariance in the  $d$ -dimensional Euclidean space and to substitute the Euclidean distance with the geodesic distance on the  $d$ -dimensional sphere. In this respect, Gneiting (2013) and Ma (2016) give sufficient conditions for the resulting model to be valid on the one- and three-dimensional spheres, in the univariate and multivariate settings, respectively. A generalization to higher dimensional spheres is provided by Nie and Ma (2019) in the univariate setting, while Beatson et al. (2014) and Xu (2018) present specific classes of compactly-supported models (the truncated power Askey covariance) - still for univariate random fields. However, none of the previous works provides an analytical expression for the spectral representation of multivariate compactly-supported covariances on the sphere.

Apart from bringing flexibility in the fitting of the spatial correlation struc-

ture of data on the sphere, compactly-supported covariance models are advantageous for parameter estimation through likelihood-based methods (Kaufman et al., 2008) and for spatial prediction (Furrer et al., 2006), insofar as they lead to sparse systems of linear equations that can be solved even when the number of available data is large.

The outline of the paper is as follows: after providing some technical background in Section 2, we prove that substituting the geodesic distance for the Euclidean distance allows converting an isotropic covariance in the  $d$ -dimensional Euclidean space into an isotropic covariance in the  $d$ -dimensional sphere, provided that  $d$  is an odd integer greater than 1 and that the range of the covariance is no greater than  $\pi$  (Section 3.1). We finalize by bringing some explicit examples where an analytical expression of both the compactly-supported covariance on the sphere and its spectral representation can be obtained (Sections 3.2 and 3.3).

## 2 Background

Throughout,  $p$  and  $d$  denote positive integers and bold letters will refer to vectors and matrices. Also, continuity, differentiability, integrability and convergence involving matrix-valued functions are understood as elementwise.

### 2.1 Elements of matrix analysis

*Positive semidefiniteness.* A real-valued symmetric matrix  $\mathbf{A}$  of size  $p \times p$  is positive semidefinite if, and only if, all its eigenvalues are nonnegative. The set of positive semidefinite matrices of a given size forms a closed convex cone in the space of all real symmetric matrices. Besides, positive semidefiniteness induces a partial order relation (called the Löwner order) between symmetric matrices of the same size:  $\mathbf{A} \geq \mathbf{B}$  if  $\mathbf{A} - \mathbf{B}$  is positive semidefinite. Likewise, a matrix-valued function  $\phi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  is said to be nonnegative if  $\phi(t) \geq \mathbf{0}$  for any  $t \in [0, +\infty)$ , where  $\mathbf{0}$  stands for the zero matrix of size  $p \times p$ .

*Matrix monotonicity.* A matrix-valued function  $\phi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  is said to be nonincreasing with respect to matrix inequality if  $\phi(t) \geq \phi(t')$  when  $0 \leq t \leq t'$  (Boyd and Vandenberghe, 2004, Example 3.46). A necessary and sufficient for  $\phi$  to be nonincreasing is that, for any vector  $\mathbf{z}$  of size  $p$ , the scalar function  $\mathbf{z}^\top \phi \mathbf{z}$  is nonincreasing.

*Matrix convexity.* A matrix-valued function  $\phi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  is convex with respect to matrix inequality if  $\omega \phi(t) + (1 - \omega) \phi(t') \geq \phi(\omega t + (1 - \omega)t')$  for all  $t, t' \in [0, +\infty)$  and all  $\omega \in [0, 1]$  (Boyd and Vandenberghe, 2004, Example 3.48). A necessary and sufficient for  $\phi$  to be convex is that, for any vector  $\mathbf{z}$  of size  $p$ , the scalar function  $\mathbf{z}^\top \phi \mathbf{z}$  is convex.

*Multiply monotone matrix-valued functions.* Let  $\mu \in \mathbb{N}$  and  $\phi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$

be a  $\mu$ -times elementwise differentiable matrix-valued function, with  $\phi^{(k)}$  denoting its elementwise  $k$ -th derivative. Following [Williamson \(1956\)](#),  $\phi$  is said to be  $(\mu + 2)$ -times monotone with respect to matrix inequality if  $(-1)^k \phi^{(k)}$  is nonnegative, nonincreasing and convex for  $k = 0, \dots, \mu$ . A 1-time monotone matrix-valued function is a nonnegative and nonincreasing function on  $[0, +\infty)$ . A necessary and sufficient for  $\phi$  to be  $(\mu + 1)$ -times monotone (with  $\mu \in \mathbb{N}$ ) is that, for any vector  $\mathbf{z}$  of size  $p$ , the scalar function  $\mathbf{z}^\top \phi \mathbf{z}$  is  $(\mu + 1)$ -times monotone.

## 2.2 Stationary isotropic covariance functions in Euclidean spaces

A matrix-valued function  $\mathbf{K} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^{p \times p}$  is the covariance of a second-order  $p$ -variate random field defined in  $\mathbb{R}^d$  if, and only if, it is positive semidefinite, i.e., the matrix of size  $np \times np$  with generic entry  $K_{ij}(\mathbf{x}_k, \mathbf{x}_\ell)$ , where  $K_{ij}$  denotes the  $(i, j)$ -th entry of  $\mathbf{K}$ , is symmetric and positive semidefinite for any choice of the positive integer  $n$  and of the set of points  $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  in  $\mathbb{R}^d$ .

The covariance function  $\mathbf{K}$  is stationary and isotropic if it can be written as follows:

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \widetilde{\mathbf{K}}(\|\mathbf{x} - \mathbf{x}'\|), \quad \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d,$$

where the matrix-valued function  $\widetilde{\mathbf{K}} : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  is called the isotropic part of  $\mathbf{K}$ , and  $\|\cdot\|$  is the Euclidean norm:

$$\|\mathbf{x} - \mathbf{x}'\|^2 = \langle \mathbf{x} - \mathbf{x}', \mathbf{x} - \mathbf{x}' \rangle$$

with  $\langle \cdot, \cdot \rangle$  the usual scalar product of the Cartesian coordinates.

