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Covariance Functions on Spheres cross Time: Beyond Spatial Isotropy and Temporal Stationarity

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Abstract

Spectral representations uniquely define the covariance functions associated to random fields defined over spheres or spheres cross time. Covariance functions on spheres cross time are usually modelled under the assumptions of either spatial isotropy or axial symmetry, and the assumption of temporal stationarity. This paper goes beyond these assumptions. In particular, we consider the problem of spatially anisotropic covariance functions on spheres. The crux of our criterion is to escape from the addition theorem for spherical harmonics. We also challenge the problem of temporal nonstationarity in nonseparable space-time covariance functions, where space is the n-dimensional sphere embedded in the $(n+1)$-dimensional Euclidean space. We finally propose a simulation routine for the models proposed in this paper.

Keywords: Gegenbauer Polynomial, Positive Definite, Space-time Random Field, Spectral Representation, Spherical Harmonic.

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1 Introduction

The literature on positive definite kernels on spheres has become ubiquitous, and we refer the reader to the essay by Gneiting (2013), with the list of references given there. Both mathematical and statistical communities have been interested in the construction of positive definite functions defined over product spaces where the sphere is involved. The recent tours de force in Barbosa and Menegatto (2016); Guella and Menegatto (2016); Guella, Menegatto and Peron (2016) in concert with the works by Gneiting (2013); Berg and Porcu (2017); Porcu, Bevilacqua and Genton (2016) and the recent review in Jeong et al. (2017) are apparent indications that there are some important branches of the mathematical and statistical communities devoted to studying such constructions.

Recently, Porcu, Alegría and Furrer (2018) have proposed an overview of statiscal approaches for global data, showing that positive definite functions have a crucial role for modeling temporally evolving phenomena defined over the sphere representing planet Earth. The importance of positive definite functions extends to statistical inferences through, *e.g.*, likelihood techniques, as well as to optimal linear prediction, called kriging in the geostatistical framework.

Recent statistical works are concerned with the construction of space-time covariances where the space is the spherical shell. Characterization theorems for positive definite kernels on n-dimensional spheres have been provided in seminal papers by Schoenberg (1942) and Narcowich (1995). Then, Berg and Porcu (2017) and Porcu, Bevilacqua and Genton (2016) extended Schoenberg's representation theorem to space-time. In particular, Porcu, Bevilacqua and Genton (2016) focus on construction principles that allow for algebraically tractable closed forms, and then analyze the discrepancy between using the correct metric on the sphere and other metrics. The literature on spatial anisotropy on spheres has instead been sparse, with the work of Hitczenko and Stein (2012) being a notable exception. Specifically, the authors show spectral representations for anisotropic processes defined over $\mathbb{R}^3$ and then restricted to the sphere. Under such a scheme, the covariance function depends on the chordal distance, being the segment *below* the arc joining any pair of points located over the spherical shell. The natural metric on the sphere is the great circle or geodesic distance, and for constructive criticism about the use of chordal distance the reader is referred to Gneiting (2013) as well as to Porcu, Alegría and Furrer (2018).

This paper goes beyond spatial anisotropy and temporal stationarity by eluding the spectral representations by Schoenberg (1942) and Berg and Porcu (2017). Specifically, we show how to avoid the addition theorem for spherical harmonics (Marinucci and Peccati, 2011) to obtain more general representations. A similar strategy is adopted by Jones (1963) and by Stein (2007) to obtain spectral representations for axially symmetric processes.

In particular, we provide spectral representations for positive definite kernels on $(\mathbb{S}^n \times T)^2$, with $\mathbb{S}^n$ being the n-dimensional sphere of $\mathbb{R}^{n+1}$ with unit radius, and where T denotes time, which might be the whole real line or a compact set. On the basis of such spectral representations, we illustrate how to obtain anisotropy with respect to space, and nonstationarity with respect to time. The paper is organized as follows. In Section 2, we give necessary notation and background. The main results of the paper are provided in Section 3. Section 4 provides some examples and a simulation technique for the models proposed in this paper. To favor a neater exposition, technical proofs are deferred to the Appendix.

2 Background

This section is largely expository and contains basic material that will be useful for the exposition of our results. Although most of our work is related to the product space $\mathbb{S}^n \times T$, it will be convenient to present some basic facts by making reference to a metric space, denoted M throughout. We call kernel on M any mapping $k : M \times M \to \mathbb{C}$, such that $\overline{k}(q,p) = k(p,q)$ for $p, q \in M$, where $\overline{a}$ denotes the complex conjugate of the complex number a. The kernel k is positive definite if, for every positive integer m and every set of points $p_1, \ldots, p_m \in M$, the $m \times m$ matrix with entries $[k(p_i, p_{i'})]_{1 \le i, i' \le m}$ satisfies, for any $c_1, \ldots, c_m \in \mathbb{C}$,

$$\sum_{i,i'=1}^{m} c_i \, \overline{c_{i'}} \, k(p_i, p_{i'}) \ge 0.$$

Kolmogorov's existence theorem implies that a real-k is positive definite if and only if there exists a zero mean real-valued Gaussian random field X defined on M such that k is the covariance function of X. Namely, we have

$$k(p_1, p_2) := \mathrm{cov}(X(p_1), X(p_2)) = \mathbb{E}[X(p_1)X(p_2)], \qquad p_1, p_2 \in M.$$

The class of positive definite kernels on M is a convex cone being stable by multiplication and closed under the topology of pointwise convergence. Furthermore, if k_1 and k_2 are positive definite kernels on M_1 and M_2 respectively, then their tensor product $k_1 \otimes k_2$, defined as $k_1 \otimes k_2((p_1, t_1), (p_2, t_2)) := k_1(p_1, t_1) k_2(p_2, t_2)$ for $p_i, t_i \in M_i$ for $i = 1, 2$, is a positive definite kernel on $M_1 \times M_2$.

