A catalogue of nonseparable positive semidefinite 1 kernels on the product of two spheres 2

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Abstract We present a catalogue of 26 parametric families of matrix-valued 7

positive semidefinite kernels for modeling the spatial correlation structure of 8 vector random fields defined over the product of two hyperspheres. Such a q geometry has been proved successful to account for complex sources of season-10 ality and direction-dependence of phenomena regionalized on a large portion of 11 planet Earth. All the kernels are nonseparable, as they cannot be written as the 12 product of positive semidefinite kernels defined on hyperspheres, and sufficient 13 validity conditions on their parameters are identified. Their analytical spectral 14 representations and a spectral simulation algorithm are also provided. A side 15 product is the derivation of new matrix-valued isotropic covariance kernels on 16 hyperspheres, together with their analytical spectral representations.

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- Keywords Space-time random fields \cdot Matrix-valued covariance kernels \cdot 18
- Schoenberg sequences · Spectral simulation · Hypertorus 19
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²¹ 1 Introduction: scope, state-of-the-art, outline

Positive semidefinite kernels are of broad interest in several fields of mathematics, such as operator theory (Aronszajn, 1950), approximation theory (Erb and Filbir, 2008), coding theory (Musin, 2008a) and distance geometry (Musin, 2008b), as well as in computer experiments (Haaland and Qian, 2011), machine learning (Hofmann et al., 2008), spatial and space-time statistics (Chen et al., 2021; Porcu et al., 2021), the latter field being the primary motivation of this work.

Space-time data in meteorological, hydrological and climate studies often 29 exhibit complex seasonal patterns. A usual approach to account for these pat-30 terns is to decompose the variable under study into a periodic deterministic 31 trend and a random residual. Removing the trend (detrending) therefore allows 32 studying the residual with the usual tools and methods of spatial statistics. 33 Another approach advocated by Porcu and White (2022) is to embed spatial 34 or space-time domains into a circle or a product of circles, i.e., to trade the 35 traditional Euclidean geometry of the time coordinates for a periodic geometry. 36 The idea of embedding time periodicities inside the geometry of the space 37 where the data are collected is not novel. In particular, Shirota and Gelfand 38 (2017) have applied such a methodology to model daily crime events using log-39 Gaussian Cox processes. Continuous-time monitoring of ground-level ozone 40 concentrations has instead been proposed by White and Porcu (2019). 41 Other relevant applications in environmental, atmospheric, oceanographic, 42

physical and earth sciences where one would benefit from using random fields 43 indexed with circular or spherical coordinates include the analysis of obser-44 vations collected over a large portion of the Earth (represented as a two-45 dimensional sphere), as well as of observations that are direction-dependent 46 (e.g., electromagnetic radiation, temperature gradient, gravity gradient, to-47 pographic slope, tectonic plate motion, average wind speed or average ocean 48 current velocity measured in a particular direction represented by a point on a 49 circle or on a sphere). Accordingly, analyzing direction-dependent or seasonal-50 dependent observations that, at the same time, are scattered over the Earth 51 would result in working with a random field with an index set consisting of 52 the product of the unit circle \mathbb{S}^1 with the unit two-dimensional sphere \mathbb{S}^2 53 (sometimes the product of two spheres $\mathbb{S}^2 \times \mathbb{S}^2$) representing TIME×SPACE or 54 DIRECTION×SPACE (Mastrantonio et al., 2016). 55

An essential challenge for this approach to be successful is to identify the structure of such a random field, in particular, its covariance kernel. One avenue is to define a separable covariance kernel, as the product of a kernel on S^1 and another one on S^2 . However, separable kernels are often simplistic and do not allow characterizing complex interactions between the spatial variations on S^1 and that on S^2 , hence the interest in finding nonseparable (and not too parameter-intensive) kernels.

To date, simpler geometries than the product of a circle and a sphere have been considered to build up nonseparable covariance kernels. For instance,

⁶⁵ Shirota and Gelfand (2017) consider random fields defined over $\mathbb{S}^1 \times \mathbb{R}^2$, where

 \mathbb{S}^1 is time wrapped over the circle and \mathbb{R}^2 is the spatial domain (a planar 66 surface). In the same line, Mastrantonio et al. (2019) and White and Porcu 67 (2019) consider a Bayesian hierarchical modeling where seasonality is modeled 68 through conditioning sets. Peron et al. (2018) propose product-sum covariance 69 kernels on $\mathbb{S}^k \times \mathbb{R}$, while Shirota and Gelfand (2017), Porcu et al. (2016), Alegría 70 et al. (2019) and Emery et al. (2021) introduce nonseparable covariance kernels 71

on $\mathbb{S}^k \times \mathbb{R}^\ell$, with k and ℓ two positive integers, motivated by applications that 72 range from climatology to geological engineering. 73

Yet, random fields defined over $\mathbb{S}^k\times\mathbb{S}^\ell$ have been considered to a limited 74 extent only. Characterizations of the covariance kernels associated with scalar-75 valued random fields that are continuously indexed over $\mathbb{S}^k \times \mathbb{S}^\ell$ have been 76 provided by Guella et al. (2015) and Guella and Menegatto (2016), while the 77 work by Porcu and White (2022) provides parametric families of such kernels. 78 The contribution by Bachoc et al. (2021) gives spectral representations for 79 vector random fields, together with some specific parametric families of matrix-80 valued covariance kernels on $\mathbb{S}^k \times \mathbb{S}^\ell$. 81 This paper provides a catalogue of parametric families of matrix-valued 82

nonseparable covariance kernels associated with vector random fields that are 83 continuously indexed over the product of two (hyper)spheres. The outline is 84 the following. Section 2 contains a succinct mathematical and statistical back-85 ground. Section 3 lists 26 new families of covariance kernels, together with 86 their spectral representations and sufficient validity conditions. A discussion on 87 these kernels (Section 4), methodological proposals for parameter estimation 88 and for random field simulation (Section 5) and concluding remarks (Section 89

6) follow. Proofs are deferred to the Appendix to ease legibility. 90

2 Background 91

2.1 Positive semidefinite and conditionally negative semidefinite matrices 92

Throughout, p is a positive integer and bold letters indicate real-valued p-93

dimensional vectors or symmetric $p \times p$ matrices. All matrix operations (prod-94

uct, ratio, or any function) are taken elementwise. For a $p \times p$ matrix a and a 95

real value ω , $\omega \pm a$ is taken as a shortcut of $\omega \mathbf{1} \pm a$, where **1** is the all-ones 96 matrix of size $p \times p$. 97

Let $\boldsymbol{a} = [a_{i,j}]_{i,j=1}^p$ be a symmetric $p \times p$ real matrix, $\boldsymbol{\omega} = [\omega_1, \dots, \omega_p]^\top \in \mathbb{R}^p$ 98 (with \top denoting the transpose operator) and the quadratic form 99

$$Q(\boldsymbol{a},\boldsymbol{\omega}) := \sum_{i=1}^{p} \sum_{j=1}^{p} \omega_i \, a_{i,j} \, \omega_j.$$
(1)

The matrix **a** is positive semidefinite when $Q(\mathbf{a}, \boldsymbol{\omega}) > 0$ for any $\boldsymbol{\omega}$. If $Q(\mathbf{a}, \boldsymbol{\omega}) > 0$ 100 0 for any nonzero $\boldsymbol{\omega}$, then the matrix is said to be positive definite. The 101 matrix **a** is conditionally negative semidefinite when $Q(\mathbf{a}, \boldsymbol{\omega}) \leq 0$ for any $\boldsymbol{\omega}$ 102 whose components add to zero. Likewise, a is said to be conditionally negative 103

definite if $Q(\boldsymbol{a}, \boldsymbol{\omega}) < 0$ for any nonzero $\boldsymbol{\omega}$ whose components add to zero. The following criteria are useful to establish the positive or conditional negative

- ¹⁰⁶ semidefiniteness of a matrix:
- ¹⁰⁷ (1) **a** is conditionally negative (semi)definite if, and only if, $[a_{ip} + a_{pj} a_{ij} a_{pp}]_{i,j=1}^{p-1}$ is positive (semi)definite (Reams, 1999, Lemma 2.4);
- (2) a is conditionally negative semidefinite if, and only if, $\exp(-ta)$ is positive semidefinite for any $t \ge 0$ (Reams, 1999, Lemma 2.5);
- ¹¹¹ (3) \boldsymbol{a} is conditionally negative semidefinite if it has nonnegative entries and ¹¹² \boldsymbol{a}^2 is conditionally negative semidefinite (Berg et al., 1984, Chapter 3, ¹¹³ Corollary 2.10);
- 114 (4) \boldsymbol{a} is conditionally negative (semi)definite if $-\boldsymbol{a}$ is positive (semi)definite;
- (5) If a_1 and a_2 are positive semidefinite, so are $a_1 a_2$ (Schur product theorem) and $a_1 + a_2$;
- (6) If a_1 and a_2 are conditionally negative semidefinite, so is $a_1 + a_2$;
- ¹¹⁸ (7) If a_1 and $-a_2$ are positive semidefinite, then $a_1 a_2$ is conditionally negative semidefinite.

¹²⁰ 2.2 Positive semidefinite kernels on hypertori

Let k, ℓ be positive integers. We define the (k, ℓ) -hyperspherical torus or (k, ℓ) -hypertorus through the identity

$$\mathbb{T}^{k,\ell} := \mathbb{S}^k \times \mathbb{S}^\ell = \{ \mathbf{x} = (x,y) : (x,y) \in \mathbb{R}^{k+1} \times \mathbb{R}^{\ell+1}, \ \|x\|_{k+1} = \|y\|_{\ell+1} = 1 \},\$$

where $\|\cdot\|_{k+1}$ and $\|\cdot\|_{\ell+1}$ are the Euclidean norms on \mathbb{R}^{k+1} and $\mathbb{R}^{\ell+1}$ respec-

122 tively. Here, \mathbb{S}^k and \mathbb{S}^{ℓ} denote the k- and ℓ -dimensional unit spheres embedded

¹²³ in \mathbb{R}^{k+1} and $\mathbb{R}^{\ell+1}$, respectively. The name hyperspherical torus is due to the

 $_{124}$ fact that $\mathbb{T}^{1,1}$, the product of two circles, is isomorphic to the classical circular

125 torus.