A continuous stationary isotropic covariance function  $\mathbf{K}$  in  $\mathbb{R}^d \times \mathbb{R}^d$  that is elementwise absolutely integrable has a Fourier representation of the form

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \int_{\mathbb{R}^d} \cos(2\pi \langle \mathbf{u}, \mathbf{x} - \mathbf{x}' \rangle) \mathbf{f}(\mathbf{u}) d\mathbf{u}, \quad \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d,$$

where  $\mathbf{f}$  is a bounded continuous matrix-valued function known as the spectral density of  $\mathbf{K}$ , such that  $\mathbf{f}(\mathbf{u})$  is real-valued, symmetric and positive semidefinite for all  $\mathbf{u} \in \mathbb{R}^d$  ([Yaglom, 1987](#)). In terms of isotropic parts, the above Fourier representation becomes a Hankel transform of order  $d$ :

$$\widetilde{\mathbf{K}}(r) = 2\pi r^{1-d/2} \int_0^{+\infty} u^{d/2} J_{d/2-1}(2\pi ur) \widetilde{\mathbf{f}}_d(u) du, \quad r \in [0, +\infty), \quad (1)$$

with  $J_\nu$  the Bessel function of the first kind of order  $\nu$  and  $\widetilde{\mathbf{f}}_d$  the isotropic part of  $\mathbf{f}$ , which can be retrieved as

$$\widetilde{\mathbf{f}}_d(u) = 2\pi u^{1-d/2} \int_0^{+\infty} r^{d/2} J_{d/2-1}(2\pi ur) \widetilde{\mathbf{K}}(r) dr, \quad u \in [0, +\infty). \quad (2)$$

### 2.3 Isotropic covariance functions on spheres

Let  $\mathbb{S}^d$  denote the unit sphere embedded in  $\mathbb{R}^{d+1}$ , *i.e.*,  $\mathbb{S}^d = \{\mathbf{s} \in \mathbb{R}^{d+1} : \|\mathbf{s}\| = 1\}$ . A matrix-valued function  $\mathbf{C} : \mathbb{S}^d \times \mathbb{S}^d \rightarrow \mathbb{R}^{p \times p}$  is the covariance of a second-order  $p$ -variate random field defined on  $\mathbb{S}^d$  if, and only if, it is positive semidefinite, *i.e.*, the matrix of size  $np \times np$  with generic entry  $C_{ij}(\mathbf{s}_k, \mathbf{s}_\ell)$ , where  $C_{ij}$  denotes the  $(i, j)$ -th entry of  $\mathbf{C}$ , is symmetric and positive semidefinite for any choice of the positive integer  $n$  and of the set of points  $\{\mathbf{s}_1, \dots, \mathbf{s}_n\}$  in  $\mathbb{S}^d$ .

The covariance  $\mathbf{C}$  is isotropic if it can be written as

$$\mathbf{C}(\mathbf{s}, \mathbf{s}') = \tilde{\mathbf{C}}(\vartheta(\mathbf{s}, \mathbf{s}')), \quad \mathbf{s}, \mathbf{s}' \in \mathbb{S}^d,$$

where the matrix-valued function  $\tilde{\mathbf{C}} : [0, \pi] \rightarrow \mathbb{R}^{p \times p}$  is called the isotropic part of  $\mathbf{C}$ , and  $\vartheta : \mathbb{S}^d \times \mathbb{S}^d \rightarrow [0, \pi]$  is the geodesic distance on the sphere, defined as

$$\vartheta(\mathbf{s}, \mathbf{s}') = \arccos(\langle \mathbf{s}, \mathbf{s}' \rangle).$$

A continuous isotropic covariance function  $\mathbf{C}$  on  $\mathbb{S}^d \times \mathbb{S}^d$  has a spectral representation of the form (Yaglom, 1987; Hannan, 2009)

$$\mathbf{C}(\mathbf{s}, \mathbf{s}') = \tilde{\mathbf{C}}(\vartheta(\mathbf{s}, \mathbf{s}')) = \sum_{n=0}^{+\infty} \mathbf{B}_{n,d} C_n^\lambda(\cos \vartheta(\mathbf{s}, \mathbf{s}')), \quad \mathbf{s}, \mathbf{s}' \in \mathbb{S}^d, \quad (3)$$

with  $\lambda = \frac{d-1}{2}$ ,  $C_n^\lambda$  the Gegenbauer or ultraspherical polynomial of degree  $n$  and order  $\lambda$  (Olver et al., 2010, formula 18.5.9), and  $\{\mathbf{B}_{n,d} : n \in \mathbb{N}\}$  a sequence of positive semidefinite matrices such that  $\sum_{n=0}^{+\infty} \mathbf{B}_{n,d} C_n^\lambda(1)$  converges elementwise. The decomposition (3) is known as the Schoenberg decomposition of  $\mathbf{C}$  (Daley et al., 2014), and the sequence  $\{\mathbf{B}_{n,d} : n \in \mathbb{N}\}$  as the  $d$ -Schoenberg sequence of  $\mathbf{C}$ , by reference to the findings of Schoenberg (1942) who examined the univariate case ( $p = 1$ ). The  $d$ -Schoenberg sequence can be retrieved as

$$\mathbf{B}_{n,d} = \frac{(2n+2\lambda)n!\Gamma^2(\lambda)}{2^{2-2\lambda}\pi\Gamma(2\lambda+n)} \int_0^\pi C_n^\lambda(\cos \vartheta)(\sin \vartheta)^{2\lambda} \tilde{\mathbf{C}}(\vartheta) d\vartheta, \quad n \in \mathbb{N}, \quad (4)$$

where  $\Gamma$  stands for the gamma function.