Next lemma provides an integral characterization of continuous positive definite kernels on $M = \mathbb{S}^n \times \mathbb{R}$. It extends the special case given by Lemma 4.3 in Berg and Porcu (2017). We do not give a proof because it is obtained by following similar arguments.

Lemma 2.1. *Let k be a continuous kernel on $\mathbb{S}^n \times \mathbb{R}$.*
Then, k is positive definite if and only if, for any continuous function $c : \mathbb{S}^n \times \mathbb{R} \to \mathbb{C}$

with compact support,

$$\int_{\mathbb{S}^n\times\mathbb{R}}\int_{\mathbb{S}^n\times\mathbb{R}} k((p_1,t_1),(p_2,t_2))\, c(p_1,t_1)\,\overline{c}(p_2,t_2)\,\mathrm{d}\sigma_n(p_1)\mathrm{d}t_1\mathrm{d}\sigma_n(p_2)\mathrm{d}t_2 \;\geq 0, \tag{2.1}$$

where σ_n is the surface measure on $\mathbb{S}^n$.

Through the manuscript we consider the geodesic (or great circle) distance as the mapping $\theta : \mathbb{S}^n \times \mathbb{S}^n \to [0,\pi]$ defined through

$$\theta(p_1,p_2) = \arccos(\langle p_1,p_2\rangle), \qquad p_1,p_2 \in \mathbb{S}^n,$$

where $\langle\cdot,\cdot\rangle$ denotes the classical inner product. Whenever no confusion can arise, we use the shortcut θ for $\theta(p_1,p_2)$. A kernel $k : \mathbb{S}^n \times \mathbb{S}^n \to \mathbb{R}$ is called isotropic if there exists a function $\psi : [0,\pi] \to \mathbb{R}$ such that

$$k(p_1,p_2) = \psi(\theta(p_1,p_2)), \qquad p_1,p_2 \in \mathbb{S}^n. \tag{2.2}$$

Isotropic covariance functions have a well established literature: Schoenberg (1942) has shown that all continuous covariance functions on n-dimensional spheres, being additionally isotropic, admit series expansions depending on spherical harmonics. We now recall some basic facts on these topics. We refer to the recent monographs by Wendland (2004) and Dai and Xu (2013) for more details.

Let

$$d_{n,\ell} = \begin{cases} \frac{(2\ell+n-1)(\ell+n-2)!}{\ell!(n-1)!} & if \quad \ell \in \mathbb{N}, \\ 1 & if \quad \ell = 0. \end{cases} \tag{2.3}$$

and let us consider $\{Y_{\ell,j} : \ell \in \mathbb{N}_0,\ j = 1,\dots,d_{n,\ell}\}$, the family of spherical harmonics on the sphere $\mathbb{S}^n$ as defined in Narcowich (1995) (see also Jones (1963) for instance in the case $n = 2$). These are complex-valued functions and they provide a complete orthonormal system in the space of the Lebesgue square integrable functions $\mathcal{L}^2(\mathbb{S}^n, \mathrm{d}\sigma_n)$. They moreover satisfy the next relation

$$\overline{Y_{\ell,j}} = Y_{\ell,d_{n,\ell}-j+1}, \qquad \ell \in \mathbb{N}_0,\ j = 1,\dots,d_{n,\ell}.$$

For any $f \in \mathcal{L}^2(\mathbb{S}^n, \mathrm{d}\sigma_n)$ and any positive integer N, let us introduce

$$f_N(p) := \sum_{\ell=0}^{N}\sum_{j=1}^{d_{n,\ell}} b_{\ell,j}Y_{\ell,j}(p), \quad p \in \mathbb{S}^n, \text{ with } \quad b_{\ell,j} = \int_{\mathbb{S}^n} f(p)\overline{Y_{\ell,j}}(p)\mathrm{d}\sigma_n(p).$$

Thus, we have

$$\int_{\mathbb{S}^n}\left|f(p) - f_N(p)\right|^2 \mathrm{d}\sigma_n(p) \to 0 \;\text{ as }\; N \to \infty,$$

and f is real-valued if and only if $\overline{b_{\ell,j}} = b_{\ell,d_{n,\ell}-j+1}$ for any ℓ and any j.