We identify $\mathbb{R}^{p \times p}$ with the set of all $p \times p$ matrices with real entries and consider a matrix-valued kernel $\boldsymbol{K} : \mathbb{T}^{k,\ell} \times \mathbb{T}^{k,\ell} \to \mathbb{R}^{p \times p}$, defined as

$$\boldsymbol{K}(\mathbf{x},\mathbf{x}') = [K_{ij}(\mathbf{x},\mathbf{x}')]_{i,j=1}^{p}, \qquad \mathbf{x},\mathbf{x}' \in \mathbb{T}^{k,\ell}.$$

 \boldsymbol{K} is positive semidefinite if, and only if, the matrix $[[K_{ij} (\mathbf{x}_m, \mathbf{x}_n)]_{i,j=1}^p]_{m,n=1}^N$ is positive semidefinite for any set of points $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{T}^{k,\ell}$. The Kolmogorov extension theorem states that such a positive semidefinite kernel is the covariance of a Gaussian vector random field $\boldsymbol{Z} = [Z_1, \ldots, Z_p]^\top$ on $\mathbb{T}^{k,\ell}$, i.e.

$$K_{ij}(\mathbf{x}, \mathbf{x}') = \mathbb{E}\left(Z_i(\mathbf{x})Z_j(\mathbf{x}')\right), \qquad \mathbf{x}, \mathbf{x}' \in \mathbb{T}^{k,\ell}, \, i, j = 1, \dots, p,$$

with \mathbb{E} denoting the mathematical expectation. Reciprocally, any covariance kernel on $\mathbb{T}^{k,\ell} \times \mathbb{T}^{k,\ell}$ is positive semidefinite.

Building covariance (positive semidefinite) kernels is mathematically challenging and simplifying assumptions are often required for modeling, estima-

¹³⁰ tion, and prediction (Chilès and Delfiner, 2012). Throughout, we assume that

there exists a continuous (continuity is intended as pointwise and elementwise) mapping $C: [-1,1]^2 \to \mathbb{R}^{p \times p}$ such that

$$K(\mathbf{x}, \mathbf{x}') = C(s, r), \quad \mathbf{x} = (x_1, y_1), \mathbf{x}' = (x'_1, y'_1),$$
 (2)

with $s := \langle x_1, x'_1 \rangle_k, r := \langle y_1, y'_1 \rangle_\ell$, for $x_1, x'_1 \in \mathbb{S}^k$, $y_1, y'_1 \in \mathbb{S}^\ell$ and where $\langle \cdot, \cdot \rangle_k$ and $\langle \cdot, \cdot \rangle_\ell$ are the usual dot products on \mathbb{R}^{k+1} and $\mathbb{R}^{\ell+1}$, respectively. Note that s and r are the cosines of the geodesic distances taken over \mathbb{S}^k and \mathbb{S}^ℓ , respectively.

Hereinafter, we call C the componentwise isotropic part of the kernel K, and denote $\mathcal{P}^p(\mathbb{T}^{k,\ell})$ the class of continuous mappings C satisfying identity (2). We use the analogous notation $\mathcal{P}^p(\mathbb{S}^k)$ for the class of continuous mappings $g: [-1,1] \to \mathbb{R}^{p \times p}$ such that the kernel $(x, x') \mapsto g(\langle x, x' \rangle_k)$, for $x, x' \in \mathbb{S}^k$, is positive semidefinite.

The componentwise isotropic part $C \in \mathcal{P}^p(\mathbb{T}^{k,\ell})$ is separable if it can be written as the product of a function of s and a function of r:

$$C(s,r) = C_1(s) C_2(r), \quad s,r \in [-1,1].$$

A wealth of separable covariance kernels on the hypertorus $\mathbb{T}^{k,\ell}$ can be obtained by multiplying isotropic covariance kernels defined on the hyperspheres \mathbb{S}^k and \mathbb{S}^ℓ . We refer the reader to Huang et al. (2011), Gneiting (2013), Guinness and Fuentes (2016), Jeong et al. (2017), Xu (2018) and Lantuéjoul et al. (2019) for examples of scalar covariance kernels on hyperspheres, and to Porcu et al. (2016), Guella and Menegatto (2019), Bevilacqua et al. (2020) and Emery et al. (2022) for matrix-valued covariance kernels.

¹⁴⁹ 2.3 Spectral representations

Guella et al. (2016) proved that a continuous mapping $C : [-1,1]^2 \to \mathbb{R}$ with $C(1,1) < \infty$ belongs to the class $\mathcal{P}^1(\mathbb{T}^{k,\ell})$ if and only if

$$C(s,r) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} b_{n,m}^{k,\ell} \mathcal{G}_n^{(k-1)/2}(s) \mathcal{G}_m^{(\ell-1)/2}(r), \quad s,r \in [-1,1],$$
(3)

where \mathcal{G}_n^{λ} stands for the Gegenbauer polynomial of degree n and order λ (for $\lambda > 0$) or the Chebychev polynomial of the first kind of degree n (for $\lambda = 0$) (Olver et al., 2010, Table 18.3.1), $b_{n,m}^{k,\ell} \ge 0$,

$$\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} b_{n,m}^{k,\ell} \mathcal{G}_n^{(k-1)/2}(1) \mathcal{G}_m^{(\ell-1)/2}(1) < \infty$$

and

$$b_{n,m}^{k,\ell} \propto \int_{-1}^{1} C(s,r) \mathcal{G}_n^{(k-1)/2}(s) \mathcal{G}_m^{(\ell-1)/2}(r) (1-s^2)^{k/2-1} (1-r^2)^{\ell/2-1} \mathrm{d}s \,\mathrm{d}r.$$

A similar series expansion holds for the class $\mathcal{P}^1(\mathbb{S}^k)$, with the reader referred to Schoenberg (1942) for details.

The characterization of a *p*-variate isotropic covariance kernel on the *k*dimensional sphere, $\mathbf{K} : \mathbb{S}^k \times \mathbb{S}^k \to \mathbb{R}^{p \times p}$, with p > 1 and k > 0, can be found in Yaglom (1987) and an alternative proof can be found in Bonfim and Menegatto (2016): the isotropic part $\mathbf{C} : [-1,1] \to \mathbb{R}^{p \times p}$ of \mathbf{K} belongs to the class $\mathcal{P}^p(\mathbb{S}^k)$ if and only if

$$\boldsymbol{C}(s) = \sum_{n=0}^{\infty} \boldsymbol{b}_n \mathcal{G}_n^{(k-1)/2}(s), \quad s \in [-1, 1],$$
(4)

where $\{\boldsymbol{b}_n\}_{n=0}^{\infty}$ is a sequence of symmetric positive semidefinite matrices of size $p \times p$ such that $\sum_{n=0}^{\infty} \boldsymbol{b}_n \mathcal{G}_n^{(k-1)/2}(1) < \infty$ (elementwise summation). This representation is a multivariate extension of Schoenberg's theorem (Schoenberg, 1942), reason for which the sequence $\{\boldsymbol{b}_n\}_{n=0}^{\infty}$ is known as the k-Schoenberg sequence of \boldsymbol{C} .

Using the techniques of Bonfim and Menegatto (2016) and Guella et al. (2016), one can infer the following result, which is an extension of (3) and agrees with the findings of Bachoc et al. (2021).

Theorem 1 Let p a positive integer. A function $C : [-1,1]^2 \to \mathbb{R}^{p \times p}$ belongs to the class $\mathcal{P}^p(\mathbb{T}^{k,\ell})$ if and only if

$$\boldsymbol{C}(s,r) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \boldsymbol{b}_{n,m}^{k,\ell} \mathcal{G}_n^{(k-1)/2}(s) \mathcal{G}_m^{(\ell-1)/2}(r), \quad s,r \in [-1,1],$$
(5)

with $\{\boldsymbol{b}_{n,m}^{k,\ell}\}_{n,m=0}^{\infty}$ a sequence of symmetric positive semidefinite matrices of size $p \times p$ such that $\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \boldsymbol{b}_{n,m}^{k,\ell} \mathcal{G}_n^{(k-1)/2}(1) \mathcal{G}_m^{(\ell-1)/2}(1) < \infty$ (elementwise summation).

Hereinafter, we call $\boldsymbol{b}_{n,m}^{k,\ell}$ the (k,ℓ) -Schoenberg matrix of \boldsymbol{C} , and $\{\boldsymbol{b}_{n,m}^{k,\ell}\}_{n,m=0}^{\infty}$ the (k,ℓ) -Schoenberg sequence of \boldsymbol{C} .

¹⁷⁴ 3 Nonseparable covariance kernels on hypertori

Throughout this section, we consider $\lambda = \frac{k-1}{2}$ and $\mu = \frac{\ell-1}{2}$. For $n \in \mathbb{N}$ and $\nu \in \mathbb{R}$, we define

$$f(\nu, n) = \begin{cases} \frac{\nu \exp(-\pi\nu/2) \sinh(\pi\nu/2)}{2\pi} & \text{if } n \text{ is even} \\ \frac{\nu \exp(-\pi\nu/2) \cosh(\pi\nu/2)}{2\pi} & \text{if } n \text{ is odd,} \end{cases}$$
(6)

with sinh and cosh the hyperbolic sine and cosine, respectively. We also use the symbols and functions listed in Table 1.

 Table 1: Symbols and ordinary and special functions

Notation	Function name	
.	Floor function	
Ī	Complex modulus	
ι	Imaginary unit	
\mathcal{G}_n^{ν}	Gegenbauer (a.k.a. ultraspherical) polynomial of degree n and order ν	
$J_{ u}$	Bessel function of the first kind of order ν	
I_{ν}	Modified Bessel function of the first kind of order ν	
Γ	Gamma function	
$(\cdot)_k$	Pochhammer symbol, a.k.a. rising factorial	
$_0F_1$	Confluent hypergeometric function	
${}_{1}F_{1}$	Kummer confluent hypergeometric function	
${}_{2}F_{1}$	Gauss hypergeometric function	

Next, we provide 26 parametric classes of nonseparable models in $\mathcal{P}^p(\mathbb{T}^{k,\ell})$,

with p > 0, k > 1 and $\ell > 1$, together with their (k, ℓ) -Schoenberg sequences

181 (Tables 2 to 11). At the end of each table, we provide sufficient conditions com-

¹⁸² mon to all the models of the table to be well-defined and positive semidefinite,

183 i.e., to be valid covariance kernels.