### 2.4 Connection formulae for Gegenbauer polynomials

The Gegenbauer polynomials of orders  $\lambda$  and  $\mu$ , with  $\lambda > (\mu - 1)/2 > -1/2$ , are connected as follows (Askey, 1965):

$$(\sin \vartheta)^{2\lambda} C_n^\lambda(\cos \vartheta) = \sum_{k=0}^{+\infty} a_{k,n,\lambda,\mu} (\sin \vartheta)^{2\mu} C_{n+2k}^\mu(\cos \vartheta), \quad n \in \mathbb{N}, \vartheta \in [0, \pi], \quad (5)$$

with

$$a_{k,n,\lambda,\mu} = \frac{\Gamma(\mu) 2^{2\mu-2\lambda} (n+2k+\mu)(n+2k)!\Gamma(n+2\lambda)\Gamma(n+k+\mu)(\mu-\lambda)_k}{\Gamma(\lambda)n!k!\Gamma(n+k+\lambda+1)\Gamma(n+2k+2\mu)},$$

where  $(\cdot)_k$  stands for the Pochhammer symbol or rising factorial (Olver et al., 2010, formula 5.2.4).

Of particular interest will be the case when  $\mu$  tends to zero, in which the  $\mu$ -Gegenbauer polynomial of degree  $n$ , properly normalized, tends to the Chebyshev polynomial of the first kind of degree  $n$ ,  $T_n$  (Olver et al., 2010, formula 18.7.25):

$$\lim_{\mu \rightarrow 0} \frac{1}{\mu} C_n^\mu(x) = \frac{2}{n} T_n(x), \quad x \in [-1, 1].$$

Accordingly, (5) provides the following connection formula between Gegenbauer and Chebyshev polynomials:

$$\begin{aligned} (\sin \vartheta)^{2\lambda} C_n^\lambda(\cos \vartheta) &= \sum_{k=0}^{+\infty} a_{k,n,\lambda} T_{n+2k}(\cos \vartheta) \\ &= \sum_{k=0}^{+\infty} a_{k,n,\lambda} \cos((n+2k)\vartheta), \quad n \in \mathbb{N}, \vartheta \in [0, \pi], \end{aligned} \quad (6)$$

with  $\lambda > -1/2$  and

$$a_{k,n,\lambda} = \frac{2^{1-2\lambda} (n+2k) \Gamma(n+2\lambda) \Gamma(n+k) (-\lambda)_k}{\Gamma(\lambda) n! k! \Gamma(n+k+\lambda+1)}. \quad (7)$$

Note that the sign of  $a_{k,n,\lambda}$  alternates for  $0 \leq k < \lambda + 1$ , then it remains the same for  $k \geq \lambda + 1$ . This implies that the series in (6) is not only convergent, but also absolutely convergent. Also, the sum of  $\{a_{k,n,\lambda} : k \in \mathbb{N}\}$  is zero, which can be seen by taking  $\theta = 0$  in (6).

## 3 Our contribution

### 3.1 Theoretical results

**Theorem 1.** *Let  $p$  and  $d$  be positive integers, with  $d \geq 2$ , and  $\lambda = \frac{d-1}{2}$ . Also, let  $\mathbf{K} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^{p \times p}$  be a continuous matrix-valued isotropic covariance function and  $\widetilde{\mathbf{K}} : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  be its isotropic part. If  $\widetilde{\mathbf{K}}(r) = \mathbf{0}$  for  $r \geq \pi$ , then the restriction of  $\widetilde{\mathbf{K}}$  to  $[0, \pi]$  admits the Schoenberg expansion (3) with the  $d$ -Schoenberg sequence given by*

$$\mathbf{B}_{n,d} = \frac{(n+\lambda) \Gamma(\lambda)}{2\pi} \sum_{k=0}^{+\infty} \frac{(n+2k) \Gamma(n+k) (-\lambda)_k}{k! \Gamma(n+k+\lambda+1)} \widetilde{\mathbf{f}}_1 \left( \frac{n+2k}{2\pi} \right), \quad n \in \mathbb{N}, \quad (8)$$

where  $\widetilde{\mathbf{f}}_1$  is the matrix-valued spectral density of the one-dimensional covariance with isotropic part  $\widetilde{\mathbf{K}}$ .

*Proof.* Arguments in [Schoenberg \(1942\)](#) based on the continuity of  $\widetilde{\mathbf{K}}$  and Abel's theorem show that the restriction of  $\widetilde{\mathbf{K}}$  to  $[0, \pi]$  can be expanded as in (3), with the  $d$ -Schoenberg matrices defined as in (4).

To prove that such an expansion matches with (8), consider the one-dimensional spectral representation (1)-(2) of  $\widetilde{\mathbf{K}}$ :

$$\widetilde{\mathbf{K}}(r) = 2 \int_0^{+\infty} \cos(2\pi ur) \widetilde{\mathbf{f}}_1(u) du, \quad r \in [0, +\infty),$$

with

$$\widetilde{\mathbf{f}}_1(u) = 2 \int_0^{+\infty} \cos(2\pi ur) \widetilde{\mathbf{K}}(r) dr, \quad u \in [0, +\infty). \quad (9)$$

In particular, we note that  $\widetilde{\mathbf{f}}_1$  is well defined because  $\widetilde{\mathbf{K}}$  is continuous and compactly supported with range less than  $\pi$ , which ensures its absolute integrability.

