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Multivariate Gaussian Random Fields over Generalized Product Spaces involving the Hypertorus

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Abstract

The paper deals with multivariate Gaussian random fields defined over generalized product spaces that involve the hypertorus. The assumption of Gaussianity implies the finite dimensional distributions to be completely specified by the covariance functions, being in this case matrix valued mappings.

We start by considering the spectral representations that in turn allow for a characterization of such covariance functions. We then provide some methods for the construction of these matrix valued mappings. Finally, we consider strategies to evade radial symmetry (called isotropy in spatial statistics) and provide representation theorems for such a more general case.

Keywords: Matrix valued covariance functions, multivariate random fields, torus, matrix spectral density.

Subject classification: Primary 62M15, 62M30; Secondary 60G12.

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1 Introduction

1.1 Context

This paper considers multivariate Gaussian random fields defined continuously over product spaces involving the torus, or generalizations of the torus obtained through the product of hyperspheres cross d -dimensional Euclidean spaces. Several applications from applied sciences motivate our work on these geometries, and we discuss some of these settings throughout the paper.

More specifically, we consider generalized product spaces, that we define here as the Cartesian product of the d -dimensional Euclidean space, \mathbb{R}^d , with the hypertorus of (d_1, d_2) dimensions, being in turn the product of two unit hyperspheres that are embedded in \mathbb{R}^{d_1+1} and \mathbb{R}^{d_2+1} , respectively. In particular, we consider multivariate Gaussian fields (vector valued fields) as in typical applications, see for instance the survey in Porcu et al. (2018), several variables are observed at the same space-time sampling points. Hence, there is a need to take into account not only the space-time dependence of one variable, but also the cross dependence between any pair of random fields that are observed over the space-time domain.

Most of the literature in the last 30 years has considered *space* as a planar domain - the Euclidean space \mathbb{R}^d - while *time* has been typically considered as linear (Porcu et al., 2020a). The main reason for considering the above generalized spaces based on the hypertorus as *space-time* index sets is that these allow for more generality for a variety of situations. For univariate (scalar valued) random fields, some special cases of these generalized spaces are provided by Porcu and White (2020). For instance, continuous-time data often exhibit multiple sources of seasonality (*e.g.*, daily and weekly). One potential strategy to address these seasonalities is by incorporating them into a covariance structure by wrapping time over the product of two circles, $\mathbb{S}^1 \times \mathbb{S}^1$, see Shirota and Gelfand (2017) and White and Porcu (2019a) on continuous-time monitoring of ground-level ozone concentrations.

As a second possible application, one might consider data over a large section of the Earth where the data exhibit strong seasonality (perhaps on a daily, weekly, or annual scale) or are indexed by a direction (*e.g.*, a bird flying southward). The planet is often approximated by a sphere \mathbb{S}^2 with a given radius (Porcu et al., 2018), and, as discussed, time can be wrapped in a circle to capture seasonality over time. Alternatively, the direction of the data could be indexed by an angle on the circle. Thus, in either case, a Gaussian random field with an index set of $\mathbb{S}^2 \times \mathbb{S}^1$ would be a natural choice to represent phenomena in SPACE×TIME or SPACE×DIRECTION (Mastrantonio et al., 2016).

Gaussian random fields have finite dimensional distributions that are completely specified by their mean, and their covariance function. Covariance functions are positive definite, and ensuring such a requirement for a given candidate mapping is a nontrivial task. For this paper, such a task is overly complicated by the fact that (a) for vector valued random fields, the covariance function

is a matrix valued function, and the mathematical machinery behind *positivity* for the matrix valued case is very challenging (see, for instance Cramer, 1940). Also, (b) generalized spaces have been considered to a very limited extent - see the subsequent literature discussion.

1.2 Literature

The last ten years have seen an unprecedented interest in random fields that are defined over non planar surfaces. For a thorough account, the reader is referred to Porcu et al. (2020a), with the references therein.

Recently, there has been some interest in modeling random fields defined over $\mathbb{R}^2 \times \mathbb{S}^1$, where \mathbb{R}^2 is *space* and \mathbb{S}^1 is time wrapped over the circle. For instance, Shirota and Gelfand (2017) challenge on daily crime events in San Francisco (space, a compact set of \mathbb{R}^2) in 2012 (time, wrapped over the circle). The same modus operandi is adopted by Mastrantonio et al. (2019), who consider Bayesian hierarchical modeling where seasonality is modeled through conditioning sets (see also White and Porcu, 2019a).

Let d, d_1 and d_2 be positive integers. Random fields defined over the product space $\mathbb{S}^{d_1} \times \mathbb{S}^{d_2}$ have only been considered to a limited extent. In mathematical analysis, Guella et al. (2015, 2016, 2017) and Guella and Menegatto (2016) provide conditions for positive definiteness. Berg and Porcu (2017) instead considered the space $\mathbb{S}^d \times G$, for G being a locally compact group. Porcu et al. (2016) and White and Porcu (2019b) considered Gaussian fields defined over \mathbb{S}^d cross linear time. The reader is referred to Porcu et al. (2018) for a recent review on the subject. Recent generalizations on product spaces involving hyperspheres have been proposed in Estrade et al. (2019), and, in more abstract settings, recent contributions can be found in Berg et al. (2018a) and Berg et al. (2018b).

1.3 The Problems, and our Contribution

We start by highlighting some aspects where the literature currently lacks.

A. Multivariate Gaussian random fields defined over generalized spaces are unexplored.

B. Characterizations theorems - that is, spectral representations - for the covariance functions associated with multivariate Gaussian random fields are not available in the current literature.

This paper is devoted to some challenges related to this topic.

1. We consider matrix valued covariance functions that are componentwise isotropic over generalized spaces. That is, they are radially symmetric in \mathbb{R}^d , and they depend on the dot product of each sphere involving the hypertorus. For this setting,

1.a) we provide a spectral representation theorem that ensures necessary and sufficient conditions for a given continuous candidate matrix valued function to be positive definite;

1.b) we provide constructive criteria that allow to build new parametric classes of matrix valued covariance functions under this setting, in particular of the

Matérn type.