A classical result provides an explicit relation between Gaussian random fields with a continuous covariance and its related expansion in terms of spherical harmonics. Formally, it states that any zero mean, real-valued and squared integrable Gaussian random field X on $\mathbb{S}^n$ with covariance function k admits the expansion

$$X(p) = \sum_{\ell=0}^{\infty} \sum_{j=1}^{d_{n,\ell}} b_{\ell,j} Y_{\ell,j}(p), \qquad p \in \mathbb{S}^n, \tag{2.4}$$

with the coefficients $\{b_{\ell,j}\}_{\ell,j}$ being complex-valued random variables with zero mean and satisfying $\overline{b_{\ell,j}} = b_{\ell,d_{n,\ell}-j+1}$ for any (ℓ, j). The representation in Equation (2.4) is also known as Karhunen-Loève expansion. Specifically, we have

$$b_{\ell,j} = \int_{\mathbb{S}^n} X(p)\overline{Y_{\ell,j}}(p)\mathrm{d}\sigma_n(p), \qquad \ell \in \mathbb{N}_0,\ j = 1, \ldots, d_{n,\ell}.$$

When the field is isotropic, the variance only depends on ℓ through

$$\mathbb{E}[b_{\ell,j}\overline{b_{\ell',j'}}] = a_\ell\, \delta_{\ell,\ell'}\delta_{j,j'}, \tag{2.5}$$

where δ is the Kronecker delta function and the associated covariance kernel admits the expression

$$\mathbb{E}[X(p_1)X(p_2)] = \sum_{\ell=0}^{\infty} a_\ell \sum_{j=1}^{d_{n,\ell}} Y_{\ell,j}(p_1)\overline{Y_{\ell,j}}(p_2), \qquad p_1, p_2 \in \mathbb{S}^n, \tag{2.6}$$

where the sequence $\{a_\ell\}_{\ell\in\mathbb{N}_0}$, identified through the relation (2.5), is called angular power spectrum.

Representation (2.6) naturally yields the family of Gegenbauer polynomials $\{C_\ell^\nu : \ell \in \mathbb{N}_0\}$ for $\nu \geq 0$, which constitutes an orthogonal basis for the space $\mathcal{L}^2([-1,1],(1-z^2)^{\nu-1/2}\mathrm{d}z)$. Actually, when $n = 2, 3, \ldots$, the $(n-1)/2$-Gegenbauer polynomial of degree ℓ can be expressed in terms of the spherical harmonics through the addition Theorem (see Equation 4.5 in Narcowich, 1995) or (Lemma 17.3 in Wendland, 2004):

$$C_\ell^{(n-1)/2}(\langle p_1, p_2\rangle) = \omega_n \frac{(n-1)}{(2\ell+n-1)} \sum_{j=1}^{d_{n,\ell}} Y_{\ell,j}(p_1)\overline{Y_{\ell,j}}(p_2), \qquad p_1, p_2 \in \mathbb{S}^n, \tag{2.7}$$

where $\omega_n = 2\pi^{(n+1)/2}/\Gamma\left((n+1)/2\right)$ is the total mass of the surface measure σ_n on $\mathbb{S}^n$, being $\Gamma(\cdot)$ the Gamma function. Note that the Gegenbauer polynomials are real-valued. Besides, for all $\ell \in \mathbb{N}_0$,

$$|C_\ell^{(n-1)/2}(z)| \leq C_\ell^{(n-1)/2}(1) = \binom{\ell+n-2}{\ell}, \qquad \forall\, z \in [-1,1], \tag{2.8}$$

and

$$\begin{aligned} \left\|C_\ell^{(n-1)/2}\right\|^2_{\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)} &= \int_0^\pi \left(C_\ell^{(n-1)/2}(\cos\theta)\right)^2 \sin\theta^{n-1}\mathrm{d}\theta \\ &= \frac{\omega_n}{\omega_{n-1}} \frac{\binom{\ell+n-2}{\ell}}{(1+\frac{2\ell}{n-1})}. \end{aligned} \tag{2.9}$$

In the case $n = 2$, the Gegenbauer polynomials coincide with the Legendre polynomials (Dai and Xu, 2013). When $n = 1$, the addition Theorem simplifies to

$$C_\ell^0(\langle p_1, p_2\rangle) = \pi \sum_{j=1}^{2} Y_{\ell,j}(p_1)\overline{Y_{\ell,j}}(p_2), \qquad p_1, p_2 \in \mathbb{S}^1,$$

and according to Equation 22.3.14 in Abramowitz and Stegun (1972), $C_\ell^0(\cos\theta) = 2\,\ell^{-1}\cos(\ell\,\theta)$ for $\ell \in \mathbb{N}$, and $C_\ell^0(\cos\theta) = 1$ for $\ell = 0$.

The ingredients in (2.6) and (2.5) sum up nicely to provide the following statement, known as Schoenberg's Theorem (Schoenberg, 1942). Let n be a positive integer. Then, any kernel $k : \mathbb{S}^n \times \mathbb{S}^n \to \mathbb{R}$ is positive definite and isotropic if and only if

$$k(p_1, p_2) = \psi(\theta(p_1, p_2)) = \sum_{\ell=0}^{\infty} \alpha_\ell^n C_\ell^{(n-1)/2}(\cos\theta), \qquad p_1, p_2 \in \mathbb{S}^n, \tag{2.10}$$

with all $\alpha_\ell^n \geq 0$ and $\sum_{\ell=0}^{\infty} \alpha_\ell^n \binom{\ell+n-2}{\ell} < \infty$ when $n = 2, 3, \ldots$ or $\sum_{\ell=1}^{\infty} \alpha_\ell^1\, \ell^{-1} < \infty$ when $n = 1$. Note that we use the upper index n in α_ℓ^n to emphasize the dependence of the Schoenberg's coefficients with respect to the dimension of the sphere $\mathbb{S}^n$.