We now make use of (7) to rewrite the expansion (8) as

$$\begin{aligned} \mathbf{B}_{n,d} &= \frac{(n+\lambda)n!\Gamma^2(\lambda)}{2^{2-\lambda}\pi\Gamma(2\lambda+n)} \sum_{k=0}^{+\infty} a_{k,n,\lambda} \widetilde{\mathbf{f}}_1\left(\frac{n+2k}{2\pi}\right) \\ &= \frac{(n+\lambda)n!\Gamma^2(\lambda)}{2^{1-\lambda}\pi\Gamma(2\lambda+n)} \sum_{k=0}^{+\infty} a_{k,n,\lambda} \int_0^{+\infty} \cos((n+2k)r) \widetilde{\mathbf{K}}(r) dr, \quad n \in \mathbb{N}, \end{aligned} \quad (10)$$

where the integral can be restricted to the interval  $[0, \pi]$  and interchanged with the sum owing to the dominated convergence theorem:

$$\mathbf{B}_{n,d} = \frac{(n+\lambda)n!\Gamma^2(\lambda)}{2^{1-\lambda}\pi\Gamma(2\lambda+n)} \int_0^\pi \sum_{k=0}^{+\infty} a_{k,n,\lambda} \cos((n+2k)r) \widetilde{\mathbf{K}}(r) dr, \quad n \in \mathbb{N},$$

which turns out to be identical to (4) on account of the connection formula (6) between Gegenbauer and Chebyshev polynomials. This identity shows that the series in (8) is convergent and completes the proof.  $\square$

**Lemma 1.** *Let  $\mathbf{K}$  be a continuous isotropic covariance in  $\mathbb{R}^d \times \mathbb{R}^d$  with  $d \geq 3$ ,  $\widetilde{\mathbf{K}}$  its isotropic part,  $\widetilde{\mathbf{f}}_1$  its one-dimensional density as per (9), and  $\lambda = \frac{d-1}{2}$ . Then, the matrix-valued function  $\phi$  defined on  $[0, +\infty)$  by*

$$\phi(t) = \widetilde{\mathbf{f}}_1(\sqrt{t}), \quad t \in [0, +\infty), \quad (11)$$

*is  $\lfloor \lambda \rfloor$ -times monotone with respect to matrix inequality and tends to the zero matrix as  $t$  tends to infinity. Here,  $\lfloor \cdot \rfloor$  stands for the floor function.*

*Proof.* The one-dimensional spectral density  $\widetilde{\mathbf{f}}_1$  can be decomposed as follows ([Yaglom, 1987](#); [Chilès and Delfiner, 2012](#), formula 2.29):

$$\begin{aligned} \widetilde{\mathbf{f}}_1(t) &= \frac{2\pi^\lambda}{\Gamma(\lambda)} \int_t^{+\infty} (u^2 - t^2)^{\lambda-1} u \widetilde{\mathbf{f}}_d(u) du \\ &= \frac{2\pi^\lambda}{\Gamma(\lambda)} \int_0^{+\infty} (u^2 - t^2)^{\lambda-1} \mathbb{I}_{u>t} u \widetilde{\mathbf{f}}_d(u) du, \quad t \in [0, +\infty), \end{aligned}$$

with  $\tilde{\mathbf{f}}_d(u)$  as defined in (2) and  $t \mapsto \mathbb{I}_{u>t}$  standing for an indicator function:  $\mathbb{I}_{u>t} = 1$  if  $u > t$ , 0 otherwise. Put another way,  $\tilde{\mathbf{f}}_1$  is the “montée” (upgrading) of order  $2\lambda$  of  $\tilde{\mathbf{f}}_d$  (Matheron, 1965, formula I.4.18), which is due to the fact that the Hankel transform of order  $d$  of the latter is the same as the Hankel transform of order 1 of the former, namely  $\tilde{\mathbf{K}}$ . It follows:

$$\begin{aligned}\phi(t) &= \frac{2\pi^\lambda}{\Gamma(\lambda)} \int_t^{+\infty} (v-t)^{\lambda-1} \tilde{\mathbf{f}}_d(\sqrt{v}) dv \\ &= \frac{2\pi^\lambda}{\Gamma(\lambda)} \int_0^{+\infty} (v-t)^{\lambda-1} \mathbb{I}_{v>t} \tilde{\mathbf{f}}_d(\sqrt{v}) dv, \quad t \in [0, +\infty).\end{aligned}\tag{12}$$

*Convergence to the zero matrix.* The fact that, for  $\lambda \geq 1$ , the integrand in (12) is a nonnegative and nonincreasing function of  $t$  implies that  $\phi$  is nonincreasing with respect to matrix inequality and lower bounded by the zero matrix. Hence, as  $t$  tends to infinity,  $\phi(t)$  tends to a limit. This limit is the zero matrix insofar as, for any sequence  $\{t_n : n \in \mathbb{N}\}$  of positive real numbers tending to infinity, the sequence of functions  $v \mapsto (v-t_n)^{\lambda-1} \mathbb{I}_{v>t_n} \tilde{\mathbf{f}}_d(\sqrt{v})$  converges uniformly to the zero matrix on any compact of  $[0, +\infty)$  as  $n$  tends to infinity.

*Elementwise differentiability.* By a repeated application of the Leibniz integral rule for differentiation under the integral sign, it is seen that, if  $\lambda \geq 2$ ,  $\phi$  is  $\lambda - 2$  times differentiable.

*Multiply monotonicity.* Let  $\mathbf{z}$  be a real-valued vector with  $p$  components and define the mapping  $\phi_{\mathbf{z}}$  on  $[0, +\infty)$  as

$$\begin{aligned}\phi_{\mathbf{z}}(t) &= \mathbf{z}^\top \phi(t) \mathbf{z} \\ &= \frac{\pi^\lambda}{\Gamma(\lambda)} \int_0^{+\infty} (v-t)^{\lambda-1} \mathbb{I}_{v>t} \left[ \mathbf{z}^\top \tilde{\mathbf{f}}_d(\sqrt{v}) \mathbf{z} \right] dv, \quad t \in [0, +\infty).\end{aligned}$$