2. We relax the hypothesis of radial symmetry in \mathbb{R}^d and provide spectral representations and convergence conditions for the spectral expansions to be well defined.

The plan of the paper is the following: Section 2 provides relevant background material. Section 3 first provides a spectral representation of covariance functions on generalized spaces and then provides new general classes of covariance functions, in particular new classes of the Matérn type. Finally, Section 4 studies a class of matrix covariance functions on generalized spaces that are not radially symmetric in \mathbb{R}^d , providing a characterization.

2 Background Material

2.1 Background from Harmonic Analysis

Let \mathbb{S}^n be the unit sphere of dimension $n \geq 1$, embedded in \mathbb{R}^{n+1} , and let Δ be the Laplace-Beltrami operator defined over \mathbb{S}^n (see Section 2.2 of Morimoto (1998)). The spectrum of Δ is discrete, real and non-positive, with eigenvalues given by $\lambda_k = -k(k+n-1)$ for $k \geq 0$ (Szegő, 1939). Let \mathcal{H}_k be the eigenspace that corresponds to the eigenvalue λ_k . It is known that (Morimoto, 1998)

$$L^2(\mathbb{S}^n) = \bigoplus_{k=0}^{\infty} \mathcal{H}_k.$$

Let $\{Y_{k,j} : k \in \mathbb{N}_0, j = 1, 2, \dots, \kappa_{n,k}\}$ be an orthonormal basis of \mathcal{H}_k having uniquely determined dimension, $\kappa_{n,k}$, defined as

$$\kappa_{n,k} = \dim \mathcal{H}_k = (2k+n-1) \frac{(k+n-2)!}{k!(n-1)!}, \quad (2.1)$$

where this expression has to be understood as being identically equal to 1 when $k=0$ and $n=1$. From (2.1) it becomes apparent that there exists a constant $c_n \geq 1$ such that

$$c_n^{-1}(k+1)^{n-1} \leq \kappa_{n,k} \leq c_n(k+1)^{n-1}. \quad (2.2)$$

The functions $Y_{k,j}$ are the well-known spherical harmonics on \mathbb{S}^n , and they satisfy the addition formula (Marinucci and Peccati, 2011; Yadrenko and Balakrishnan, 1983)

$$\sum_{j=1}^{\kappa_{n,k}} Y_{k,j}(x) \overline{Y_{k,j}(y)} = \frac{\kappa_{n,k}}{\omega_n} C_k^{(n-1)/2}(\langle x, y \rangle), \quad x, y \in \mathbb{S}^n, \quad (2.3)$$

where $\omega_n = (2\pi^{(n+1)/2})/\Gamma((n+1)/2)$ is the total area of \mathbb{S}^n , with

$$C_k^n(r) = \frac{c_k^{\frac{n-1}{2}}(r)}{c_k^{\frac{n-1}{2}}(1)}, \quad r \in [-1, 1],$$

where c_k^λ is a Gegenbauer polynomial of degree k and order $\lambda > -1/2$ (Szegő, 1939). Fundamentally, if $\lambda > -1/2$, then there exists a constant $c = c_\lambda > 0$ such that

$$\sup_{r \in [-1, 1]} c_k^\lambda(r) \leq c(k+1)^{2\lambda-1}, \quad \text{for every } k = 0, 1, \dots \quad (2.4)$$

2.2 Gaussian Fields on Generalized Product Spaces involving the Hypertorus

Let d_1, d_2 be positive integers. We define the (d_1, d_2) -hypertorus with index (d_1, d_2) through the identity

$$\mathbb{T}^{d_1, d_2} := \mathbb{S}^{d_1} \times \mathbb{S}^{d_2} = \{\mathbf{x} = (x_1, x_2) : x_i \in \mathbb{R}^{d_i+1}, \|x_i\|_{d_i+1} = 1, i = 1, 2\},$$

where $\|\cdot\|_{d_i+1}$ is the Euclidean norm on \mathbb{R}^{d_i+1} . The name *hypertorus* is due to $\mathbb{T}^{1,1} = \mathbb{S}^1 \times \mathbb{S}^1$, the product of two circles, being isomorphic to the classical torus.

Let p, d be positive integers, and let \top be the transpose of a column vector. The paper considers zero mean p -variate (or simply, multivariate) Gaussian random fields $\{\mathbf{Z}(\mathbf{x}, \mathbf{u}) = (Z_1(\mathbf{x}, \mathbf{u}), \dots, Z_p(\mathbf{x}, \mathbf{u}))^\top, \mathbf{x} \in \mathbb{T}^{d_1, d_2}, \mathbf{u} \in \mathbb{R}^d\}$ and focuses on their covariance function $\mathbf{K}_Z : (\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d) \times (\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d) \rightarrow \mathbb{R}^{p \times p}$, having elements $K_{ij, \mathbf{Z}}, i, j = 1, \dots, p$, that are defined as

$$K_{ij, \mathbf{Z}}((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')) = \mathbb{E}\left(Z_i(\mathbf{x}, \mathbf{u})Z_j(\mathbf{x}', \mathbf{u}')\right), \quad \mathbf{x}, \mathbf{x}' \in \mathbb{T}^{d_1, d_2}, \mathbf{u}, \mathbf{u}' \in \mathbb{R}^d.$$

For spectral representations for Gaussian fields, the reader is referred to Malarenko and Ostoja-Starzewski (2018). Covariance functions are a linear measure of dependence between any pair of random variables $Z_i(\mathbf{x}, \mathbf{u}), Z_j(\mathbf{x}', \mathbf{u}')$ located at points $(\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}') \in \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d$. The function \mathbf{K}_Z is positive definite (Schoenberg, 1942): for any collection $\{\mathbf{a}_k\}_{k=1}^N \subset \mathbb{R}^{pN}$ and points $\{(\mathbf{x}_k, \mathbf{u}_k)\}_{k=1}^N \in (\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d)^N$,

$$\sum_{k, h=1}^N \mathbf{a}_k^\top \mathbf{K}_Z((\mathbf{x}_k, \mathbf{u}_k), (\mathbf{x}_h, \mathbf{u}_h)) \mathbf{a}_h \geq 0.$$