184 3.1 Models based on elementary and gamma functions

The kernels $(s, r) \mapsto C(s, r)$ listed in Tables 2 and 3 are defined by sums, products and compositions of finitely many polynomial, rational, inverse trigono-

metric, logarithmic and exponential functions of the input parameters a, b,

¹⁸⁸ ν and ρ . Two other kernels also involving gamma functions are provided in

Tables 4 and 5. Examples of graphical representations of the kernel marginals

190 $s \mapsto C(s, 1)$ and $r \mapsto C(1, r)$ are shown in Figure 1.

 Table 2: Elementary covariance kernels, part 1.

Elementary model 1
Covariance kernel:
$C = \rho (1 - 2r \exp(\nu(s - a) - b) + \exp(2\nu(s - a) - 2b))^{-\mu}$
Schoenberg matrices:
$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b}) 2^{\lambda} \Gamma(\lambda)(\lambda+n)(m\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}(m\boldsymbol{\nu})$
Elementary model 2
Covariance kernel:
$C = \rho (1 - r \exp(\nu(s - a) - b)) (1 - 2r \exp(\nu(s - a) - b)) + \exp(2\nu(s - a) - 2b))^{-\nu - 1}$
Schoenberg matrices:
$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \frac{m+2\mu}{4\mu} \exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b}) 2^{\lambda} \Gamma(\lambda) (\lambda+n) (m\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}(m\boldsymbol{\nu})$

Table 2	(continued)
Table 2	(continued)

Elementary model 3
Covariance kernel:
$C = \rho 2^{\mu - 1/2} (1 - 2r \exp(\nu(s - a) - b) + \exp(2\nu(s - a) - 2b))^{-1/2} \\ \times \left(1 - r \exp(\nu(s - a) - b) + \sqrt{1 - 2r \exp(\nu(s - a) - b)} + \exp(2\nu(s - a) - 2b) \right)^{1/2 - \mu}$
$\times \left(1 - r \exp(\boldsymbol{\nu}(s-\boldsymbol{a}) - \boldsymbol{b}) + \sqrt{1 - 2r \exp(\boldsymbol{\nu}(s-\boldsymbol{a}) - \boldsymbol{b})} + \exp(2\boldsymbol{\nu}(s-\boldsymbol{a}) - 2\boldsymbol{b})\right)^{1/2 - \mu}$
Schoenberg matrices:
$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \frac{(\mu + \frac{1}{2})_m}{(2\mu)_m} \exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b}) 2^{\lambda} \Gamma(\lambda)(\lambda + n)(m\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}(m\boldsymbol{\nu})$
Elementary model 4
Covariance kernel:
$\boldsymbol{C} = \boldsymbol{\rho} \left(1 + 2r \exp(\boldsymbol{\nu}(s-\boldsymbol{a}) - \boldsymbol{b}) + \exp(2\boldsymbol{\nu}(s-\boldsymbol{a}) - 2\boldsymbol{b}) \right)^{\kappa/2}$
$r + \exp(\boldsymbol{\nu}(s-\boldsymbol{a}) - \boldsymbol{b})$
$\times \mathcal{G}^{\mu}_{\kappa} \left(\frac{r + \exp(\boldsymbol{\nu}(s - \boldsymbol{a}) - \boldsymbol{b})}{\sqrt{1 + 2r \exp(\boldsymbol{\nu}(s - \boldsymbol{a}) - \boldsymbol{b}) + \exp(2\boldsymbol{\nu}(s - \boldsymbol{a}) - 2\boldsymbol{b})}} \right)$
Schoenberg matrices:
(0 if $m > \kappa$
$\boldsymbol{b}_{n,m}^{k,\ell} = \begin{cases} \boldsymbol{0} & \text{if } m > \kappa \\ \boldsymbol{\rho} \frac{\exp(-(\kappa - m)(\boldsymbol{a}\boldsymbol{\nu} + \boldsymbol{b})) \Gamma(\kappa + 2\mu)}{(\kappa - m)! \Gamma(m + 2\mu)} 2^{\lambda} \Gamma(\lambda)(\lambda + n)((\kappa - m)\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}((\kappa - m)\boldsymbol{\nu}) & \text{otherwise} \end{cases}$ Elementary model 5
Elementary model 5
Covariance kernel:
$\boldsymbol{C} = \boldsymbol{\rho} \left(1 + 2r \exp(\boldsymbol{\nu}(s-\boldsymbol{a}) - \boldsymbol{b}) + \exp(2\boldsymbol{\nu}(s-\boldsymbol{a}) - 2\boldsymbol{b}) \right)^{\kappa/2}$
$\times \mathcal{G}^{\mu}_{\kappa} \left(\frac{1 + r \exp(\boldsymbol{\nu}(s - \boldsymbol{a}) - \boldsymbol{b})}{\sqrt{1 + 2r \exp(\boldsymbol{\nu}(s - \boldsymbol{a}) - \boldsymbol{b}) + \exp(2\boldsymbol{\nu}(s - \boldsymbol{a}) - 2\boldsymbol{b})}} \right)$
$\left(\mathbf{V} + \mathbf{F} + \mathbf{F} \right) = \left[\mathbf{V} + \mathbf{F} + \mathbf{F} \right]$
Schoenberg matrices:
$\int 0 \text{if } m > \kappa$
$\boldsymbol{b}_{n,m}^{k,\ell} = \begin{cases} \boldsymbol{0} & \text{if } m > \kappa \\ \boldsymbol{\rho} \frac{\exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b}) \Gamma(\kappa + 2\mu)}{(\kappa - m)! \Gamma(m + 2\mu)} 2^{\lambda} \Gamma(\lambda)(\lambda + n)(m\boldsymbol{\nu})^{-\lambda} I_{\lambda + n}(m\boldsymbol{\nu}) & \text{otherwise} \end{cases}$
Sufficient conditions for convergence:
$\kappa \in \mathbb{N}, \nu \text{ and } \boldsymbol{b} + (\boldsymbol{a} - 1)\nu \text{ with entries in } (0, \infty), \text{ and } \boldsymbol{\rho} \text{ with entries in } \mathbb{R}$
Sufficient conditions for positive semidefiniteness:
(A) (1) \boldsymbol{a} is conditionally negative semidefinite
(2) \boldsymbol{b} is conditionally negative semidefinite
$(3) \boldsymbol{\nu} = \boldsymbol{\nu} 1$
(4) $\boldsymbol{\rho}$ is positive semidefinite
or (B) (1) $-a$ is positive semidefinite
(B) (1) $-a$ is positive semidemine (2) b is conditionally negative semidefinite
(2) $\boldsymbol{\nu}$ is conditionally negative semidefinite (3) $\boldsymbol{\nu}$ is positive semidefinite
(d) ρ is positive semidefinite (4) ρ is positive semidefinite

 Table 3: Elementary covariance kernels, part 2.

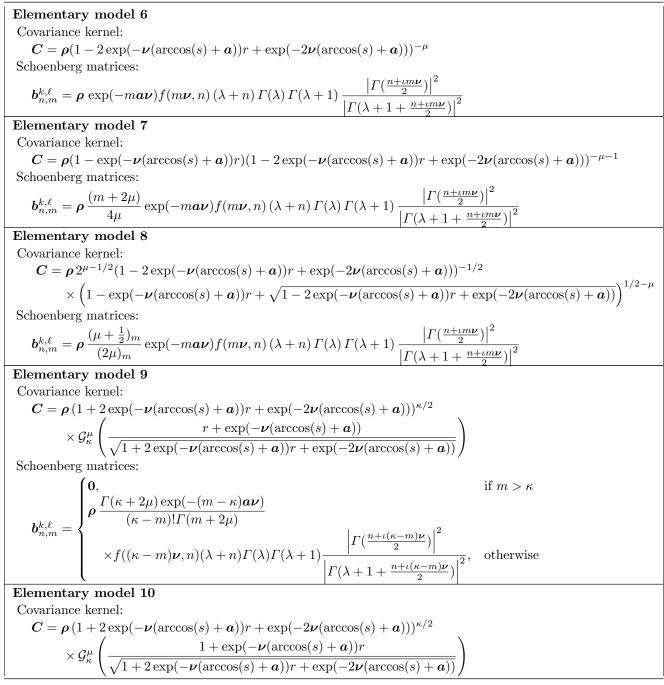
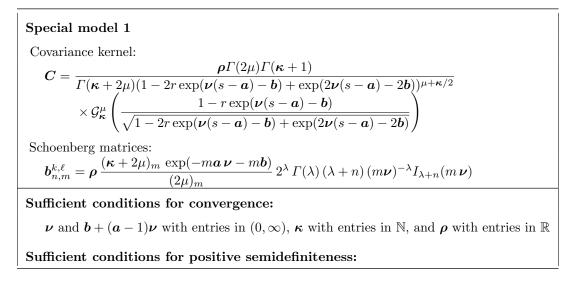


Table 3 (continued)

Schoenberg matrices:		
(0,	if $m > \kappa$	
$\boldsymbol{b}_{n,m}^{k,\ell} = \begin{cases} \boldsymbol{b}, \\ \boldsymbol{\rho} \frac{\Gamma(\kappa+2\mu)\exp(-m\boldsymbol{a}\boldsymbol{\nu})}{(\kappa-m)!\Gamma(m+2\mu)} f(m\boldsymbol{\nu},n) \left(\lambda+n\right)\Gamma(\lambda)\Gamma(\lambda+1) \frac{\left \Gamma(\frac{n+\iota m\boldsymbol{\nu}}{2})\right ^2}{\left \Gamma(\lambda+1+\frac{n+\iota m\boldsymbol{\nu}}{2})\right ^2}, \end{cases}$	otherwise	
Sufficient conditions for convergence:		
$\kappa \in \mathbb{N}, a \text{ and } \boldsymbol{\nu} \text{ with entries in } (0, \infty), \text{ and } \boldsymbol{\rho} \text{ with entries in } \mathbb{R}$		
Sufficient conditions for positive semidefiniteness:		
(A) (1) \boldsymbol{a} is conditionally negative semidefinite		
(2) $\boldsymbol{\nu} = \boldsymbol{\nu} 1$		
(3) $\boldsymbol{\rho}$ is positive semidefinite		
or		
(B) (1) $a = a1$		
(2) ν^2 is conditionally negative semidefinite		
(3) $\rho f(\nu, 0)$ is positive semidefinite		
(4) $\rho f(\nu, 1)$ is positive semidefinite		

 Table 4: Covariance kernels involving elementary and gamma functions, part 1.