The claim follows from the fact that, for any fixed vector  $\mathbf{z}$  and positive real  $v$ , the integrand is a  $\lfloor \lambda \rfloor$ -times monotone function of the form  $t \mapsto (v-t)^{\lambda-1} \mathbb{I}_{v>t}$  (Williamson, 1956) weighted by the nonnegative real number  $\mathbf{z}^\top \tilde{\mathbf{f}}_d(\sqrt{v}) \mathbf{z}$ . Therefore, for any  $\mathbf{z}$ ,  $t \mapsto \phi_{\mathbf{z}}(t)$  is  $\lfloor \lambda \rfloor$ -times monotone, as a nonnegative scale mixture of  $\lfloor \lambda \rfloor$ -times monotone functions.  $\square$

**Lemma 2.** *Let  $\lambda$  be a positive integer,  $n$  a nonnegative integer, and let  $\{a_{k,n,\lambda} : k \in \mathbb{N}\}$  be the coefficients defined in (7). Then, the matrix  $\mathbf{B}_{\psi,n,\lambda}$ , defined through*

$$\mathbf{B}_{\psi,n,\lambda} = \sum_{k=0}^{+\infty} a_{k,n,\lambda} \psi((n+2k)^2 - n^2)\tag{13}$$

*is positive semidefinite for any matrix-valued function  $\psi : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  that is  $\lambda$ -times monotone with respect to matrix inequality.*

*Proof.* First of all, observe that the series in (13) is convergent for any  $n \in \mathbb{N}$ , insofar as the sequence  $\{a_{k,n,\lambda} : k \in \mathbb{N}\}$  only has finitely many nonzero terms when  $\lambda$  is a positive integer. The lemma can now be proven by induction. For  $\lambda = 1$  and  $n \in \mathbb{N}$ , one has  $a_{0,n,1} = -a_{1,n,1} > 0$  and  $a_{k,n,1} = 0$  when  $k \geq 2$ . If  $\psi$  is 1-time monotone on  $[0, +\infty)$ , then it is nonincreasing on  $[0, +\infty)$ , which implies

$$\mathbf{B}_{\psi,n,1} = a_{0,n,1}(\psi(0) - \psi((n+2)^2 - n^2)) \geq \mathbf{0},$$

so the lemma is true for  $\lambda = 1$ . Assume now that the lemma is true up to some positive integer  $\lambda - 1$  and consider a  $\lambda$ -times monotone matrix-valued function  $\psi$  defined on  $[0, +\infty)$ . Accounting for the fact that the coefficients  $\{a_{k,n,\lambda} : k \in \mathbb{N}\}$  add to zero, one has

$$\begin{aligned} \mathbf{B}_{\psi,n,\lambda} &= \sum_{k=1}^{+\infty} a_{k,n,\lambda}(\psi((n+2k)^2 - n^2) - \psi(0)) \\ &= \sum_{k=1}^{+\infty} a_{k-1,n+2,\lambda-1} \frac{-\lambda(n+1)(n+2)}{4k(n+k)(\lambda-1)} (\psi((n+2k)^2 - n^2) - \psi(0)) \\ &= \frac{\lambda(n+1)(n+2)}{4(\lambda-1)} \sum_{k=0}^{+\infty} a_{k,n+2,\lambda-1} \frac{\psi(0) - \psi((n+2+2k)^2 - n^2)}{(k+1)(n+k+1)}, \\ &= \frac{\lambda(n+1)(n+2)}{\lambda-1} \sum_{k=0}^{+\infty} a_{k,n+2,\lambda-1} \zeta((n+2+2k)^2), \quad n \in \mathbb{N}, \end{aligned}$$

with

$$\zeta(t) = \frac{\psi(0) - \psi(t - n^2)}{t - n^2} = - \int_0^1 \psi^{(1)}(u(t - n^2)) du, \quad t \geq n^2.$$

Since  $-\psi^{(1)}$  (opposite of the first-order derivative of  $\psi$ ) is  $(\lambda-1)$ -times monotone on  $[0, +\infty)$ , so is  $\zeta$  on  $[n^2, +\infty)$ , as a nonnegative scale mixture of such functions, and one can apply the recursion assumption to conclude that  $\mathbf{B}_{\psi,n,\lambda}$  is positive semidefinite for any  $n \in \mathbb{N}$ .  $\square$

**Theorem 2.** *Let  $p$  be a positive integer,  $d$  an odd integer greater than 1, and  $\widetilde{\mathbf{K}} : [0, +\infty) \rightarrow \mathbb{R}^{p \times p}$  a matrix-valued function such that  $\widetilde{\mathbf{K}}(r) = \mathbf{0}$  for  $r \geq \pi$ . If  $\widetilde{\mathbf{K}}$  is the isotropic part of a valid covariance in  $\mathbb{R}^d \times \mathbb{R}^d$ , then the restriction of  $\widetilde{\mathbf{K}}$  to  $[0, \pi]$  is the isotropic part of a valid covariance function on  $\mathbb{S}^d \times \mathbb{S}^d$ .*

*Proof.* Let  $\mathbf{K}$  be the covariance function in  $\mathbb{R}^d \times \mathbb{R}^d$  whose isotropic part is  $\widetilde{\mathbf{K}}$ . According to Crum (1956),  $\mathbf{K}$  can be written as the sum of a matrix-valued nugget effect and a continuous isotropic component, both of which are positive semidefinite functions in  $\mathbb{R}^d \times \mathbb{R}^d$ . The nugget effect is clearly a valid covariance on  $\mathbb{S}^d \times \mathbb{S}^d$ , so one can restrict the proof to a continuous mapping  $\mathbf{K}$ . Based on the Schoenberg expansion given in Theorem 1, it suffices to prove that the