Building covariance functions is mathematically challenging and simplifying assumptions are often required for modeling, estimation, and prediction. Section 3 assumes that there exists a continuous (continuity is intended as pointwise) mapping $\mathbf{K} : [-1, 1]^2 \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ with $K_{ii}(1, 1, 0) = 1$, such that

$$\mathbf{K}_Z((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')) = \Sigma^{1/2} \mathbf{K}(s, r, h) \Sigma^{1/2}, \quad (2.5)$$

with $s := \langle x_1, x'_1 \rangle_1, r := \langle x_2, x'_2 \rangle_2, h := \|\mathbf{u} - \mathbf{u}'\|$ for $\mathbf{x} = (x_1, x_2), \mathbf{x}' = (x'_1, x'_2), x_i, x'_i \in \mathbb{S}^{d_i}$ and where $\langle \cdot, \cdot \rangle_i$ denotes the classical dot product on \mathbb{R}^{d_i+1} $i = 1, 2$.

Here, $\Sigma^{1/2}$ is a diagonal matrix such that $(\Sigma^{1/2})^\top \Sigma^{1/2} = \Sigma = \text{diag}(\sigma_1, \dots, \sigma_p)$ with σ_i denoting the variance of Z_i .

We call the covariance functions \mathbf{K}_Z componentwise isotropic. In Equation (2.5), s and r are the cosine of the great circle distances taken over \mathbb{S}^{d_1} and \mathbb{S}^{d_2} , respectively. How to relax the hypothesis of componentwise isotropy will be discussed in Section 4. Throughout the rest of the paper, we say that \mathbf{K} is positive definite to mean that the composition of \mathbf{K} with the triplet $(\langle \cdot, \cdot \rangle_1, \langle \cdot, \cdot \rangle_2, \|\cdot\|)$ is a positive definite matrix valued function. This abuse of notation will allow to have a simplified exposition of the results coming subsequently.

2.3 Conditionally Negative Definite Functions

Let X be any nonempty set. A matrix valued function $\gamma : X \times X \rightarrow \mathbb{R}^{p \times p}$ is a cross variogram if it is conditionally negative definite, that is

$$\sum_{k,h=1}^N \mathbf{a}_k^\top \gamma(\mathbf{x}_k, \mathbf{x}_h) \mathbf{a}_h \leq 0,$$

for all $\{\mathbf{x}_k\}_{k=1}^N$ being points in X and $\{\mathbf{a}_k\}_{k=1}^N$ being a collection of vectors summing up to the zero vector. A similar definition applies to matrices $\mathbf{A} = [a_{ij}]_{i,j=1}^p$. We observe that γ is conditionally negative definite if and only if $-\gamma$ is conditionally positive definite (that is, the sign in the inequality above is changed by greater or equal): we refer Menegatto and Peron (2004); Menegatto et al. (2006) for results related to characterizations of conditional positive definiteness when $p = 1$ and X is respectively \mathbb{S}^d or \mathbb{R}^d , and Guella and Menegatto (2020) when $X = \mathbb{R}^d$, $p \geq 1$ and N is fixed.

3 Theoretical Results

3.1 Spectral Representations

We start with a characterization theorem that will provide the basis to subsequent findings. The result provides a spectral representation for all functions \mathbf{K} that are defined through Equation (2.5).

Theorem 3.1. *Let \mathbf{K}_Z be the mapping defined through Equation (2.5). Then, \mathbf{K}_Z is positive definite if and only the mapping \mathbf{K} on the right hand side of (2.5) is uniquely determined through the expansion*

$$\mathbf{K}(s, r, h) = \sum_{\mathbf{k}=(k_1, k_2) \in \mathbb{N}_0^2} \mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(h) C_{k_1}^{\frac{d_1-1}{2}}(s) C_{k_2}^{\frac{d_2-1}{2}}(r), \quad s, r \in [-1, 1], h \geq 0, \quad (3.1)$$

where $\{\mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(\cdot)\}$ is a sequence of continuous functions from $[0, \infty)$ into $\mathbb{R}^{p \times p}$ such that

1. $\sum_{\mathbf{k}} \mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(0) = \mathbf{B}$, where \mathbf{B} is a matrix with ones in the diagonal.

2. For every $\mathbf{k} \in \mathbb{N}_0^2$, the function $\mathbb{R}^d \ni \mathbf{h} \mapsto \mathbf{B}_{\mathbf{k},Z}(\mathbf{h})$, defined as

$$\mathbf{B}_{\mathbf{k},Z}(\mathbf{h}) = \mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(\|\mathbf{h}\|), \quad \mathbf{h} \in \mathbb{R}^d,$$

is the covariance function of a multivariate Gaussian random field $\mathbf{Z}_{\mathbf{k}}$.

The proof is based on the following

Lemma 3.2. *Let $\mathbf{K} : [-1, 1] \times [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$. Then, \mathbf{K} is positive definite if and only if*

$$\int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} d\boldsymbol{\mu}(x_1, x_2, \mathbf{u})^\top \mathbf{K} \left(\langle x_1, x'_1 \rangle, \langle x_2, x'_2 \rangle, \|\mathbf{u} - \mathbf{u}'\| \right) \overline{d\boldsymbol{\mu}(x'_1, x'_2, \mathbf{u}')}, \geq 0, \quad (3.2)$$

for every complex-valued Radon measure $\boldsymbol{\mu} : \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d \rightarrow \mathbb{C}^p$.