(A) (1) \boldsymbol{a} is conditionally negative semidefinite
(2) \boldsymbol{b} is conditionally negative semidefinite
(3) $\nu = \nu 1$
(4) $\boldsymbol{\kappa}$ is positive semidefinite
(5) $\boldsymbol{\rho}$ is positive semidefinite
or
(B) (1) $-a$ is positive semidefinite
(2) \boldsymbol{b} is conditionally negative semidefinite
(3) $\boldsymbol{\nu}$ is positive semidefinite
(4) $\boldsymbol{\kappa}$ is positive semidefinite
(5) $\boldsymbol{\rho}$ is positive semidefinite

Table 5: Covariance kernels involving elementary and gamma functions, part 2.

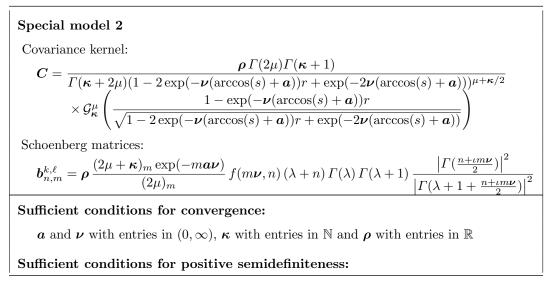


Table 5 (continued)

- (A) (1) \boldsymbol{a} is conditionally negative semidefinite
 - (2) $\boldsymbol{\nu} = \boldsymbol{\nu} \mathbf{1}$
 - (3) κ is positive semidefinite
 - (4) $\boldsymbol{\rho}$ is positive semidefinite

$\stackrel{\text{or}}{(B)(1)} \boldsymbol{a} = a \boldsymbol{1}$

(2) ν^2 is conditionally negative semidefinite

(3) κ is positive semidefinite

- (4) $\rho f(\boldsymbol{\nu}, 0)$ is positive semidefinite
- (5) $\rho f(\nu, 1)$ is positive semidefinite

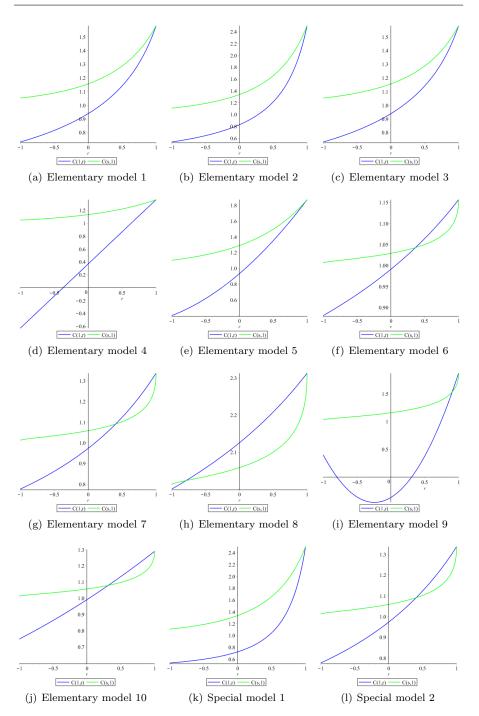


Fig. 1: Examples of elementary models and special models involving elementary and gamma functions. Representation of the marginals $s \mapsto C(s, 1)$ (green) and $r \mapsto C(1, r)$ (blue) for s and r ranging from -1 to 1

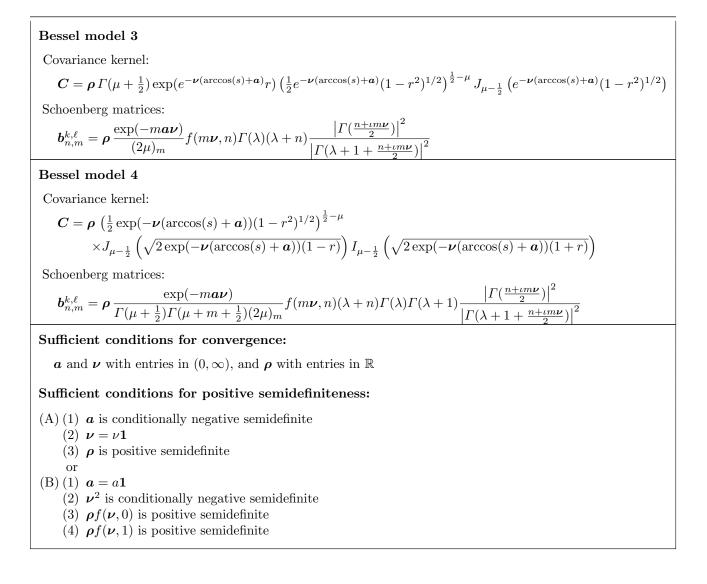
¹⁹¹ 3.2 Bessel and hypergeometric models

- ¹⁹² Tables 6 to 11 list covariance kernels involving Bessel or hypergeometric func-
- ¹⁹³ tions, while Figures 2 and 3 show examples of kernel marginals.

 Table 6: Bessel covariance kernels, part 1.

Bessel model 1
Covariance kernel:
$\boldsymbol{C} = \boldsymbol{\rho} \Gamma(\mu + \frac{1}{2}) \exp(r \exp(\boldsymbol{\nu}(s - \boldsymbol{a}) - \boldsymbol{b}))$
$\times \left(\frac{1}{2}\exp(\boldsymbol{\nu}(s-\boldsymbol{a})-\boldsymbol{b})(1-r^2)^{1/2}\right)^{\frac{1}{2}-\mu} J_{\mu-\frac{1}{2}}(\exp(\boldsymbol{\nu}(s-\boldsymbol{a})-\boldsymbol{b})(1-r^2)^{1/2})$
Schoenberg matrices:
$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \frac{\exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b})}{(2\mu)_m} 2^{\lambda} \Gamma(\lambda)(\lambda+n)(m\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}(m\boldsymbol{\nu})$
Bessel model 2
Covariance kernel:
$C = ho \left(rac{1}{2} \exp(oldsymbol{ u}(s-oldsymbol{a}) - oldsymbol{b})(1-r^2)^{1/2} ight)^{rac{1}{2}-\mu}$
$\times J_{\mu-\frac{1}{2}}\left(\sqrt{2\exp(\boldsymbol{\nu}(s-\boldsymbol{a})-\boldsymbol{b})(1-r)}\right)I_{\mu-\frac{1}{2}}\left(\sqrt{2\exp(\boldsymbol{\nu}(s-\boldsymbol{a})-\boldsymbol{b})(1+r)}\right)$
Schoenberg matrices:
$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \frac{\exp(-m\boldsymbol{a}\boldsymbol{\nu} - m\boldsymbol{b})}{\Gamma(\mu + \frac{1}{2})\Gamma(\mu + m + \frac{1}{2})(2\mu)_m} 2^{\lambda} \Gamma(\lambda)(\lambda + n)(m\boldsymbol{\nu})^{-\lambda} I_{\lambda+n}(m\boldsymbol{\nu})$
Sufficient conditions for convergence:
$\boldsymbol{\nu}$ and $\boldsymbol{b} + (\boldsymbol{a} - 1)\boldsymbol{\nu}$ with entries in $(0, \infty)$, and $\boldsymbol{\rho}$ with entries in \mathbb{R}
Sufficient conditions for positive semidefiniteness:
(A) (1) \boldsymbol{a} is conditionally negative semidefinite
(2) b is conditionally negative semidefinite (3) $\boldsymbol{\nu} = \boldsymbol{\nu} 1$
(3) $\nu = \nu 1$ (4) ρ is positive semidefinite
$\begin{array}{c} \text{Or} \\ \text{(D)} (1) \\ \text{(1)} \end{array}$
(B) (1) $-a$ is positive semidefinite (2) b is conditionally negative semidefinite
(3) $\boldsymbol{\nu}$ is positive semidefinite
(4) $\boldsymbol{\rho}$ is positive semidefinite

Table 7: Bessel covariance kernels, part 2.



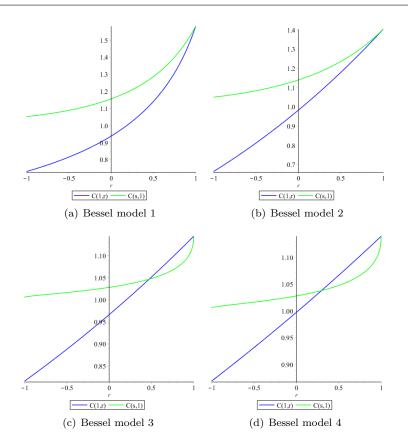
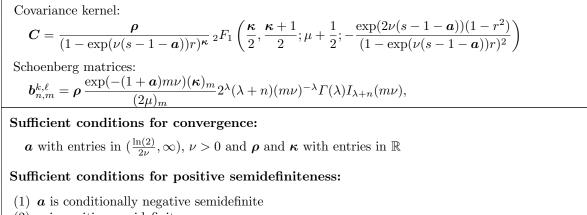


Fig. 2: Examples of Bessel models. Representation of the marginals $s \mapsto C(s, 1)$ (green) and $r \mapsto C(1, r)$ (blue) for s and r ranging from -1 to 1

 Table 8: Hypergeometric covariance kernels, part 1.

Table 8 (continued)



- (2) $\pmb{\rho}$ is positive semidefinite
- (3) $\boldsymbol{\kappa}$ is positive semidefinite

Table 9: Hypergeometric covariance kernels, part 2.