Schoenberg matrix  $\mathbf{B}_{n,d}$  is positive semidefinite for any  $n \in \mathbb{N}$ . Accounting for (10) and (11), one has:

$$\begin{aligned}\mathbf{B}_{n,d} &= \frac{(n+\lambda)n!\Gamma^2(\lambda)}{2^{2-\lambda}\pi\Gamma(2\lambda+n)} \sum_{k=0}^{+\infty} a_{k,n,\lambda} \phi\left(\left(\frac{n+2k}{2\pi}\right)^2\right) \\ &= \frac{(n+\lambda)n!\Gamma^2(\lambda)}{2^{2-\lambda}\pi\Gamma(2\lambda+n)} \sum_{k=0}^{+\infty} a_{k,n,\lambda} \psi((n+2k)^2 - n^2),\end{aligned}$$

with

$$\psi(t) = \phi\left(\frac{t+n^2}{4\pi^2}\right), \quad t \in [0, +\infty).$$

Since  $\phi$  is  $\lambda$ -times monotone on  $[0, +\infty)$  (lemma 1), so is  $\psi$ , and the positive semidefiniteness of  $\mathbf{B}_{n,d}$  stems from lemma 2.  $\square$

**Remark 1.** *Theorem 2 generalizes results by Gneiting (2013) (in a univariate setting) and Ma (2016) (in a multivariate setting), corresponding to  $d = 3$ , and the finding by Nie and Ma (2019) that has been established only for scalar-valued covariance functions, with all these works focusing only on continuous covariance functions.*

**Remark 2.** *The reciprocal of Theorem 2 does not hold: if  $\widetilde{\mathbf{K}}$  is a matrix-valued function that vanishes for  $r \geq \pi$  and its restriction to  $[0, \pi]$  is the isotropic part of a valid covariance function on  $\mathbb{S}^d \times \mathbb{S}^d$ , with  $d \geq 3$ , then  $\widetilde{\mathbf{K}}$  may not be the isotropic part of a valid covariance in  $\mathbb{R}^d \times \mathbb{R}^d$ . A counterexample is the tent function  $\widetilde{\mathbf{K}} : r \mapsto (1 - \frac{r}{\pi})\mathbb{I}_{r < \pi} = (\frac{1}{2} + \frac{1}{2}(1 - \frac{2r}{\pi}))\mathbb{I}_{r < \pi}$ , which is the isotropic part of a valid covariance on  $\mathbb{S}^d \times \mathbb{S}^d$  (Alegría et al., 2020), but not in  $\mathbb{R}^d \times \mathbb{R}^d$  (Chilès and Delfiner, 2012).*

### 3.2 Example 1: the Gauss hypergeometric covariance

A wide parametric family of compactly-supported univariate covariance functions in  $\mathbb{R}^d \times \mathbb{R}^d$  is the Gauss hypergeometric covariance, the isotropic part of which is of the form (Emery and Alegría, 2021):

$$\begin{aligned}\widetilde{K}(r; a, \alpha, \beta, \gamma) &= \frac{\Gamma(\beta - \frac{d}{2})\Gamma(\gamma - \frac{d}{2})}{\Gamma(\beta - \alpha + \gamma - \frac{d}{2})\Gamma(\alpha - \frac{d}{2})} \left(1 - \frac{r^2}{a^2}\right)_+^{\beta - \alpha + \gamma - \frac{d}{2} - 1} \\ &\quad \times {}_2F_1\left(\beta - \alpha, \gamma - \alpha; \beta - \alpha + \gamma - \frac{d}{2}; \left(1 - \frac{r^2}{a^2}\right)_+\right), \quad r \in [0, +\infty),\end{aligned}\tag{14}$$

where  $(\cdot)_+$  stands for the positive part function,  ${}_2F_1$  for the Gauss hypergeometric function (Olver et al., 2010, formula 15.2.1), and  $(a, \alpha, \beta, \gamma)$  are positive parameters such that

- $\pi \geq a > 0$ ;

- $\alpha > \frac{d}{2}$ ;
- $2(\beta - \alpha)(\gamma - \alpha) \geq \alpha$ ;
- $2(\beta + \gamma) \geq 6\alpha + 1$ .

The first restriction has been set so that the range  $a$  of the covariance is less than  $\pi$ , which will be required to obtain a valid model when substituting the geodesic distance  $\vartheta$  for the Euclidean distance  $r$ . Parameter  $\alpha$  relates to the smoothness, as it controls the behavior of the covariance at the origin, while  $\beta$  and  $\gamma$  are shape parameters that control the decay and curvature of the covariance function. As particular cases, one finds the Euclid's hat (spherical) covariance family (Gneiting, 1999) when choosing  $\beta = \alpha + \frac{1}{2}$  and  $\gamma = 2\alpha$ , the Askey (truncated power) covariance family (Askey, 1973) when choosing  $\alpha = \frac{d+1}{2}$ ,  $\beta \geq \frac{3\alpha}{2}$  and  $\gamma = \beta + \frac{1}{2}$ , and the generalized Wendland covariance family (Hubbert, 2012) when choosing  $\alpha > \frac{d+1}{2}$ ,  $\beta \geq \frac{3\alpha}{2}$  and  $\gamma = \beta + \frac{1}{2}$ .

The one-dimensional spectral density associated with this covariance is (Emery and Alegría, 2021)

$$\begin{aligned} \tilde{f}_1(u; a, \alpha, \beta, \gamma) &= \frac{\pi^{\frac{1}{2}} a \Gamma(\alpha - \frac{d-1}{2}) \Gamma(\beta - \frac{d}{2}) \Gamma(\gamma - \frac{d}{2})}{\Gamma(\alpha - \frac{d}{2}) \Gamma(\beta - \frac{d-1}{2}) \Gamma(\gamma - \frac{d-1}{2})} \\ &\times {}_1F_2\left(\alpha - \frac{d-1}{2}; \beta - \frac{d-1}{2}, \gamma - \frac{d-1}{2}; -(\pi a u)^2\right), \end{aligned} \quad (15)$$

where  ${}_1F_2$  stands for a generalized hypergeometric function (Olver et al., 2010, formula 16.2.1).