Proof. It is clear that if \mathbf{K} satisfies (3.2), then \mathbf{K} is positive definite. Let \mathbf{K} be positive definite. Then, \mathbf{K} is bounded (Berg and Porcu, 2017). Take $\boldsymbol{\mu}$ as

$$\boldsymbol{\mu}(x_1, x_2, \mathbf{u}) = \sum_{j=1}^n \boldsymbol{\alpha}_j \delta_{(x_{1,j}, x_{2,j}, \mathbf{u}_j)}(x_1, x_2, \mathbf{u}), \quad (x_{1,j}, x_{2,j}, \mathbf{u}_j) \in \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d,$$

for $\boldsymbol{\alpha}_j \in \mathbb{R}^p$ and with δ denoting the Kronecker delta. Then, the left hand side of Equation (3.2) can be written as

$$\sum_{k, \ell} \boldsymbol{\alpha}_k^\top \mathbf{K} \left(\langle x_{1,k}, x_{1,\ell} \rangle, \langle x_{2,k}, x_{2,\ell} \rangle, \|\mathbf{u}_k - \mathbf{u}_\ell\| \right) \boldsymbol{\alpha}_\ell,$$

which is apparently nonnegative because \mathbf{K} is positive definite. Now, for a general $\boldsymbol{\mu}$, consider the number

$$I := \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} d\boldsymbol{\mu}(x_1, x_2, \mathbf{u})^\top \mathbf{K} \left(\langle x_1, x'_1 \rangle, \langle x_2, x'_2 \rangle, \|\mathbf{u} - \mathbf{u}'\| \right) \overline{d\boldsymbol{\mu}(x'_1, x'_2, \mathbf{u}')}. \quad \square$$

We will prove that $I \geq 0$ by showing that for every $\epsilon > 0$ there exists $J \geq 0$ such that $|I - J| < \epsilon \|\boldsymbol{\mu}\|^2$, with $\|\cdot\|$ denoting the total variation of a complex valued measure with image in \mathbb{C}^p (Rudin, 1964). The rest of the proof follows straight by invoking the same arguments as in the proof of Lemma 4.3 of Berg and Porcu (2017). \square

Proof of Theorem 3.1. We start by supposing that \mathbf{K} is positive definite. Then, we apply Lemma 3.2 under the choice

$$\boldsymbol{\mu} = \sigma_{d_1} \otimes \sigma_{d_2} \otimes \boldsymbol{\sigma},$$

where \otimes denotes tensor product, σ_n is the Lebesgue measure for \mathbb{S}^n , and $\boldsymbol{\sigma}$ is an arbitrary Radon vector valued measure with compact support. Thus, we have

that the integral

$$\frac{\int_{(\mathbb{T}^{d_1, d_2})^2} \int_{\mathbb{R}^{2d}} d\sigma_{d_1}(x_1) d\sigma_{d_2}(x_2) d\boldsymbol{\sigma}(\mathbf{u})^\top \mathbf{K}(\langle x_1, x'_1 \rangle, \langle x_2, x'_2 \rangle, \|\mathbf{u} - \mathbf{u}'\|)}{d\sigma_{d_1}(x'_1) d\sigma_{d_2}(x'_2) d\boldsymbol{\sigma}(\mathbf{u}')}$$
 (3.3)

is nonnegative. Using the tensor product measure as above allows to write

$$\begin{aligned} & \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{T}^{d_1, d_2}} d\sigma_{d_1}(x_1) d\sigma_{d_2}(x_2) \mathbf{K}(\langle x_1, x'_1 \rangle, \langle x_2, x'_2 \rangle, \|\mathbf{u} - \mathbf{u}'\|) \overline{d\sigma_{d_1}(x'_1) d\sigma_{d_2}(x'_2)} \\ = & \omega_{d_1} \omega_{d_2} \int_{\mathbb{T}^{d_1, d_2}} \mathbf{K}(\langle \mathbf{e}_1, \eta_1 \rangle, \langle \mathbf{e}_1, \eta_2 \rangle, \|\mathbf{u} - \mathbf{u}'\|) d\sigma_{d_1}(\eta_1) d\sigma_{d_2}(\eta_2), \end{aligned}$$

with $\mathbf{e}_1 = (1, 0, \dots, 0)^\top$. Hence, (3.3) can be rewritten as

$$\int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} d\boldsymbol{\sigma}(\mathbf{u})^\top \mathbf{K}(\langle \mathbf{e}_1, \eta_1 \rangle, \langle \mathbf{e}_1, \eta_2 \rangle, \|\mathbf{u} - \mathbf{u}'\|) \overline{d\boldsymbol{\sigma}(\mathbf{u}')} d\sigma_{d_1}(\eta_1) d\sigma_{d_2}(\eta_2) \geq 0. \quad (3.4)$$

We now apply (3.4) to the matrix valued function $\mathbf{K}(\cdot, \cdot, \cdot) C_{k_1}^{\frac{d_1-1}{2}}(\cdot) C_{k_2}^{\frac{d_2-1}{2}}(\cdot)$ (that is positive definite because \mathbf{K} is positive definite by hypothesis, and the Gegenbauer polynomials are positive definite by construction) to obtain

$$\begin{aligned} & \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} d\boldsymbol{\sigma}(\mathbf{u})^\top \mathbf{K}(\langle \mathbf{e}_1, \eta_1 \rangle, \langle \mathbf{e}_1, \eta_2 \rangle, \|\mathbf{u} - \mathbf{u}'\|) \\ \times & C_{k_1}^{\frac{d_1-1}{2}}(\langle \mathbf{e}_1, \eta_1 \rangle) C_{k_2}^{\frac{d_2-1}{2}}(\langle \mathbf{e}_1, \eta_2 \rangle) \overline{d\boldsymbol{\sigma}(\mathbf{u}')} d\sigma_{d_1}(\eta_1) d\sigma_{d_2}(\eta_2) \geq 0. \end{aligned} \quad (3.5)$$