When $n = 2$ and $T = \mathbb{R}$, a direct way to extend representation (2.4) to processes defined over $\mathbb{S}^2 \times \mathbb{R}$ is proposed by Jones (1963):

$$X(p, t) = \sum_{\ell=0}^{\infty} \sum_{j=1}^{d_{2,\ell}} b_{\ell,j}(t) Y_{\ell,j}(p), \qquad p \in \mathbb{S}^2, t \in \mathbb{R}, \tag{2.11}$$

where $\{b_{\ell,j}(\cdot)\}$ is a uniquely determined sequence of stochastic processes defined over the real line. Again, the hypothesis on such sequence are crucial to determine the properties of the associated covariance. If $\mathbb{E}[b_{\ell,j}(\cdot)] = 0$ and $\mathbb{E}[b_{\ell,j}(t_1)\overline{b_{\ell',j'}}(t_2)] = a_\ell(t_1 - t_2)\delta_{\ell,\ell'}\delta_{j,j'}$, then the associated covariance is isotropic in space and stationary in time. Berg and Porcu (2017) show that all covariance functions being isotropic in space and stationary in time are uniquely defined as

$$\begin{aligned} k(p_1, t_1, p_2, t_2) &= \psi(\theta(p_1, p_2), t_1 - t_2) \\ &= \sum_{\ell=0}^{\infty} a_\ell(t_1 - t_2) C_\ell^{(n-1)/2}(\cos\theta), \quad (p_i, t_i) \in \mathbb{S}^n \times \mathbb{R}, \end{aligned}$$

for a uniquely determined sequence $\{a_\ell(\cdot)\}$ of positive definite functions with the requirement that $\sum_\ell a_\ell(0) < \infty$ (otherwise X in (2.11) would have infinite variance). In view of Jones (1963)'s result, it becomes apparent that the spectral representation (2.11) is the building block for considering alternatives to isotropy. The following results show that we can go beyond these spectral representations, by inducing spatial anisotropy and temporal non-stationarity.

3 Beyond Spatial Isotropy and Temporal Stationarity

Recall that T denotes either a compact interval in $\mathbb{R}$ or $\mathbb{R}$ itself. We are concerned with the representation of real-valued positive definite kernels on $\mathbb{S}^n \times T$. It should be remarked that isotropy and stationarity occur in a separate way in each respective space.

Definition 1. *Let k be a continuous positive definite kernel on $\mathbb{S}^n \times T$.*

i.- k is called isotropic with respect to space when there exists a function $\widetilde{k}_S : [0,\pi] \times T \times T \to \mathbb{R}$ such that

$$k(p_1,t_1,p_2,t_2) = \widetilde{k}_S(\theta(p_1,p_2),t_1,t_2), \qquad p_1,p_2 \in \mathbb{S}^n,\ t_1,t_2 \in T.$$

ii.- k is called stationary with respect to time when there exists a function $\widetilde{k}_T : \mathbb{S}^n \times \mathbb{S}^n \times \mathbb{R} \to \mathbb{R}$ such that

$$k(p_1,t_1,p_2,t_2) = \widetilde{k}_T(p_1,p_2,t_2-t_1), \qquad p_1,p_2 \in \mathbb{S}^n,\ t_1,t_2 \in T.$$

We first focus on a class of kernels defined on the product space $\mathbb{S}^n \times T$. We call $\mathcal{E}(\mathbb{S}^n,T)$ the set of continuous symmetric maps $k : (\mathbb{S}^n \times T)^2 \to \mathbb{R}$ that satisfy the following: for any $t_1,t_2 \in T$ fixed, there exists a sequence $\{\varphi^n_{\ell,j}(t_1,t_2)\}_{\ell,j}$ of complex numbers such that

$$k(p_1,t_1,p_2,t_2) = \sum_{\ell=0}^{\infty}\sum_{j=1}^{d_{n,\ell}} \varphi^n_{\ell,j}(t_1,t_2) Y_{\ell,j}(p_1)\overline{Y_{\ell,j}}(p_2), \qquad p_1,p_2 \in \mathbb{S}^n, \tag{3.1}$$

where the convergence holds uniformly with respect to (p_1,p_2) in $\mathbb{S}^n \times \mathbb{S}^n$ and the sequence $\{\varphi^n_{\ell,j}(t_1,t_2)\}_{\ell,j}$ satisfies

$$\overline{\varphi^n_{\ell,j}}(t_1,t_2) = \varphi^n_{\ell,d_{n,\ell}-j+1}(t_1,t_2), \qquad \ell \in \mathbb{N}_0,\ j = 1,\dots,d_{n,\ell}.$$