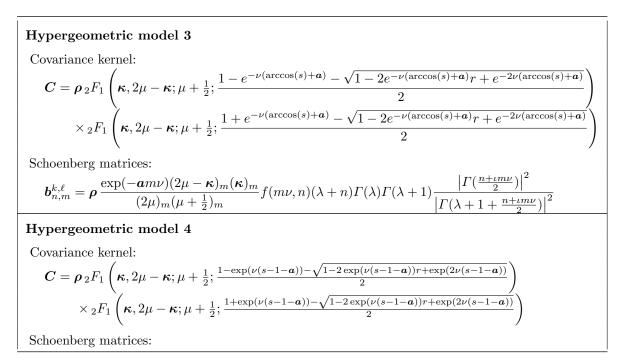


Table 9 (continued)

$$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\rho} \, \frac{\exp(-(1+\boldsymbol{a})m\nu)(2\mu-\boldsymbol{\kappa})_m(\boldsymbol{\kappa})_m}{(2\mu)_m(\mu+\frac{1}{2})_m} \, 2^{\lambda}(\lambda+n)(m\nu)^{-\lambda} \Gamma(\lambda)I_{\lambda+n}(m\nu),$$

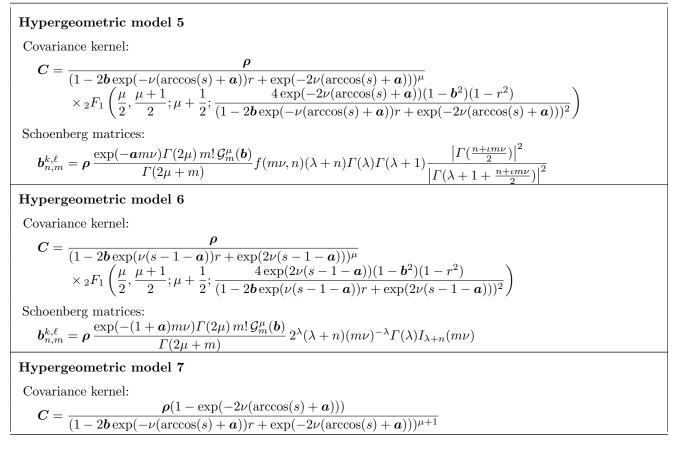
Sufficient conditions for convergence:

 \boldsymbol{a} with entries in $(0,\infty)$, $\nu > 0$ and $\boldsymbol{\rho}$ and $2\mu\boldsymbol{\kappa} - \boldsymbol{\kappa}^2$ with entries in \mathbb{R}

Sufficient conditions for positive semidefiniteness:

- (1) \boldsymbol{a} is conditionally negative semidefinite
- (2) $\boldsymbol{\rho}$ is positive semidefinite
- (3) $2\mu\kappa \kappa^2$ is positive semidefinite

Table 10: Hypergeometric covariance kernels, part 3.

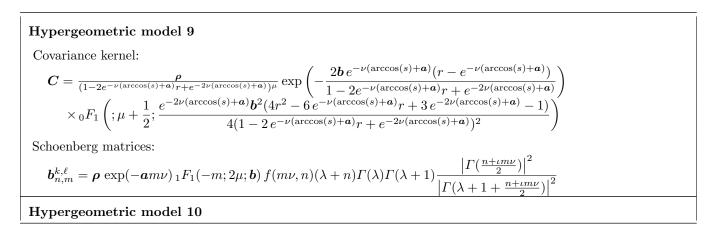


 $\times {}_{2}F_{1}\left(\frac{\mu+1}{2},\frac{\mu}{2}+1;\mu+\frac{1}{2};\frac{4\exp(-2\nu(\arccos(s)+a))(1-b^{2})(1-r^{2})}{(1-2b\exp(-\nu(\arccos(s)+a))r+\exp(-2\nu(\arccos(s)+a)))^{2}}\right)$ Schoenberg matrices: $b_{n,m}^{k,\ell} = \rho \frac{\exp(-am\nu)\Gamma(2\mu)m!(1+\frac{m}{\mu})\mathcal{G}_{m}^{\mu}(b)}{\Gamma(2\mu+m)} f(m\nu,n)(\lambda+n)\Gamma(\lambda)\Gamma(\lambda+1)\frac{\left|\Gamma(\frac{n+im\nu}{2})\right|^{2}}{\left|\Gamma(\lambda+1+\frac{n+im\nu}{2})\right|^{2}}$ Hypergeometric model 8 Covariance kernel: $C = \frac{\rho(1-\exp(2\nu(s-1-a)))}{(1-2b\exp(\nu(s-1-a))r+\exp(2\nu(s-1-a)))^{\mu+1}} \times {}_{2}F_{1}\left(\frac{\mu+1}{2},\frac{\mu}{2}+1;\mu+\frac{1}{2};\frac{4\exp(2\nu(s-1-a))(1-b^{2})(1-r^{2})}{(1-2b\exp(\nu(s-1-a))r+\exp(2\nu(s-1-a)))^{2}}\right)$ Schoenberg matrices: $b_{n,m}^{k,\ell} = \rho \frac{\exp(-(1+a)m\nu)\Gamma(2\mu)m!(1+\frac{m}{\mu})\mathcal{G}_{m}^{\mu}(b)}{\Gamma(2\mu+m)} 2^{\lambda}(\lambda+n)(m\nu)^{-\lambda}\Gamma(\lambda)I_{\lambda+n}(m\nu)$ Sufficient conditions for convergence: $a \text{ with entries in } (0,\infty), b = [\langle s_{i},s_{j}\rangle_{l}]_{i,j=1}^{p} \text{ for a set of points } s_{1},\ldots,s_{p} \in \mathbb{S}^{\ell}, \nu > 0 \text{ and } \rho \text{ with entries in } \mathbb{R}$ Sufficient conditions for positive semidefiniteness:

(1) \boldsymbol{a} is conditionally negative semidefinite

(2) $\boldsymbol{\rho}$ is positive semidefinite

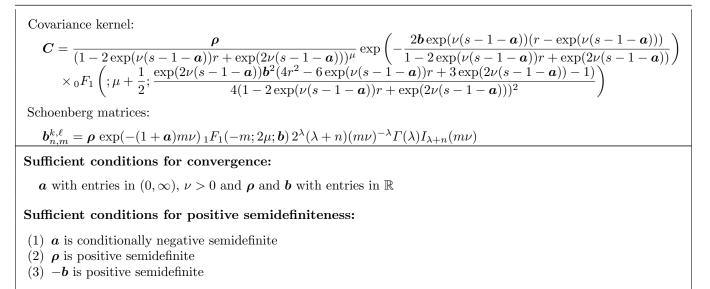
Table 11: Hypergeometric covariance kernels, part 4.



To be continued

Table 10 (continued)

Table 11 (continued)



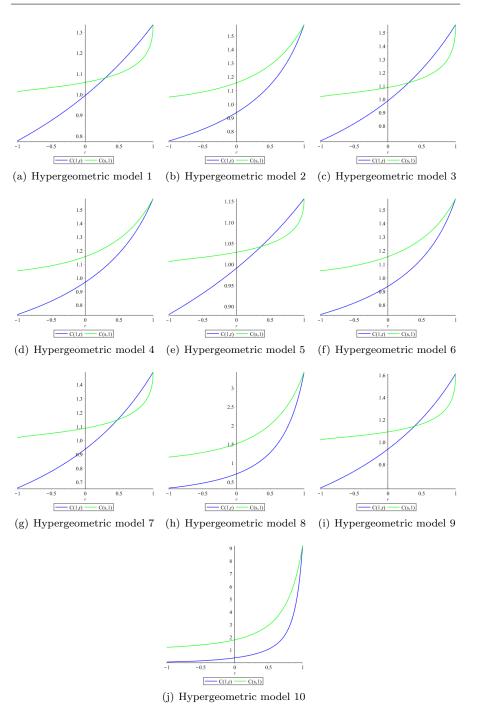


Fig. 3: Examples of hypergeometric models. Representation of the marginals $s \mapsto C(s, 1)$ (green) and $r \mapsto C(1, r)$ (blue) for s and r ranging from -1 to 1

¹⁹⁴ 4 Discussion

All the covariance kernels presented in Tables 2 to 11 are nonseparable, i.e., 195 the componentwise isotropic part $(s,r) \mapsto C(s,r)$ cannot be written as the 196 elementwise product of a function of s with a function of r; equivalently, the 197 Schoenberg matrix $oldsymbol{b}_{n,m}^{k,\ell}$ cannot be written as the elementwise product of a 198 matrix depending on n with a matrix depending on m. This is illustrated in 199 Figure 4, which shows the full covariance maps (not only the marginals) for two 200 specific models of the above list: in both cases, the curvature of the isopleths 201 is not compatible with a separable covariance. The interest in nonseparable 202 covariance kernels for random fields defined on $\mathbb{S}^k \times \mathbb{S}^\ell$ lies in the fact that 203 they allow modeling complex interactions between the spatial variations on 204 \mathbb{S}^k and that on \mathbb{S}^{ℓ} . To date, many nonseparable covariance kernels have been 205 designed for modeling data indexed in a Euclidean space (Cressie and Huang, 206 1999; Gneiting, 2002; Stein, 2005; Apanasovich and Genton, 2010; Rodrigues 207 and Diggle, 2010; Allard et al., 2022) or the product of a Euclidean space with 208 a sphere (Shirota and Gelfand, 2017; Porcu et al., 2016; Alegría et al., 2019; 209 Emery et al., 2021), but we are not aware of such kernels for modeling data 210 indexed in the product of two spheres, except for the recent works of Bachoc 211 et al. (2021) and Porcu and White (2022). 212

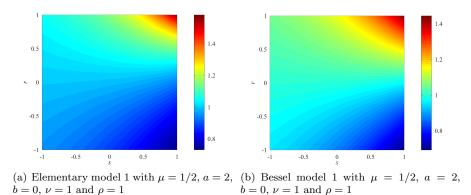


Fig. 4: Mapping $(s, r) \mapsto C(s, r)$ for s and r ranging from -1 to 1, for the elementary model 1 and Bessel model 1 whose marginals are shown in Figures 1 and 2, respectively

The expression of the proposed kernels contain up to five matrix-valued parameters, which are often necessary to ensure the convergence of the Schoenberg sequence, i.e., the existence of the kernel. As an exception, in Tables 2, 4 and 6, either the matrix-valued parameter a or the matrix-valued parameter bcan be set to zero, but not both simultaneously, while b can also be set to zero to yield more parsimonious kernels in Table 11. However, all these are minor simplifications, and dealing with 3 to 5 parameters allows an interesting trade-

off between the number of parameters and the structural features that can be 220 fitted. In particular, from the previous figures, one sees that the behavior at 221 short distances (s or r close to 1), shape and monotonicity of the marginal 222 covariances can be different. The same happens with multivariate kernels: the 223 parameters controlling the shape, large-scale and short-scale behaviors can be 224 different for all the entries of the covariance, which offers much more versa-225 tility to the practitioners than traditional modeling approaches such as the 226 well-known and parameter-intensive linear model of coregionalization (Chilès 227 and Delfiner, 2012; Genton and Kleiber, 2015). In our constructions, the con-228 ditions on the matrix-valued parameters refer to positive semidefiniteness and 229 negative conditional semidefiniteness and are straightforward to check (see cri-230 teria in Section 2.1). 231