We can now define the sequence of functions $\mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}$ through the identity

$$\begin{aligned} \mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(h) &= \frac{\kappa_{d_1, k_1} \kappa_{d_2, k_2}}{\omega_{d_1} \omega_{d_2}} \int_{\mathbb{T}^{d_1, d_2}} \mathbf{K}(\langle \mathbf{e}_1, \eta_1 \rangle, \langle \mathbf{e}_1, \eta_2 \rangle, h) \\ &\times C_{k_1}^{\frac{d_1-1}{2}}(\langle \mathbf{e}_1, \eta_1 \rangle) C_{k_2}^{\frac{d_2-1}{2}}(\langle \mathbf{e}_1, \eta_2 \rangle) d\sigma_{d_1}(\eta_1) d\sigma_{d_2}(\eta_2), \end{aligned}$$

$h \geq 0$. Equation (3.5) shows that $\mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}$ is positive definite on \mathbb{R}^d for every fixed $\mathbf{k} = (k_1, k_2) \in \mathbb{N}_0^2$. Clearly, the identity above can be simplified into

$$\begin{aligned} & \mathbf{B}_{\mathbf{k}}^{(d_1, d_2)}(h) \\ = & \frac{\kappa_{d_1, k_1} \kappa_{d_2, k_2}}{\omega_{d_1} \omega_{d_2}} \int_{-1}^1 \int_{-1}^1 \mathbf{K}(r, s, h) C_{k_1}^{\frac{d_1-1}{2}}(r) C_{k_2}^{\frac{d_2-1}{2}}(s) \frac{(1-r^2)^{d_1/2-1}}{\mathcal{B}(d_1/2, 1/2)} \frac{(1-s^2)^{d_2/2-1}}{\mathcal{B}(d_2/2, 1/2)} dr ds. \end{aligned}$$

Here, \mathcal{B} denotes the Beta function. The rest of the proof follows the same arguments as in Berg and Porcu (2017) and is thus omitted. \square

3.2 New Classes of Covariance Functions

The previous theorem is actually the key to prove the following results.

Theorem 3.3. Let $\gamma : [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ such that $-\gamma(s, h)$ is a cross variogram over $(\mathbb{S}^{d_2} \times \mathbb{R}^{d_1})^2$. Additionally, suppose the elements γ_{ij} of γ are all strictly positive valued. Let \mathbf{K} have elements K_{ij} that are defined as

$$K_{ij}(s, r, h) = \frac{1}{\gamma_{ij}(r, h)} + \frac{\pi \sinh \sqrt{\gamma_{ij}(r, h)(\pi - \arccos s)}}{2 \sinh \sqrt{\gamma_{ij}(r, h)}}, \quad s, r \in [-1, 1], \quad h \geq 0. \quad (3.6)$$

Then, $\mathbf{K}(s, r, h)$ is positive definite on $\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d$ for $d_1 = 1$ and for all $d, d_2 = 1, 2, \dots$

Proof. We start by noting that the Online Supplement in Porcu et al. (2019) proves the identity

$$\frac{1}{\gamma_{ij}(r, h)} + \frac{\pi \sinh \sqrt{\gamma_{ij}(r, h)(\pi - \arccos s)}}{2 \sinh \sqrt{\gamma_{ij}(r, h)}} = \sum_{k=0}^{\infty} \frac{\cos(k \arccos s)}{(k^2 + \gamma_{ij}(r, h))}, \quad s, r \in [-1, 1], \quad h \geq 0.$$

Hence, the function \mathbf{K} as in (3.6) can be written as

$$\mathbf{K}(s, r, h) = \sum_k \cos(k \arccos s) \mathbf{B}_k(r, h), \quad s, r \in [-1, 1], h \geq 0,$$

with $\{\mathbf{B}_k\}$ being a sequence of matrix valued functions having entries $B_{ij,k}$ defined as

$$B_{ij,k}(r, h) = \frac{1}{(k^2 + \gamma_{ij}(r, h))}, \quad r \in [-1, 1], \quad h \geq 0.$$

Hence, the proof is completed if we prove that $\{\mathbf{B}_k(\cdot, \cdot)\}_k$ is a sequence of positive definite functions that are summable at $(r, h) = (1, 0)$. Indeed, we have that, for every $k = 0, 1, \dots$,

$$B_{ij,k}(r, h) = \int_0^{\infty} e^{-\xi k^2} e^{-\xi \gamma_{ij}(r, h)} d\xi.$$

Since $-\gamma$ is a cross variogram, a direct application of Theorem 1 in Schlather (2010) shows that \mathbf{B}_k is positive definite for every fixed k . Summability of $\mathbf{B}_k(1, 0)$ is obtained through direct inspection. The proof is completed. \square

We now define the parametric class of functions $\mathcal{F}(\cdot; \alpha, \tau, \nu)$ through the identity

$$\mathcal{F}(t; \alpha, \tau, \nu) = \frac{\mathcal{B}(\alpha, \nu + \tau)}{\mathcal{B}(\alpha, \nu)} {}_2F_1(\tau, \alpha; \alpha + \nu + \tau; -t), \quad t \in [-1, 1], \quad (3.7)$$

where ${}_2F_1$ is an hypergeometric function (Olver et al., 2010), and where α, ν, τ are strictly positive. Here, \mathcal{B} denotes the Beta function.