According to Theorems 1 and 2, provided that  $d$  is an odd integer greater than 1 and the previous restrictions on the model parameters  $(a, \alpha, \beta, \gamma)$  hold, then  $\vartheta \mapsto \tilde{K}(\vartheta; a, \alpha, \beta, \gamma)$  is the isotropic part of a valid covariance on  $\mathbb{S}^d \times \mathbb{S}^d$ , and its Schoenberg expansion is given by (8), with the sum containing finitely many nonzero terms and with  $f_1$  defined in (15). This generalizes results given by Beatson et al. (2014) and Xu (2018), related to the Askey covariance family.

Having an analytical expression of the Schoenberg sequence allows simulating random fields with this hypergeometric covariance, by use of spectral algorithms (Ma, 2016; Lantuéjoul et al., 2019; Emery and Porcu, 2019; Alegría et al., 2020). Figure 1 presents an example of realizations obtained with the turning arcs algorithm of Alegría et al. (2020), consisting of a weighted sum of  $N = 50,000$  Gegenbauer waves, for three covariance models of the Euclid's hat family (spherical, cubic and penta, corresponding to a smoothness parameter  $\alpha = \frac{d+1}{2}$ ,  $\frac{d+3}{2}$  and  $\frac{d+5}{2}$ , respectively) and three correlation ranges (0.5, 1.5 and 3). The simulation has been performed on the three-dimensional sphere  $\mathbb{S}^3$  and then restricted to the two-dimensional sphere  $\mathbb{S}^2$  for visualization purposes.

The previous examples can be extended to multivariate covariance models, by considering matrix-valued functions  $\tilde{\mathbf{K}}$  and  $\tilde{\mathbf{f}}_1$  and matrix-valued parameters

$(\mathbf{a}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma})$  instead of scalar functions and parameters. The reader is referred to [Emery and Alegría \(2021\)](#) for a list of sufficient conditions on these parameters to ensure the validity of the multivariate covariance model.

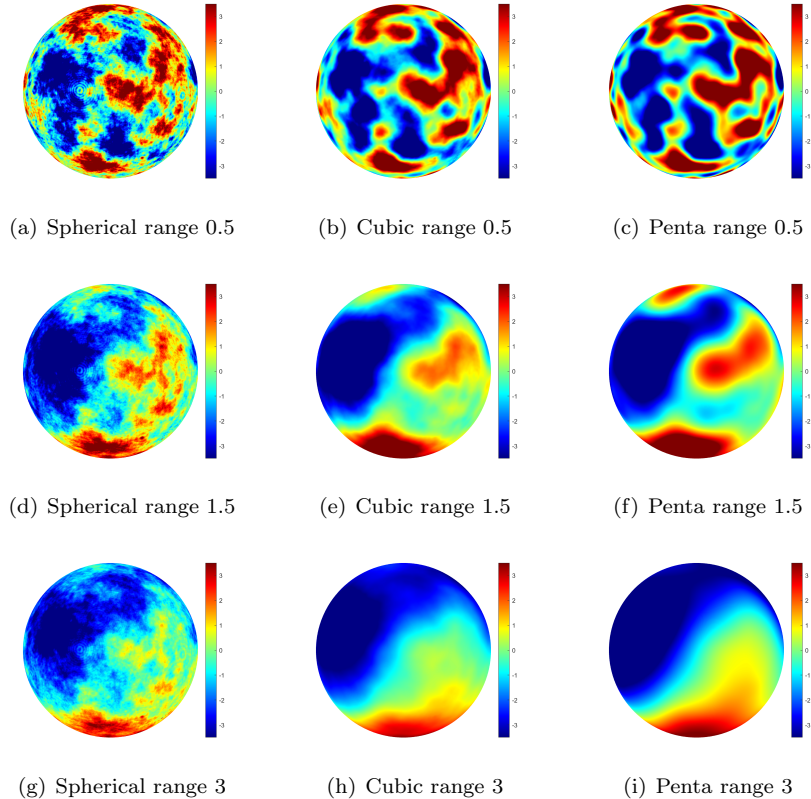


Figure 1: Realizations of isotropic random fields with spherical (left), cubic (middle) or penta (right) covariance functions, with short (top), medium (center) or high (bottom) ranges. The simulation is performed on  $\mathbb{S}^3$  via the turning arcs algorithm, using 50,000 Gegenbauer waves with degrees following a shifted zeta distribution of parameter 2. The visualization is restricted to  $\mathbb{S}^2$  discretized into 250,000 points. The higher the smoothness parameter of the covariance, the more regular are the realizations

### 3.3 Example 2: a hole effect model

The Gauss hypergeometric covariance is nonnegative and unimodal (the isotropic part is nonincreasing), but it can be the building block of more complex models exhibiting nonmonotone variations, in particular hole effects. As an example, consider a pentaspherical covariance  $K_5$  in  $\mathbb{R}^5 \times \mathbb{R}^5$ , the isotropic part of which

( $\tilde{K}_5$ ) is given by (14) with  $a \in (0, \pi]$ ,  $\alpha = 3$ ,  $\beta = \frac{7}{2}$  and  $\gamma = 6$ , i.e.:

$$\tilde{K}_5(r; a) = \left(1 - \frac{15r}{8a} + \frac{5r^3}{4a^3} - \frac{3r^5}{8a^5}\right)_+, \quad r \in [0, +\infty).$$

The isotropic part (15) of the associated spectral density  $f_5$  is

$$\tilde{f}_5(u; a) = \frac{\pi^2 a^5}{60} {}_1F_2\left(3; \frac{7}{2}, 6; -(\pi a u)^2\right), \quad u \in [0, +\infty),$$

which can also be expressed as a squared Bessel function (Arroyo and Emery, 2021). Consider now the isotropic covariance  $K_3$  in  $\mathbb{R}^3 \times \mathbb{R}^3$  obtained by applying the turning bands operator (from  $\mathbb{R}^5$  to  $\mathbb{R}^3$ ) to such a pentaspherical covariance. The isotropic parts of  $K_3$  and of its spectral density are (Matheron, 1972)

$$\begin{aligned} \tilde{K}_3(r; a) &= \frac{1}{3r^2} \frac{d}{dr} [r^3 \tilde{K}_5(r; a)] \\ &= \left(1 - \frac{5r}{2a} + \frac{5r^3}{2a^3} - \frac{r^5}{a^5}\right)_+, \quad r \in [0, +\infty), \end{aligned}$$

and

$$\tilde{f}_3(u; a) = \frac{2\pi u^2}{3} \tilde{f}_5(u; a), \quad u \in [0, +\infty).$$