An example of a kernel k belonging to $\mathcal{E}(\mathbb{S}^n,T)$ is given by the covariance function of a real-valued random field X on $\mathbb{S}^n \times T$ with a spectral representation similar to (2.11),

$$X(p,t) = \sum_{\ell=0}^{\infty}\sum_{j=1}^{d_{n,\ell}} b_{\ell,j}(t) Y_{\ell,j}(p), \qquad p \in \mathbb{S}^n, t \in \mathbb{R}, \tag{3.2}$$

where $\{b_{\ell,j}(t) : \ell \in \mathbb{N}_0,\ j = 1,\dots,d_{n,\ell}\}$ is a family of complex-valued centered random processes on T such that, for all $t \in T$,

$$\overline{b_{\ell,j}}(t) = b_{\ell,d_{n,\ell}-j+1}(t) \qquad \text{and} \qquad \mathbb{E}\left[\sum_{\ell=0}^{\infty}\sum_{j=1}^{d_{n,\ell}} |b_{\ell,j}(t)|^2\right] < \infty,$$

and for all $t_1, t_2 \in T$,

$$\mathbb{E}[b_{\ell,j}(t_1)\overline{b_{\ell',j'}}(t_2)] = 0 \quad \text{for} \quad (\ell, j) \neq (\ell', j'). \tag{3.3}$$

In that case, the covariance function associated with X satisfies Equation (3.1) with

$$\varphi^n_{\ell,j}(t_1, t_2) = \mathbb{E}[b_{\ell,j}(t_1)\overline{b_{\ell,j}}(t_2)], \qquad t_1, t_2 \in T.$$

Let us remark that writing (3.3) with $\ell' = \ell$ and $j' = d_{n,\ell} - j + 1$ yields

$$\text{if} \quad j \neq d_{n,\ell} - j + 1 \quad \text{then} \quad \mathbb{E}[b_{\ell,j}(t)^2] = 0, \quad \forall t \in T.$$

In particular, it prevents $b_{\ell,j}$ to be real-valued except if vanishing.

Theorem 3.1. *Let k belong to $\mathcal{E}(\mathbb{S}^n, T)$. Then, the following holds.*

a) For every $t_1, t_2 \in T$, the series $\sum_{\ell=0}^{\infty} \sum_{j=1}^{d_{n,\ell}} |\varphi^n_{\ell,j}(t_1, t_2)|^2$ converges. Additionally, for any $\ell \in \mathbb{N}_0$ and any $j \in \{1, \ldots, d_{n,\ell}\}$,

$$\varphi^n_{\ell,j}(t_1, t_2) = \int_{\mathbb{S}^n} \int_{\mathbb{S}^n} k(p_1, t_1, p_2, t_2)\overline{Y_{\ell,j}}(p_1) Y_{\ell,j}(p_2) \mathrm{d}\sigma_n(p_1) \mathrm{d}\sigma_n(p_2). \tag{3.4}$$

Moreover, $\varphi^n_{\ell,j}$ is continuous on $T \times T$ for every $\ell \in \mathbb{N}_0$ and $j \in \{1, \ldots, d_{n,\ell}\}$.

b) The kernel k is a positive definite kernel on $\mathbb{S}^n \times T$ if and only if, for any $\ell \in \mathbb{N}_0$ and any $j \in \{1, \ldots, d_{n,\ell}\}$, $\varphi^n_{\ell,j}$ is a positive definite kernel on T.

Next result provides a spectral representation for the positive definite kernels that are isotropic with respect to the space $\mathbb{S}^n$ and not necessarily stationary with respect to time. On the one hand, it is a generalization of the main result given in Berg and Porcu (2017), which provides a characterization for the stationary case. On the other hand, it is a corollary of Theorem 3.1.

Theorem 3.2. *Let k be a continuous kernel on $\mathbb{S}^n \times T$.*
Then, k is positive definite and isotropic with respect to space if and only if we have, for every $(p_i, t_i) \in \mathbb{S}^n \times T, \quad i = 1, 2,$

$$k(p_1, t_1, p_2, t_2) = \sum_{\ell=0}^{\infty} \alpha^n_\ell(t_1, t_2)\, C_\ell^{(n-1)/2}(\cos\theta), \tag{3.5}$$

where,

i) for every $\ell \in \mathbb{N}_0$, α^n_ℓ is a real-valued continuous positive definite kernel on T;

ii) for every t in T, $\sum_{\ell=1}^{\infty} \alpha^n_\ell(t, t)\ell^{n-2} < \infty$;

iii) let $\widetilde{k}_S(\theta, t_1, t_2) = k(p_1, t_1, p_2, t_2)$. Then, for every $t_1, t_2 \in T$, the convergence in (3.5) is uniform with respect to $\theta \in [0, \pi]$.