Proposition 3.4. Let $\mathbf{C} : [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ be positive definite in $\mathbb{S}^{d_2} \times \mathbb{R}^d$ with entries C_{ij} such that $|C_{ij}(\cdot)| \leq 1$. Let $[\alpha_{ij}]$, $[\beta_{ij}]$ be conditionally negative definite matrices. Then, the function $\mathbf{K} : [-1, 1] \times [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ having entries K_{ij} defined as

$$K_{ij}(s, r, h) = \mathcal{B}(\alpha_{ij}, \beta_{ij}) \mathcal{F}(sC_{ij}(r, h); \alpha_{ij}, \tau, \nu_{ij}),$$

is positive definite on $\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d$ for all $d_1 = 1, 2, \dots$

Proof. We start by considering the class

$$\mathcal{N}_{\delta, \tau}(s) = \left(\frac{1 - \delta}{1 - \delta s} \right)^\tau, \quad s \in [-1, 1], \quad \delta \in (0, 1), \quad \tau > 0. \quad (3.8)$$

Direct inspection shows that $\mathcal{N}_{\delta, \tau}$ admits the following expansion:

$$\mathcal{N}_{\delta, \tau}(s) = \sum_{k=0}^{\infty} s^k b_k(\delta, \tau), \quad s \in [-1, 1],$$

where $b_k(\delta, \tau) = \binom{k+\tau-1}{k} \delta^k (1-\delta)^\tau$. Hence, the function

$$\mathcal{N}_{i,j;\delta,\tau}(s) = \sum_{k=0}^{\infty} s^k b_k(\delta, \tau) C_{ij}(r, h)^k, \quad s, r \in [-1, 1], h \geq 0,$$

is the (i, j) -th entry of a positive definite function, \mathcal{N} . We now apply the arguments in theorem 1 of Alegria et al. (2021) to infer that

$$\mathcal{F}(sC_{ij}(r, h); \alpha_{ij}, \tau, \nu_{ij}) = \int_0^1 \mathcal{N}_{i,j;\delta,\tau}(s) \frac{\delta^{\alpha_{ij}-1} (1-\delta)^{\beta_{ij}-1}}{\mathcal{B}(\alpha_{ij}, \beta_{ij})} d\delta.$$

We now observe that, since $[\alpha_{ij}]_{i,j=1}^p$ and $[\beta_{ij}]_{i,j=1}^p$ are conditionally negative definite matrices, we get $\delta^{\alpha_{ij}} = \exp(\alpha_{ij} \log \delta)$, proving that the matrix $[\delta^{\alpha_{ij}}]_{i,j=1}^p$ is positive definite, from a theorem by Schoenberg (see for instance Theorem A.3 in Bachoc et al. (2017) or Berg et al. (1984)). So is the matrix $[(1-\delta)^{\beta_{ij}}]$ by the same arguments. The proof is completed. \square

3.3 A Multivariate Matérn Model

Theorem 3.5. Let $\mathbf{F} : [-1, 1] \times [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ be a continuous mapping such that

1. $\mathbf{F}(\cdot, \cdot, \omega)$ is positive definite on \mathbb{T}^{d_1, d_2} for all $\omega \geq 0$;
2. $\mathbf{F}(0, 0, \cdot)$ is pointwise integrable.

Let

$$\mathbf{K}(s, r, h) := \int_{\mathbb{R}^d} e^{i\langle \omega, h \rangle} \mathbf{F}(s, r, \|\omega\|) d\omega. \quad (3.9)$$

Then, \mathbf{K} is a positive definite matrix valued function on $\mathbb{T}^{d_1, d_2} \times \mathbb{R}^d$.

Proof. By Assumption 1, and as a corollary of Theorem 3.4 of Berg and Porcu (2017), we have that for every fixed ω , the mapping \mathbf{F} can be uniquely written as

$$\mathbf{F}(s, r, \omega) = \sum_{\mathbf{k}=(k_1, k_2) \in \mathbb{N}_0^2} \mathbf{B}_{\mathbf{k}}(\omega) C_{k_1}^{(d_1-1)/2}(s) C_{k_2}^{(d_2-1)/2}(r), \quad s, r \in [-1, 1], \quad \omega \geq 0,$$

where, for every fixed ω , $\{\mathbf{B}_{\mathbf{k}}(\omega)\}_{\mathbf{k} \in \mathbb{N}_0^2}$ is a sequence of positive definite matrices with the additional requirement that $\sum_{\mathbf{k}} \mathbf{B}_{\mathbf{k}}(0)$ is finite.

We now rewrite the function \mathbf{K} as in (3.9) as

$$\begin{aligned} \mathbf{K}(s, r, h) &= \int_{\mathbb{R}^d} e^{i\langle \boldsymbol{\omega}, \mathbf{h} \rangle} \mathbf{F}(s, r, \|\boldsymbol{\omega}\|) d\boldsymbol{\omega} \\ &= \sum_{\mathbf{k}} \int_{\mathbb{R}^d} e^{i\langle \boldsymbol{\omega}, \mathbf{h} \rangle} \mathbf{B}_{\mathbf{k}}(\|\boldsymbol{\omega}\|) d\boldsymbol{\omega} C_{k_1}^{(d_1-1)/2}(s) C_{k_2}^{(d_2-1)/2}(r) \\ &=: \sum_{\mathbf{k}} \tilde{\mathbf{B}}_{\mathbf{k}}(h) C_{k_1}^{(d_1-1)/2}(s) C_{k_2}^{(d_2-1)/2}(r) \quad s, r \in [-1, 1], \quad h = \|\mathbf{h}\|, \quad \mathbf{h} \in \mathbb{R}^d. \end{aligned}$$

By Cramér's theorem (Cramer, 1940), the functions $\tilde{\mathbf{B}}_{\mathbf{k}}$ are positive definite in \mathbb{R}^d for all $\mathbf{k} \in \mathbb{N}_0^2$. Thus, we can invoke Theorem 3.1 and the proof will be completed if we show that the sequence $\{\tilde{\mathbf{B}}_{\mathbf{k}}(0)\}_{\mathbf{k}}$ is convergent. This comes from Assumption 2 which guarantes that \mathbf{K} is bounded at $(0, 0, 0)$. The proof is completed. \square

For the following result, we need to define the Matérn family of functions $\mathcal{M}(\cdot; \alpha, \nu)$ through the identity

$$\mathcal{M}(h; \alpha, \nu) = \frac{2^{1-\nu}}{\Gamma(\nu)} (\alpha h)^\nu \mathcal{K}_\nu(\alpha h), \quad h \geq 0, \quad (3.10)$$

for α, ν being strictly positive, and where \mathcal{K}_ν denotes the modified Bessel function of the second kind of order $\nu > 0$. Some works related to this family when analyzed over spheres can be found in Terdik (2015) and Leonenko and Malyarenko (2017).