232

The case of the hypertorus $\mathbb{T}^{1,\ell}$ deserves a separate treatment. Tables 2 233 to 11 provide covariance kernels on $\mathbb{T}^{k,\ell} \times \mathbb{T}^{k,\ell}$ together with their (k,ℓ) -234 Schoenberg sequences, for any integers k and ℓ greater than 1. In particular, 235 the following holds: 236

- 237
- Each (k, ℓ)-Schoenberg matrix b^{k,ℓ}_{n,m} is positive semidefinite.
 The series ∑[∞]_{n=0} ∑[∞]_{m=0} b^{k,ℓ}_{n,m} G^{(k-1)/2}_n(s)G^{(ℓ-1)/2}_m(r) converges (pointwise and componentwise) to C(s, r) for any s, r ∈ [-1, 1]. 238 239
- For all the presented models, the analytical expression of C depends on ℓ (3)240 (equivalently, μ) but not on k (equivalently, λ). 241
- Looking at the proofs in Appendix A and in Emery et al. (2022), it is seen 242 that the positive semidefiniteness of the Schoenberg matrices (1) and the con-243 vergence of the Schoenberg series (2) actually hold for any real numbers (not 244 necessarily integers) k and ℓ greater than 1. If one makes k tend to 1, with 245 $\ell > 1$ fixed, it becomes possible to extend the previous kernels to the hy-246 pertorus $\mathbb{T}^{1,\ell}$, which is of interest for modeling variables evolving in time or 247 direction-dependent variables (recall Section 1). 248

Specifically, for each fixed natural integer m, define

$$\boldsymbol{b}_{n,m}^{1,\ell} = \begin{cases} \lim_{k \to 1} \boldsymbol{b}_{n,m}^{k,\ell} \text{ if } n = 0\\ \lim_{k \to 1} \frac{2\lambda}{n} \boldsymbol{b}_{n,m}^{k,\ell} \text{ if } n > 0 \end{cases}$$

The above limits exist and are finite for all the models of Tables 2 to 11, insofar as the Schoenberg matrix always contains a term $\Gamma(\lambda)(\lambda+n)$, with $\lambda = \frac{k-1}{2}$ and

$$\begin{cases} \lim_{\lambda \to 0} \Gamma(\lambda)(\lambda + n) = 1 \text{ if } n = 0\\ \lim_{\lambda \to 0} \frac{2\lambda}{n} \Gamma(\lambda)(\lambda + n) = 2 \text{ if } n > 0. \end{cases}$$

Also, $\boldsymbol{b}_{n,m}^{1,\ell}$ is the limit of a sequence of positive semidefinite matrices, hence it is positive semidefinite for any n and m. Accordingly, taking the limit of both sides of (5) as k tends to 1, one obtains:

$$\begin{split} \lim_{k \to 1} \boldsymbol{C}(s,r) &= \lim_{k \to 1} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \boldsymbol{b}_{n,m}^{k,\ell} \mathcal{G}_{n}^{(k-1)/2}(s) \mathcal{G}_{m}^{(\ell-1)/2}(r) \\ &= \lim_{k \to 1} \sum_{m=0}^{\infty} \boldsymbol{b}_{0,m}^{k,\ell} \mathcal{G}_{0}^{(k-1)/2}(s) \mathcal{G}_{m}^{(\ell-1)/2}(r) \\ &+ \lim_{k \to 1} \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} \frac{2\lambda}{n} \boldsymbol{b}_{n,m}^{k,\ell} \frac{n}{2\lambda} \mathcal{G}_{n}^{(k-1)/2}(s) \mathcal{G}_{m}^{(\ell-1)/2}(r), \quad s,r \in [-1,1], \end{split}$$

249 i.e.,

$$\boldsymbol{C}(s,r) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \boldsymbol{b}_{n,m}^{1,\ell} \mathcal{G}_n^0(s) \mathcal{G}_m^{(\ell-1)/2}(r), \quad s,r \in [-1,1],$$
(7)

where \mathcal{G}_n^0 is the Chebyshev polynomial of the first kind (Olver et al., 2010, formula 18.7.25):

$$\mathcal{G}_n^0 = \begin{cases} 1 \text{ if } n = 0 \\\\ \lim_{\lambda \to 0} \frac{n}{2\lambda} \mathcal{G}_n^\lambda \text{ if } n > 0. \end{cases}$$

The identity (7) gives a valid $(1, \ell)$ -Schoenberg sequence for the mapping C,

viewed as the componentwise isotropic part of a covariance on the hypertorus $\mathbb{T}^{1,\ell}$.

253

Finally, a side product of this work is the design of new *p*-variate isotropic covariance kernels on spheres or hyperspheres, together with sufficient validity conditions on their parameters. Indeed, for all the models presented in Tables 2 to 11, the marginals $s \mapsto C(s, 1)$ and $r \mapsto C(1, r)$ belong to $\mathcal{P}^p(\mathbb{S}^k)$ and $\mathcal{P}^p(\mathbb{S}^\ell)$, respectively. The marginals obtained by setting *s* to 1 have already been studied in Emery et al. (2022). Likewise, the marginals obtained by setting *r* to 1 are members of $\mathcal{P}^p(\mathbb{S}^k)$ and their spectral representation is derived from (5):

$$C(s,1) = \sum_{n=0}^{\infty} \boldsymbol{b}_n^k \, \mathcal{G}_n^{(k-1)/2}(s), \quad s \in [-1,1],$$

with

$$\boldsymbol{b}_n^k = \sum_{m=0}^\infty \boldsymbol{b}_{n,m}^{k,\ell} \, \mathcal{G}_m^{(\ell-1)/2}(1), \quad n \in \mathbb{N}.$$

²⁵⁴ 5 Estimation and simulation

A common challenge in spatial statistics is the estimation of the covariance parameters from a set of sampling data (observations). Having chosen a parametric class of covariance models among those presented in Tables 2 to 11 and assuming that the random field under study is Gaussian, maximum likelihood

techniques can be used to specify the model parameters. In the presence of 259

large datasets, composite or pairwise likelihood may be good alternatives to 260

full likelihood (Curriero and Lele, 1999; Varin and Vidoni, 2005). Also, the 261

maximization of the likelihood function can be done with iterative optimiza-262

tion algorithms that work sequentially on a subset of parameters and leave the 263

other parameters fixed to the values previously attained; the reader is referred 264 to Bourotte et al. (2016) and Allard et al. (2022) for details on the proce-265 dure and convincing examples. Although it has been developed for modeling 266

data in Euclidean spaces, this procedure can be adapted to data on hypertori 267

and benefits from the fact that all the kernels presented in this work are rela-268 tively parsimonious (with two to five matrix-valued parameters), so as to reach 269 a trade-off between model complexity, interpretability and versatility and to 270

avoid overfitting. 271

272

We now turn into the simulation of Gaussian vector random fields that are 273 continuously indexed over the hypertorus. 274

For each model in Tables 2 to 11, the Schoenberg sequence has a known an-275

alytic expression, which makes possible to simulate a Gaussian vector random 276

field on the hypertorus by spectral algorithms. A straightforward extension of 277

the arguments exposed in Alegría et al. (2020) implies that a zero-mean vector 278

random field Z on $\mathbb{T}^{k,\ell}$ with matrix-valued covariance K associated with the 279

Schoenberg sequence $\{ \boldsymbol{b}_{n,m}^{k,\ell} \}_{n,m=0}^{\infty}$ can be obtained by putting 280

$$\boldsymbol{Z}(\mathbf{x}) = \varepsilon \sqrt{\frac{p(2\kappa_1 + k - 1)(2\kappa_2 + \ell - 1)}{a_{\kappa_1,\kappa_2}(k - 1)(\ell - 1)}} \,\boldsymbol{\gamma}_{\kappa_1,\kappa_2,k,\ell}^{(q)} \,\mathcal{G}_{\kappa_1}^{(k-1)/2}(\langle \omega_1, x \rangle_k) \,\mathcal{G}_{\kappa_2}^{(\ell-1)/2}(\langle \omega_2, y \rangle_\ell),$$
(8)

where: 281

- (1) $\mathbf{x} = (x, y) \in \mathbb{T}^{k, \ell} = \mathbb{S}^k \times \mathbb{S}^\ell$, with $k, \ell > 1$ 282
- (2) ε is a random variable with a Rademacher distribution (symmetric two-283 point distribution concentrated at 1 and +1) 284
- (3) $\boldsymbol{\kappa} = (\kappa_1, \kappa_2)$, where κ_1 and κ_2 are random integers with joint probability 285
- mass $\mathbb{P}(\kappa_1 = n, \kappa_2 = m) = a_{n,m}$ for any nonnegative integers n and m286
- (4) $a_{n,m} > 0$ for any (n,m) such that $b_{n,m}^{k,\ell}$ is nonzero 287
- (5) q is a random integer uniformly distributed in $\{1, \ldots, p\}$ (6) $\gamma_{n,m,k,\ell}$ is the positive semidefinite square root of $\boldsymbol{b}_{n,m}^{k,\ell}$ 288
- 289
- (7) $\boldsymbol{\gamma}_{n,m,k,\ell}^{(q)}$ is the q-th column of $\boldsymbol{\gamma}_{n,m,k,\ell}$ 290
- (8) ω_1 and ω_2 are random vectors uniformly distributed on \mathbb{S}^k and \mathbb{S}^ℓ , respec-291 tively 292
- (9) ε , κ , q, ω_1 and ω_2 are mutually independent. 293

Other constructions are possible, e.g., by using hyperspherical harmonics 294 instead of Gegenbauer polynomials in (8) (Emery and Porcu, 2019). 295

For k = 1 and $\ell > 1$, the simulated random field takes the form

$$\boldsymbol{Z}(\mathbf{x}) = \varepsilon \sqrt{\frac{2p(2\kappa_2 + \ell - 1)}{a_{\kappa_1,\kappa_2}(\ell - 1)}} \boldsymbol{\gamma}_{\kappa_1,\kappa_2,1,\ell}^{(q)} \mathcal{G}_{\kappa_1}^0(\langle \omega_1, x \rangle_k) \mathcal{G}_{\kappa_2}^{(\ell - 1)/2}(\langle \omega_2, y \rangle_\ell), \qquad (9)$$
$$\mathbf{x} = (x, y) \in \mathbb{T}^{1,\ell}.$$

Finally, a zero-mean Gaussian random field with covariance K can be obtained via a central limit approximation of the form

$$\widetilde{\boldsymbol{Z}}(\mathbf{x}) = \frac{1}{\sqrt{J}} \sum_{j=1}^{J} \boldsymbol{Z}_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{T}^{k,\ell},$$
(10)

where J is a large integer and $\{Z_j : j = 1, ..., J\}$ is a set of independent copies of Z as defined in (8) (if k > 1) or (9) (if k = 1).