Moreover, for every $t_1, t_2 \in T$ and $\ell \in \mathbb{N}_0$,

$$\alpha_\ell^n(t_1,t_2) = \frac{\omega_{n-1}}{\omega_n} \frac{(1+\frac{2\ell}{n-1})}{\binom{\ell+n-2}{\ell}} \int_0^\pi \widetilde{k}_S(\theta,t_1,t_2)\, C_\ell^{(n-1)/2}(\cos\theta)\, \sin^{n-1}\theta \,\mathrm{d}\theta, \quad \text{for } n = 2,3,\dots\ , \tag{3.6}$$

and

$$\alpha_\ell^1(t_1,t_2) = \begin{cases} \frac{\ell}{\pi}\int_0^\pi \widetilde{k}_S(\theta,t_1,t_2)\, \cos(\ell\theta)\,\mathrm{d}\theta, & \text{for} \quad \ell = 1,2,\dots \\ \frac{1}{\pi}\int_0^\pi \widetilde{k}_S(\theta,t_1,t_2)\,\mathrm{d}\theta, & \text{for} \quad \ell = 0. \end{cases} \tag{3.7}$$

Next result comes from Theorems 3.1 and 3.2.

Corollary 3.3. *Let $k : (\mathbb{S}^n \times T)^2 \to \mathbb{R}$ be a kernel in $\mathcal{E}(\mathbb{S}^n, T)$. Assume moreover that k is positive definite.*

Then, k is isotropic with respect to space if and only if the functions $\{\varphi_{\ell,j}^n\}_{\ell,j}$ appearing in Expansion (3.1) do not depend on the j index, i.e. they are such that

$$\varphi_{\ell,j}^n \equiv \varphi_{\ell,j'}^n\ , \quad \text{for all} \quad j,j' \in \{1,\dots,d_{n,\ell}\}\ ,\ \ell \in \mathbb{N}_0.$$

Furthermore, the functions $\{\varphi_{\ell,j}^n\}_{\ell,j}$ are linked with the functions $\{\alpha_\ell^n\}_\ell$ in Expansion (3.5) by the following. For $n \geq 2$,

$$\varphi_{\ell,j}^n(t_1,t_2) = \frac{\omega_n\,(n-1)}{2\ell+n-1}\,\alpha_\ell^n(t_1,t_2)\ ,\ t_1,t_2 \in T, \tag{3.8}$$

and $\varphi_{\ell,j}^1(t_1,t_2) = \pi\,\alpha_\ell^1(t_1,t_2)$ for $n = 1$.

4 Examples and Simulations

In this section, we consider random fields given by Expansion (3.2) where we choose a family of independent Gaussian complex-valued centered Gaussian processes $\{b_{\ell,j} : \ell \in \mathbb{N}_0,\ j = 1,\dots,d_{n,\ell}\}$ such that $\overline{b_{\ell,j}} = b_{\ell,d_{n,\ell}-j+1}$. Note that independence yields relation (3.3) to be satisfied.

4.1 A Spatially Isotropic and Time Nonstationary Model

We propose the kernel $k(p_1,t_1,p_2,t_2) = \widetilde{k}_S(\theta(p_1,p_2),t_1,t_2)$, such that

$$\widetilde{k}_S(\theta,t_1,t_2) = \exp\left\{\lambda(g(t_1,t_2)\cos\theta\ -1)\right\}, \qquad (\theta,t_1,t_2) \in [0,\pi]\times\mathbb{R}\times\mathbb{R}, \tag{4.1}$$

with λ a nonnegative constant and g the nonstationary positive definite kernel on $\mathbb{R}$ given by

$$g(t_1,t_2) = \frac{1}{t_1^2+t_2^2+1}, \qquad t_1,t_2\ \in \mathbb{R}.$$

We note that the kernel (4.1) is nonseparable, isotropic with respect to space and nonstationary with respect to time. It is called Poisson model, the stationary analogue

case is shown in Table 1 in Porcu, Bevilacqua and Genton (2016), where one can see other properties of the model. The Schoenberg's functions $\{\alpha_\ell^n\}_{\ell\in\mathbb{N}_0}$ that appear in (3.5) when expanding the isotropic kernel, are given by (3.6). In the case $n = 2$, it yields for every $t_1, t_2 \in \mathbb{R}$,

$$\alpha_\ell^2(t_1,t_2) = 2\,\exp(-\lambda)\,(1+2\ell)\int_0^\pi \exp\left\{\lambda g(t_1,t_2)\cos\theta\right\} C_\ell^{1/2}(\cos\theta)\sin\theta\,\mathrm{d}\theta \qquad \ell\in\mathbb{N}_0. \tag{4.2}$$

We now simulate in R Software (2013), a realization of a Gaussian random field on $\mathbb{S}^2\times\mathbb{R}$ whose covariance function is given by (4.1). First, we compute the α_ℓ^2 following (4.2) using the Package *orthopolynom* by Novomestky (2015) in the computation of the Gegenbauer polynomials (see Figure 1). Then, we take four time instants $t_1 = 0.1$, $t_2 = 0.2$, $t_3 = 0.3$ and $t_4 = 0.4$ in order to observe the temporal evolution of the process. We choose $\lambda = 2$ and a mesh on $\mathbb{S}^2$ with 40.000 points. For each time instant we use the spectral representation of the field given by the spherical harmonics series expansion (3.2), *i.e.*, we simulate

$$X_N(p,t_i) = \sum_{\ell=0}^{N}\sum_{j=1}^{2\ell+1} b_{\ell,j}(t_i)Y_{\ell,j}(p), \quad p\in\mathbb{S}^2,\ i=1,\dots,4.$$

In this way, we need to simulate the coefficients $\{b_{\ell,j}(t_i)\}_{\ell,j}$ for each instant of time. The truncation of the series expansion was put at $N = 10$, which means $\ell = 0,1,\dots,10$, since in this case the decay of α_ℓ^2 is fast enough as ℓ increases.