Theorem 3.6. Let $[\nu_{ij}(\cdot, \cdot)]_{i,j=1}^p$ be a matrix of functions $\nu_{ij} : [-1, 1]^2 \rightarrow (0, \infty)$ that are continuous and such that $\nu_{ij}(\cdot, \cdot) = (\nu_{ii}(\cdot, \cdot) + \nu_{jj}(\cdot, \cdot))/2$. Let

$$\rho_{ij}(s, r) = \beta_{ij} \frac{\Gamma(\nu_{ij}(s, r))}{\Gamma(\nu_{ij}(s, r) + d/2)}, \quad s, r \in [-1, 1], \quad (3.11)$$

where $[\beta_{ij}]$ is a matrix with $\beta_{ii}=1$. Assume that for any $0 < a \leq 1$, the matrix-valued function $(s, r) \mapsto [\beta_{ij} a^{\nu_{ij}(s, r)}]$ is positive definite in \mathbb{T}^{d_1, d_2} . Let $\mathbf{K} : [-1, 1] \times [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ have elements K_{ij} that are defined as

$$K_{ij}(s, r, h) = \sigma_i \sigma_j \rho_{ij}(s, r) \mathcal{M}(h; \alpha, \nu_{ij}(s, r)), \quad (3.12)$$

with $\sigma_i > 0$, $i = 1, \dots, p$. Then, \mathbf{K} is positive definite.

Proof. Let

$$f(\omega; \alpha, \nu) = \frac{\Gamma(\nu + d/2)\alpha^{2\nu}}{\Gamma(\nu)\pi^{d/2}} (\alpha^2 + \omega^2)^{-\nu-d/2}, \quad \omega = \|\boldsymbol{\omega}\|, \boldsymbol{\omega} \in \mathbb{R}^d,$$

with α and ν being strictly positive. The Fourier transform in \mathbb{R}^d of the function f is the function $\mathcal{M}(\cdot; \alpha, \nu)$, defined at (3.10). We now define

$$\tilde{f}(\omega; \alpha, \nu) = \frac{\Gamma(\nu)\pi^{d/2}}{\Gamma(\nu + d/2)} f(\omega; \alpha, \nu), \quad \omega \geq 0,$$

having Fourier transform the function

$$\widetilde{\mathcal{M}}(h; \alpha, \nu) = \frac{\Gamma(\nu)\pi^{d/2}}{\Gamma(\nu + d/2)} \mathcal{M}(h; \alpha, \nu), \quad h \geq 0.$$

We consider the function $\mathbf{F} : [-1, 1] \times [-1, 1] \times [0, \infty) \rightarrow \mathbb{R}^{p \times p}$ having elements F_{ij} that are identically defined as

$$\begin{aligned} F_{ij}(s, r, \omega) &= \sigma_i \sigma_j \beta_{ij} \tilde{f}(\omega; \alpha, \nu_{ii}(s, r))^{1/2} \tilde{f}(\omega; \alpha, \nu_{jj}(s, r))^{1/2} \\ &= \sigma_i \sigma_j \beta_{ij} \alpha^{2\nu_{ij}(s, r)} (\alpha^2 + \omega^2)^{-\nu_{ij}(s, r) - d/2}. \end{aligned}$$

Clearly, \mathbf{F} satisfies the two hypothesis in Theorem 3.5. Thus, we can calculate the function \mathbf{K} as in (3.9) to obtain a matrix valued mapping \mathbf{K} with elements K_{ij} defined as in (3.12). The proof is completed by direct application of Theorem 3.5. \square

4 Evading from Stationarity and Isotropy in \mathbb{R}^d

We have explored so far the constructions related to spherical isotropy on \mathbb{T}^{d_1, d_2} coupled with Euclidean isotropy in \mathbb{R}^d . The next findings show characterizations related to relaxing this last hypothesis. Specifically, we refer to covariance functions $\mathbf{K}_{\mathbf{Z}}$ such that

$$\mathbf{K}_{\mathbf{Z}}((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')) = \left(\Sigma^{1/2}\right)^\top \mathbf{K}(s, r, \mathbf{u}, \mathbf{u}') \Sigma^{1/2}, \quad (4.1)$$

with $s = \langle x_1, x'_1 \rangle_1$, $r = \langle x_2, x'_2 \rangle_2$, $\mathbf{x} = (x_1, x_2)$, $\mathbf{x}' = (x'_1, x'_2) \in \mathbb{T}^{d_1, d_2}$, $\mathbf{u}, \mathbf{u}' \in \mathbb{R}^d$. The matrix $\Sigma^{1/2}$ is being defined around (2.5). Under this setting, the mapping \mathbf{K} is defined over $[-1, 1]^2 \times (\mathbb{R}^d)^2$ with image on $\mathbb{R}^{p \times p}$. Characterizations for this class have been elusive so far. We call $\Xi(\mathbb{T}^{d_1, d_2}, \mathbb{R}^d)$ the class of mappings $\mathbf{K} : \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d \times \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d \rightarrow \mathbb{R}^{p \times p}$ such that

$$\mathbf{K}((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')) = \sum_{\mathbf{k} \in \mathbb{N}_0^2} \sum_{j=1}^{\kappa_{d_1, k_1}} \sum_{j'=1}^{\kappa_{d_2, k_2}} \Upsilon_{\mathbf{k}, j, j'}(\mathbf{u}, \mathbf{u}') Y_{k_1, j}(x_1) \overline{Y_{k_1, j'}(x'_1)} Y_{k_2, j}(x_2) \overline{Y_{k_2, j'}(x'_2)},$$

for $s = \langle x_1, x'_1 \rangle_1$, $r = \langle x_2, x'_2 \rangle_2$, $\mathbf{k} = (k_1, k_2)$, $\{Y_{k_i, j}\}_{k_i=0}^\infty$ denoting the set of spherical harmonics in \mathbb{S}^{d_i} , having a uniquely determined finite dimension κ_{d_i, k_i}

that is given by (2.1). The expansion is uniformly convergent with respect to $(\mathbf{x}, \mathbf{x}') \in \mathbb{T}^{d_1, d_2}$. The next result is providing some insight into the knowledge of the class $\Xi(\mathbb{T}^{d_1, d_2}, \mathbb{R}^d)$.