Although any bivariate probability mass function such that $a_{n,m} > 0$ if $\mathbf{b}_{n,m}^{k,\ell} \neq \mathbf{0}$ is acceptable for simulating the random degrees (κ_1, κ_2) , some choices are more judicious than others to improve the central limit approximation. In particular, if $\mathbf{b}_{n,m}^{k,\ell} = \mathbf{0}$, then $\gamma_{n,m,k,\ell} = \mathbf{0}$ and the pair (n,m) contributes with a zero (constant) field to the sum (8) or (9). Accordingly, it is good practice to choose $a_{n,m} = 0$ when $\mathbf{b}_{n,m}^{k,\ell} = \mathbf{0}$, in order not to use a copy of \mathbf{Z} that does not add any spatial variability. Also, for the sake of simplicity, it is suggested that κ_1 and κ_2 are independent. Based on these arguments, a good choice for $a_{n,m}$ is the product of two long-tailed probability mass functions, for instance (shifted zeta distributions of parameter 2)

$$a_{n,m} = \frac{36}{\pi^4} (1+n)^{-2} (1+m)^{-2}, \quad n,m \in \mathbb{N}.$$

This choice is certainly not the best option for the elementary models 4, 5, 9 and 10, for which $\mathbf{b}_{n,m}^{k,\ell} = \mathbf{0}$ for $m > \kappa$. In such cases, one suggestion is the product of a shifted zeta distribution with a uniform distribution:

$$a_{n,m} = \begin{cases} \frac{6}{(1+\kappa)\pi^2} (1+n)^{-2}, & n \in \mathbb{N} \text{ and } m \le \kappa \\\\ 0, & n \in \mathbb{N} \text{ and } m > \kappa. \end{cases}$$

The computational cost for constructing a realization of \widetilde{Z} as in (10) is essentially proportional to the number of copies J and to the number of target locations on the hypertorus, while the memory requirements are minimal (the simulated values can be exported as soon as they are generated). The calculations are furthermore parallelizable, which makes the proposed spectral algorithm an attractive approach when large-scale simulations are required.

308 6 Concluding remarks

The present paper has provided a rich catalogue of matrix-valued covariance 309 kernels, together with their spectral representations and sufficient validity con-310 ditions on the parameters, for vector random fields indexed over hypertori. 311 This catalogue may be useful for practitioners who deal with the modeling 312 of direction-dependent (e.g., electromagnetic radiation, temperature gradient, 313 gravity gradient, topographic slope, tectonic plate motion, wind speed, ocean 314 current velocity) or seasonal-dependent (e.g., temperature, precipitation, hu-315 midity, pressure, air quality, solar radiation) variables observed over a large 316 portion of planet Earth. The paper has also provided a straightforward sim-317 ulation algorithm for random fields on hypertori, for which the knowledge of 318 the spectral representation of the covariance kernel is relevant. 319

Understanding the regularity properties of random fields is a subject of major importance in probability theory and statistics, for which an abundant literature is available. The works by Lang and Schwab (2015), Clarke et al. (2018) and Cleanthous et al. (2021) suggest that extensions of the mentioned approaches to our models might be doable. This is certainly a subject of interest for future researches.

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329 Conflict of interest

³³⁰ The authors declare that they have no conflict of interest.

331 Declarations

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337 nolo 338

- Availability of data and material. Not applicable.
- 340

³⁴¹ Code availability. Not applicable.

342

- ³⁴³ Ethics approval. Not applicable.
- ³⁴⁵ Consent to participate. Not applicable.
- 346

Consent for publication. Not applicable. 347

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28

A Appendix: Proofs for the models in Tables 2 to 11 349

Lemma 1 Let k be a positive integer and $\lambda = \frac{k-1}{2}$. Let $\{\mathbf{b}_n\}_{n=0}^{\infty}$ be a sequence of symmetric positive semidefinite matrices, such that the series $\sum_{n=0}^{\infty} \mathbf{b}_n \mathcal{G}_n^{\lambda}(s)$ converges elementwise 350 351 for all $s \in [-1, 1]$. Then, the series is not only convergent, but also absolutely convergent. 352

Proof For $n \in \mathbb{N}$, let $\mathbf{b}_n = [b_{ij,n}]_{i,j=1}^p$. The diagonal entries $b_{ii,n}$, $i = 1, \ldots, p$, are nonnegative, while the absolute value of the off-diagonal entries can be upper bounded by use of Cauchy-Schwarz's and AM-GM inequalities:

$$|b_{ij,n}| \le \sqrt{b_{ii,n} \, b_{jj,n}} \le \frac{b_{ii,n} + b_{jj,n}}{2}.$$

Accordingly, the absolute convergence of the series $\sum_{n=0}^{\infty} b_n \mathcal{G}_n^{\lambda}(s)$ stems from the fact that, for any $s \in [-1,1]$, $|\mathcal{G}_n^{\lambda}(s)| \leq \mathcal{G}_n^{\lambda}(1)$ (Olver et al., 2010, formula 18.14.4):

$$\sum_{n=0}^{\infty} |b_{ij,n}\mathcal{G}_n^{\lambda}(s)| \le \frac{1}{2} \left(\sum_{n=0}^{\infty} b_{ii,n}\mathcal{G}_n^{\lambda}(1) + \sum_{n=0}^{\infty} b_{jj,n}\mathcal{G}_n^{\lambda}(1) \right) < \infty, \quad s \in [-1,1], i, j = 1, \dots, p.$$

353

Lemma 2 Let k, ℓ be positive integers, $\lambda = \frac{k-1}{2}$ and $\mu = \frac{\ell-1}{2}$. Also, let $\{b_{n,m}^{k,\ell}\}_{n,m=0}^{\infty}$ be a doubly-indexed sequence of symmetric positive semidefinite matrices such that the double series $\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{n,m}^{k,\ell} \mathcal{G}_{n}^{\lambda}(s) \mathcal{G}_{m}^{\mu}(r)$ converges elementwise for all $s, r \in [-1, 1]$. Then, this series is absolutely convergent and one can interchange the order of the summations:

$$+\infty < \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{n,m}^{k,\ell} \mathcal{G}_n^{\lambda}(s) \mathcal{G}_m^{\mu}(r) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} b_{n,m}^{k,\ell} \mathcal{G}_m^{\mu}(r) \mathcal{G}_n^{\lambda}(s) < \infty, \quad s,r \in [-1,1].$$

354

Proof The absolute convergence can be established in the same way as in Lemma 1. The 355 interchange of the summation order follows from Fubini's theorem for the counting measure 356 357 on \mathbb{N} .

359 We can now prove the results given in Tables 2 to 11.

Let k and ℓ be integers greater than 1, $\lambda = \frac{k-1}{2}$ and $\mu = \frac{\ell-1}{2}$. Let $C_0(\cdot; \alpha, \theta)$ be the 360 isotropic part of a continuous *p*-variate covariance kernel on \mathbb{S}^{ℓ} , i.e., $C_0 \in \mathcal{P}^p(\mathbb{S}^{\ell})$, where α 361 and θ are real matrices of parameters, the former with size $p \times p$ and entries in $(\alpha_{\min}, \alpha_{\max})$ 362 such that $\alpha_{\max} > 0 \ge \alpha_{\min}$. Assume that C_0 has a spectral representation of the form 363

$$C_0(r; \boldsymbol{\alpha}, \boldsymbol{\theta}) = \sum_{m=0}^{\infty} \boldsymbol{\alpha}^{\phi_m} \, \boldsymbol{\theta}_m \, \mathcal{G}_m^{\mu}(r), \quad r \in [-1, 1], \tag{11}$$

where ϕ_m and θ_m are a nonnegative integer and a $p \times p$ matrix, respectively, that depend 364 analytically on θ and m, but not on α . 365

Let now $C_1(\cdot;\beta)$ be the isotropic part of a continuous p-variate covariance kernel on \mathbb{S}^k , 366 i.e., $C_1 \in \mathcal{P}^p(\mathbb{S}^k)$, where β is a real matrix of parameters, such that, for any nonnegative 367 integer m, the k-Schoenberg sequence of $[C_1]^{\phi_m}$ has a known analytical expression:

$$\boldsymbol{C}_{1}(s;\boldsymbol{\beta})]^{\phi_{m}} = \sum_{n=0}^{\infty} \boldsymbol{\beta}_{n,\phi_{m}} \, \boldsymbol{\mathcal{G}}_{n}^{\lambda}(s), \quad s \in [-1,1].$$
(12)

³⁵⁸

The series (12) converges elementwise for any $s \in [-1, 1]$ and $m \in \mathbb{N}$, insofar as $[C_1]^{\phi_m} \in \mathcal{P}^p(\mathbb{S}^k)$ for any $m \in \mathbb{N}$.

For $n, m \in \mathbb{N}$, define the matrix

$$\boldsymbol{b}_{n,m}^{k,\ell} = \boldsymbol{\beta}_{n,\phi_m} \,\boldsymbol{\theta}_m. \tag{13}$$

Based on the previous statements and on Lemma 2, if the entries of C_1 take values in the

open interval $(\alpha_{\min}, \alpha_{\max})$ and $b_{n,m}^{k,\ell}$ is positive semidefinite for any $n, m \in \mathbb{N}$, the composite function $(s, r) \mapsto C(s, r) := C_0(r; C_1(s; \beta), \theta)$ defined on $[-1, 1]^2$ has a representation of the form (5) and belongs to $\mathcal{P}^p(\mathbb{T}^{k,\ell})$.