We like to remark that our simulation procedure follows the approximation described in Lang and Schwab (2013) (see Lemma 5.1 in this reference).

To compute the spherical harmonic functions, we use the function *legendre_sphPlm* included in the Package *gsl* by Hankin et al. (2017), defined as follows

$$Y_{\ell,j}(\vartheta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{\ell-j}{\ell+j}}P_{\ell,j}(\cos\vartheta)\,e^{ij\varphi}, \qquad p = p(\vartheta,\varphi)\in\mathbb{S}^2,$$

where $P_{\ell,j}$ denote the associated Legendre function and $(\vartheta,\varphi)\in[0,\pi]\times[0,2\pi)$.

The variables $\{b_{\ell,j}(t_i) : \ell = 0,1,\dots,10,\ j = 1,\dots,2\ell+1,\ i = 1,2,3,4\}$ are simulated as centered complex-valued Gaussian random variables following the next dependence rule: for each fixed t_i, $\{b_{\ell,j}(t_i) : \ell = 0,1,\dots,10,\ j = 1,\dots,2\ell+1\}$ are uncorrelated and for each fixed ℓ, j,

$$\mathrm{cov}(b_{\ell,j}(t_i), b_{\ell,j}(t_k)) = \varphi_{\ell,j}(t_i,t_k) = \frac{\pi}{2\ell+1}\alpha_\ell^2(t_i,t_k),$$

with α_ℓ^2 given by (4.2). Moreover, following Corollary 2.5 in Lang and Schwab (2013), for $j\neq 0$, we have that $\mathrm{Re}(b_{\ell,j}(t_i))$ and $\mathrm{Im}(b_{\ell,j}(t_i))$ are equal in law, uncorrelated and

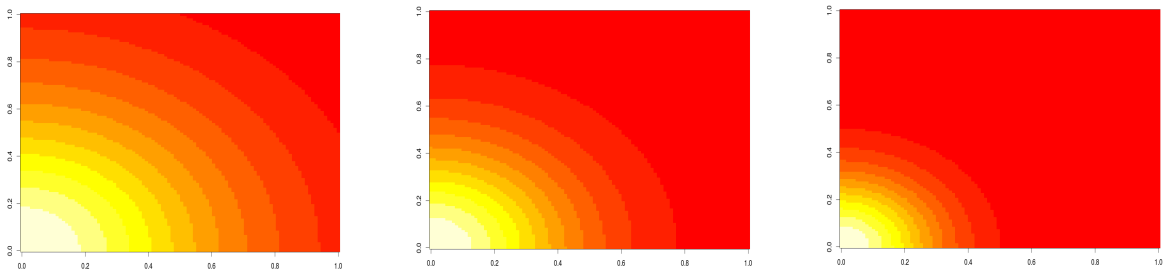

Figure 1. $\alpha_\ell^2(\cdot,\cdot)$ for $\ell = 1, 6$ and 12, with $\lambda = 2$.

satisfy

$$\mathbb{E}[\mathrm{Re}(b_{\ell,j}(t_i))^2] = \mathbb{E}[\mathrm{Im}(b_{\ell,j}(t_i))^2] = \frac{\varphi_{\ell,j}(t_i,t_i)}{2},$$

and for $j = 0$, the elements $\{b_{\ell,0}(t_i)\}_\ell$ are real-valued and satisfy

$$\mathbb{E}[b_{\ell,0}(t_i)^2] = \varphi_{\ell,0}(t_i,t_i).$$

Note that the above covariances $\varphi_{\ell,j}$ do not depend on the j index. This fact induces isotropy with respect to space following Corollary 3.3. By a usual regression, we get that $b_{\ell,j}(t_2)$ follows a conditional Gaussian distribution given $b_{\ell,j}(t_1)$, *i.e*

$$b_{\ell,j}(t_2) \mid b_{\ell,j}(t_1) \sim \mathcal{N}\left(\frac{\varphi_{\ell,j}^2(t_1,t_2)}{\varphi_{\ell,j}^2(t_1,t_1)} b_{\ell,j}(t_1), \varphi_{\ell,j}^2(t_2,t_2) - \frac{\varphi_{\ell,j}^2(t_1,t_2)^2}{\varphi_{\ell,j}^2(t_1,t_1)}\right).$$