Theorem 4.1. *Let $\mathbf{K}: \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d \times \mathbb{T}^{d_1, d_2} \times \mathbb{R}^d \rightarrow \mathbb{R}^{p \times p}$ belong to $\Xi(\mathbb{T}^{d_1, d_2}, \mathbb{R}^d)$.*

Then,

(i) for every fixed $\mathbf{u}, \mathbf{u}' \in \mathbb{R}^d$,

$$\sum_{\mathbf{k}} \sum_j \sum_{j'} \left| \Upsilon_{\mathbf{k}, j, j'}^{(\ell, m)}(\mathbf{u}, \mathbf{u}') \right|^2 < \infty,$$

where $\Upsilon_{\mathbf{k}, j, j'}^{(\ell, m)}$ denotes the (ℓ, m) -element of $\Upsilon_{\mathbf{k}, j, j'}$. Additionally,

$$\Upsilon_{\mathbf{k}, j, j'}(\mathbf{u}, \mathbf{u}') = \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{T}^{d_1, d_2}} \mathbf{K}\left((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')\right) d\lambda_{d_1, d_2}(\mathbf{x}) d\lambda_{d_1, d_2}(\mathbf{x}'),$$

where $d\lambda_{d_1, d_2} = d\sigma_{d_1} \otimes d\sigma_{d_2}$, with $d\sigma_{d_i}$ denoting the Lebesgue measure on \mathbb{S}^{d_i} , $i = 1, 2$.

(ii) \mathbf{K} is positive definite if and only if $\{\Upsilon_{\mathbf{k}, j, j'}\}$ is a sequence of positive definite functions.

Proof. Let $N, N' \in \mathbb{N}$. Define

$$\begin{aligned} & \mathbf{K}_{N, N'}\left((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')\right) \\ &= \sum_{k_1=0}^N \sum_{k_2=0}^{N'} \sum_{j=1}^{\kappa_{d_1, k_1}} \sum_{j'=1}^{\kappa_{d_2, k_2}} \Upsilon_{\mathbf{k}, j, j'}(\mathbf{u}, \mathbf{u}') Y_{k_1, j}(x_1) \overline{Y_{k_1, j'}(x'_1)} Y_{k_2, j}(x_2) \overline{Y_{k_2, j'}(x'_2)}. \end{aligned} \quad (4.2)$$

Clearly, $\mathbf{K}_{N, N'}$ converges uniformly on $\mathbb{T}^{d_1, d_2} \times \mathbb{T}^{d_1, d_2}$ to \mathbf{K} as N, N' tend to infinity for any fixed \mathbf{u}, \mathbf{u}' . This implies convergence in $\mathcal{L}_2(\mathbb{T}^{d_1, d_2} \times \mathbb{T}^{d_1, d_2}, \sigma_{d_1} \otimes \sigma_{d_2})$, the space of square integrable functions on $\mathbb{T}^{d_1, d_2} \times \mathbb{T}^{d_1, d_2}$ with respect to the tensor product measure $\sigma_{d_1} \otimes \sigma_{d_2}$. Here, square integrability is intended as finiteness of the Frobenius norm $|\cdot|$, so that we have

$$\begin{aligned} \infty &> \int_{\mathbb{T}^{d_1, d_2}} \int_{\mathbb{T}^{d_1, d_2}} \left| \mathbf{K}\left((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')\right) - \mathbf{K}_{N, N'}\left((\mathbf{x}, \mathbf{u}), (\mathbf{x}', \mathbf{u}')\right) \right|^2 d\sigma_{d_1}(\mathbf{x}) d\sigma_{d_2}(\mathbf{x}') \\ &= \sum_{k_1=N}^{\infty} \sum_{k_2=N'}^{\infty} \sum_{j=1}^{\kappa_{d_1, k_1}} \sum_{j'=1}^{\kappa_{d_2, k_2}} |\Upsilon_{\mathbf{k}, j, j'}(\mathbf{u}, \mathbf{u}')|^2, \end{aligned}$$

where the second line is due to legitimate inversion of series with integrals, in concert with the fact that the spherical harmonics are orthonormal basis in their respective spaces. Point (i) is established. Point (ii) can be proved by following the same arguments as in Theorem 3.1. \square

5 Conclusions

We have provided characterization theorems for the covariance functions of vector valued random fields that are continuously indexed over generalized spaces involving the hypertorus. In turn, we have proposed several parametric classes available in closed form. This work opens for several research directions. For instance, it might be extremely useful to study conditions for equivalence of Gaussian measures defined over compact subsets of these generalized spaces. This would have important consequences for maximum likelihood estimation, as well as for kriging prediction, under infill asymptotics (Yadrenko and Balakrishnan, 1983; Stein, 1999; Bevilacqua et al., 2019; Arafat et al., 2018; Bachoc et al., 2020). Such conditions would allow to evaluate the covariance functions proposed in this paper in terms of estimation and prediction. Another relevant problem is related to modeling anisotropies in these generalized spaces, and how to estimate such structure.

We should also mention that recent approaches allow to define reducibility over hyperspheres (Allard et al., 2016; Porcu et al., 2020b; Senoussi and Porcu, 2021). It would be definitely mandatory to study such approaches over the generalized spaces introduced in this paper.

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