In particular,  $\tilde{K}_3$  is compactly supported, with the same range  $a$  as the original pentaspherical covariance  $\tilde{K}_5$ , but is no longer monotone; instead, it presents a hole effect, with an interval of distances in which the covariance is negative (Figure 2). The one-dimensional spectral density associated with  $\tilde{K}_3$  (viewed as the isotropic part of a covariance in  $\mathbb{R}$ ) is the montée of order 2 of  $\tilde{f}_3$ , that is (Matheron, 1965, formula I.4.8)

$$\tilde{f}_1(t; a) = 2\pi \int_t^{+\infty} u \tilde{f}_3(u; a) du, \quad t \in [0, +\infty).$$

One finds

$$\begin{aligned} \tilde{f}_1(t; a) &= \frac{4\pi^2}{3} \int_t^{+\infty} u^3 \tilde{f}_5(u; a) du \\ &= \frac{\pi^4 a^5}{45} \int_t^{+\infty} u^3 {}_1F_2\left(3; \frac{7}{2}, 6; -(\pi a u)^2\right) du \\ &= \tilde{f}_1(0; a) - \frac{\pi^4 a^5 t^4}{180} {}_1F_2\left(2; \frac{7}{2}, 6; -(\pi a t)^2\right) du, \quad t \in [0, +\infty), \end{aligned}$$

where the generalized hypergeometric function has the following elementary representation (Wolfram Research, 2021):

$$\begin{aligned} &{}_1F_2\left(2; \frac{7}{2}, 6; -x^2\right) \\ &= \frac{75(2x^6 - 6x^4 - 9x^2 - 6x(x^2 - 6)) \sin(2x) - 9(3x^2 - 2) \cos(2x) - 18}{2x^{10}}, \quad x \in [0, +\infty). \end{aligned}$$

Accordingly, the Schoenberg expansion of  $\tilde{K}_3$  is given by (8), where the series terminates after the term associated with  $k = 1$ . The knowledge of the constant  $\tilde{f}_1(0; a)$  is unnecessary, as it is filtered out since  $a_{0,n,1} + a_{1,n,1} = 0$ .

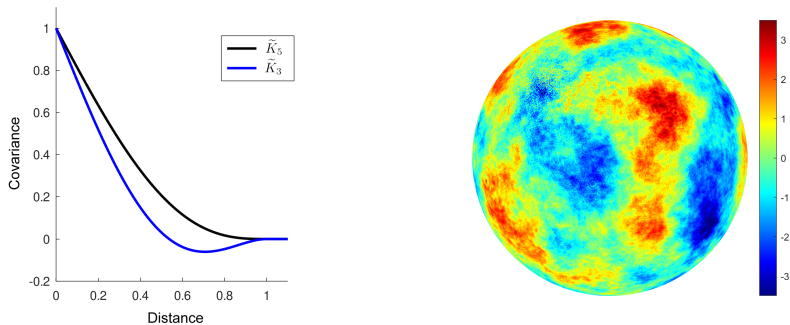


Figure 2: Left: isotropic parts of a pentaspherical covariance  $K_5$  in  $\mathbb{R}^5 \times \mathbb{R}^5$  with unit range (black) and of the covariance  $K_3$  in  $\mathbb{R}^3 \times \mathbb{R}^3$  obtained by applying the turning bands operator (blue). Both isotropic parts are compactly supported, with the former being monotone, while the latter exhibits a hole effect. Right: a realization of an isotropic random field with covariance  $K_3$ , obtained with the turning arcs algorithm, using 50,000 Gegenbauer waves with degrees following a shifted zeta distribution of parameter 2. The visualization is restricted to  $\mathbb{S}^2$  discretized into 250,000 points

## 4 Conclusions

The main result of this work can be summarized as follows: if a matrix-valued function on the nonnegative half-line with support in  $[0, \pi]$  is the isotropic part of a covariance function in  $\mathbb{R}^d \times \mathbb{R}^d$ , with  $d$  an odd integer greater than 1, then it is also the isotropic part of a covariance function on  $\mathbb{S}^d \times \mathbb{S}^d$ . This result generalizes findings by Gneiting (2013) and Ma (2016), which are restricted to continuous functions and to  $d = 3$ , and a result by Nie and Ma (2019), which is restricted to continuous scalar functions (univariate covariances). Our proof, apart from differing from that of the previous authors, furthermore allows deriving an analytical expression of the  $d$ -Schoenberg sequence associated with the covariance on the sphere, which is a key input in spectral simulation algorithms. The examples of the Gauss hypergeometric covariance and of a hole effect covariance have been provided, for which the  $d$ -Schoenberg sequences can be expressed by means of the generalized hypergeometric function  ${}_1F_2$ .

The case of spaces of even dimension turns out to be quite more complex and could not be solved, as it seemingly involves less tractable montée operators of odd order and multiply monotone functions of fractional order. Yet, counterex-

amples that would make Theorem 2 fail in even dimensional spaces could not be found either, which leaves open the conjecture of whether this theorem is valid or not for even  $d$ . In practice, a covariance model on the  $d$ -dimensional sphere, with even  $d$ , can be obtained by restricting a model on the  $(d + 1)$ -dimensional sphere, so that the restriction imposed by the unevenness of the Euclidean space and sphere dimensions has little consequence in practice.

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