Tables 12 and 13 indicate the functions C_0 and C_1 used to construct the 26 kernels presented in Tables 2 to 11, and give the analytical expressions of ϕ_m , θ_m and $\beta_{n,m}$ as defined in (11) and (12). We refer the reader to Emery et al. (2022) for a derivation of such expressions and for a proof that C_0 and C_1 belong to $\mathcal{P}^p(\mathbb{S}^{\ell})$ and $\mathcal{P}^p(\mathbb{S}^{k})$, respectively. From this information, it is straightforward to derive the analytical expressions of the kernels and of their Schoenberg sequences (as per (13)) given in Tables 2 to 11.

382

³⁸³ Convergence of the Schoenberg sequence (5) of C. $(\alpha_{\min}, \alpha_{\max}) = (-1, 1)$ for all the entries ³⁸⁴ of Table 12, except for the one associated with the hypergeometric kernels 1 and 2, in which ³⁸⁵ case $(\alpha_{\min}, \alpha_{\max}) = (-\sqrt{2}/2, \sqrt{2}/2)$. The fact that the entries of C_1 take values in the open ³⁸⁶ interval $(\alpha_{\min}, \alpha_{\max})$ can easily be verified on the basis of the convergence conditions given ³⁸⁷ in Tables 2 to 11.

Positive semidefiniteness of the Schoenberg matrix $\mathbf{b}_{n,m}^{k,\ell}$. Based on the criteria given in Section 2.1 and on the positive semidefiniteness conditions given in Emery et al. (2022), the conditions indicated in Tables 2 to 11 ensure that $\boldsymbol{\theta}_m$ and $\boldsymbol{\beta}_{n,m}$ are positive semidefiniteness of the schoenberg matrix (13) follows from the Schur product theorem, which concludes the proof.

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Kernel	$C_0(r; oldsymbol{lpha}, oldsymbol{ heta})$	ϕ_m	θ_m
Elementary 1 & 6	$ ho (1-2lpha r+lpha^2)^{-\mu}$	m	ρ
Elementary 2 & 7	$\rho (1-\alpha r)(1-2\alpha r+\alpha^2)^{-\mu-1}$	m	$ ho rac{(m+2\mu)}{4\mu}$
Elementary 3 & 8	$\rho 2^{\mu - \frac{1}{2}} (1 - 2\alpha r + \alpha^2)^{-\frac{1}{2}} (1 - \alpha r + \sqrt{1 - 2\alpha r + \alpha^2})^{\frac{1}{2} - \mu}$	m	$\frac{\rho\left(\mu+\frac{1}{2}\right)_m}{(2\mu)_m}$
Elementary 4 & 9	$\rho \left(1 + 2\alpha r + \alpha^2\right)^{\frac{\kappa}{2}} \mathcal{G}^{\mu}_{\kappa} \left(\frac{r + \alpha}{\sqrt{1 + 2\alpha r + \alpha^2}}\right)$	$\kappa - m$	$\begin{cases} 0 & \text{if } m > \kappa \\ \boldsymbol{\rho} \frac{\Gamma(\kappa+2\mu)}{(\kappa-m)!\Gamma(m+2\mu)} & \text{otherwise} \\ 0 & \text{if } m > \kappa \\ \boldsymbol{\rho} \frac{\Gamma(\kappa+2\mu)}{(\kappa-m)!\Gamma(m+2\mu)} & \text{otherwise} \end{cases}$
Elementary 5 & 10	$\rho \left(1 + 2\alpha r + \alpha^2\right)^{\frac{\kappa}{2}} \mathcal{G}^{\mu}_{\kappa} \left(\frac{1 + \alpha r}{\sqrt{1 + 2\alpha r + \alpha^2}}\right)$	m	$\begin{cases} 0 & \text{if } m > \kappa \\ \rho \frac{\Gamma(\kappa + 2\mu)}{(\kappa - m)! \Gamma(m + 2\mu)} & \text{otherwise} \end{cases}$
Special 1 & 2	$\rho_{\frac{\Gamma(2\mu)\Gamma(\kappa+1)}{\Gamma(\kappa+2\mu)(1-2\alpha r+\alpha^2)^{\mu+\kappa/2}}}\mathcal{G}^{\mu}_{\kappa}\left(\frac{1-\alpha r}{\sqrt{1-2\alpha r+\alpha^2}}\right)$	m	$ ho rac{(\kappa+2\mu)_m}{(2\mu)_m}$
Bessel 1 & 3	$\rho \Gamma(\mu + \frac{1}{2}) \exp(\alpha r) \left(\frac{1}{2} \alpha (1 - r^2)^{1/2}\right)^{\frac{1}{2} - \mu} J_{\mu - \frac{1}{2}}(\alpha (1 - r^2)^{1/2})$	m	$\frac{oldsymbol{ ho}}{(2\mu)_m}$
Bessel 2 & 4	$\rho\left(\frac{1}{2}\alpha(1-r^2)^{1/2}\right)^{\frac{1}{2}-\mu} J_{\mu-\frac{1}{2}}(\sqrt{2\alpha(1-r)}) I_{\mu-\frac{1}{2}}(\sqrt{2\alpha(1+r)})$	m	$rac{oldsymbol{ ho}}{\Gamma(\mu+rac{1}{2})\Gamma(\mu+m+rac{1}{2})(2\mu)_m}$
Hypergeometric 1 & 2	$\frac{\rho}{(1-\alpha r)^{\kappa}} _2F_1\left(\frac{\kappa}{2}, \frac{\kappa+1}{2}; \mu+\frac{1}{2}; -\frac{\alpha^2(1-r^2)}{(1-\alpha r)^2}\right)$	m	$ ho rac{(m{\kappa})_m}{(2\mu)_m}$
Hypergeometric 3 & 4	$\rho_{2}F_{1}\left(\kappa, 2\mu-\kappa; \mu+\frac{1}{2}; \frac{1-\alpha-\sqrt{1-2\alpha r+\alpha^{2}}}{2}\right)$	m	$ ho rac{(2\mu-m{\kappa})_n(m{\kappa})_m}{(2\mu)_m(\mu+rac{1}{2})_m}$
	$\times {}_2F_1\left(\kappa,2\mu-\kappa;\mu+rac{1}{2};rac{1+lpha-\sqrt{1-2lpha r+lpha^2}}{2} ight)$		
Hypergeometric 5 & 6	$\frac{\rho}{(1-2\alpha br+\alpha^2)^{\mu}} _2F_1\left(\frac{\mu}{2}, \frac{\mu+1}{2}; \mu+\frac{1}{2}; \frac{4\alpha^2(1-b^2)(1-r^2)}{(1-2\alpha br+\alpha^2)^2}\right)$	m	$oldsymbol{ ho}rac{\Gamma(2\mu)m!}{\Gamma(2\mu+m)}\mathcal{G}^{\mu}_m(oldsymbol{b})$
Hypergeometric 7 & 8	$\frac{\rho(1-\alpha^2)}{(1-2\alpha br+\alpha^2)^{\mu+1}} _2F_1\left(\frac{\mu+1}{2},\frac{\mu}{2}+1;\mu+\frac{1}{2};\frac{4\alpha^2(1-b^2)(1-r^2)}{(1-2\alpha br+\alpha^2)^2}\right)$	m	$ ho rac{\Gamma(2\mu)m!}{\Gamma(2\mu+m)}\left(1+rac{m}{\mu} ight){\cal G}_m^\mu(m{b})$
Hypergeometric 9 & 10	$\frac{\rho}{(1-2\alpha r+\alpha^2)^{\mu}} \exp\left(-\frac{2\alpha b(r-\alpha)}{1-2\alpha r+\alpha^2}\right)$	m	$\boldsymbol{\rho}_{1}F_{1}\left(-m;2\mu;\boldsymbol{b}\right)$
	$\times {}_0F_1\left(;\mu+\frac{1}{2};\frac{\alpha^2 b^2 (4r^2-6\alpha r+3\alpha^2-1)}{4(1-2\alpha r+\alpha^2)^2}\right)$		

Table 12: List of functions C_0 and associated parameters used to construct the covariance kernels given in Tables 2 to 11

Table 13: List of functions C_1 and associated parameters used to construct the covariance kernels given in Tables 2 to 11

Kernel	$C_1(s;oldsymbol{eta})$	$eta_{n,m}$
Elementary 1 to 5, Bessel 1 & 2	$\exp(-oldsymbol{ u} oldsymbol{a} - oldsymbol{b}) \exp(oldsymbol{ u} s)$	$\exp(-m\boldsymbol{\nu}\boldsymbol{a}-m\boldsymbol{b})2^{\lambda}\Gamma(\lambda)(\lambda+n)(m\boldsymbol{\nu})^{-\lambda}I_{\lambda+n}(m\boldsymbol{\nu})$
Elementary 6 to 10, Bessel 3 & 4	$\exp(- u a)\exp\left(- u rccos(s) ight)$	$\exp(-m\boldsymbol{\nu}\boldsymbol{a})f(m\boldsymbol{\nu},n)\left(\lambda+n\right)\Gamma(\lambda)\Gamma(\lambda+1)\frac{\left \Gamma\left(\frac{n+\iotam\boldsymbol{\nu}}{2}\right)\right ^{2}}{\left \Gamma\left(\lambda+1+\frac{n+\iotam\boldsymbol{\nu}}{2}\right)\right ^{2}}$
Hypergeometric $1, 3, 5, 7, 9$	$\exp(-\nu a)\exp(-\nu \arccos(s))$	$\exp(-m\nu a)f(m\nu,n)\left(\lambda+n\right)\Gamma(\lambda)\Gamma(\lambda+1)\frac{\left \Gamma\left(\frac{n+\iota}{2}m^{2}\right)\right ^{2}}{\left \Gamma\left(\lambda+1+\frac{n+\iota}{2}m^{2}\right)\right ^{2}}$
Hypergeometric 2, 4, 6, 8, 10	$\exp(-\nu(1+\boldsymbol{a}))\exp\left(\nus\right)$	$\exp(-m\nu(1+a))2^{\lambda}\Gamma(\lambda)(\lambda+n)(m\nu)^{-\lambda}I_{\lambda+n}(m\nu)$

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