We do subsequently the same conditioning for $b_{\ell,j}(t_3)$ given $\{b_{\ell,j}(t_i) : i = 1,2\}$ and for $b_{\ell,j}(t_4)$ given $\{b_{\ell,j}(t_i) : i = 1,2,3\}$, with $j = 1,\dots,2\ell+1$, either for the real or for the imaginary part, separately. At the end, it is possible to evaluate the error of the approximation applying Proposition 5.2 of Lang and Schwab (2013), since for every $t_i \in \mathbb{R}$, $\alpha_\ell^2(t_i,t_i)$ decays algebraically with order $\beta > 2$ *i.e.*, for $i = 1,\dots,4$, there exist constants $C_i > 0$ and $\ell_0 \geq 0$ such that $\alpha_\ell^2(t_i,t_i) \leq C_i\,\ell^{-\beta}$ for all $\ell \geq \ell_0$. Thus, it holds

$$\|X(\cdot,t_i) - X_N(\cdot,t_i)\|_{\mathcal{L}^2(\mathbb{S}^2)} \leq \hat{C}_i\, N^{-(\beta-2)/2},$$

for $N \geq \ell_0$, where $\hat{C}_i^{\,2} = C_i\left(\frac{2}{\beta-2} + \frac{1}{\beta-1}\right)$. As an example, the decay of $\alpha_\ell^2(t_i,t_i)$ for $i = 1,2$, is compared with a function in $\mathcal{O}(\ell^{-3})$ in Figure 2.

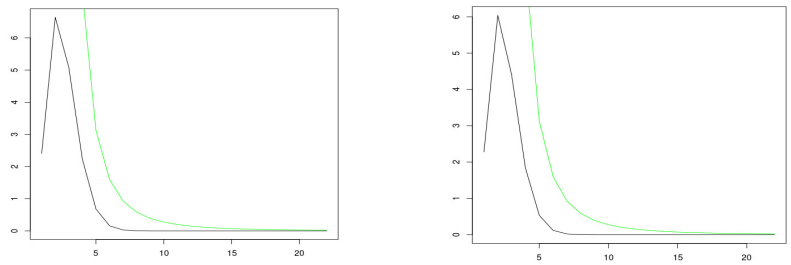

Figure 2. $\ell \mapsto \alpha_\ell^2(t_1, t_1)$ and $\ell \mapsto \alpha_\ell^2(t_2, t_2)$ respectively in color black with curves in $\mathcal{O}(\ell^{-3})$ in green.

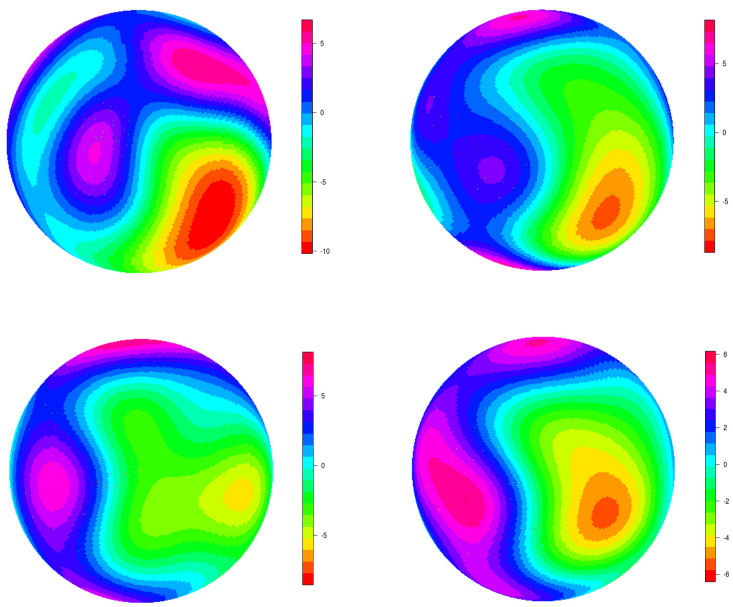

Figure 3. Isotropic nonstationary Gaussian random field simulated at time instants $t_1 = 0.1$, $t_2 = 0.2$, $t_3 = 0.3$ and $t_4 = 0.4$ respectively, with $N = 10$ over a mesh in $\mathbb{S}^2$ with 40.000 points.

In Figure 3, we can see the variation of the field through time.

4.2 A Spatially Anisotropic and Time Nonstationary Model

In this section, we provide an anisotropic nonstationary covariance model on $\mathbb{S}^n \times \mathbb{R}$, modifying the model given in the previous section. We consider a random field X on $\mathbb{S}^n \times \mathbb{R}$ that admits an expansion of the type (3.2). We again choose a family of independent complex-valued centered Gaussian processes $\{b_{\ell,j} \,:\, \ell \in \mathbb{N}_0,\ j = 1, \ldots, d_{n,\ell}\}$ satisfying $\overline{b_{\ell,j}} = b_{\ell,d_{n,\ell}-j+1}$. Introducing the covariance functions,

$$\mathbb{E}[b_{\ell j}(t_1)\overline{b_{\ell j}}(t_2)] = \varphi_{\ell,j}^n(t_1, t_2),$$

we now impose that $\varphi^n_{\ell,j}$ depends on the j index, in order to elude the isotropy assumption with respect to space. In particular, when $n = 2$ we propose to use

$$\varphi^2_{\ell j}(t_1, t_2) = \frac{2j+1}{2\ell+1}\alpha^2_\ell(t_1, t_2), \qquad t_1, t_2 \in \mathbb{R}, \tag{4.3}$$

with α^2_ℓ being defined by (4.2).

We now simulate a Gaussian random field on $\mathbb{S}^2 \times \mathbb{R}$ at two time instants. The procedure to apply is analogous to the one explained in Section 4.1, simulating in this case the $\{b_{\ell,j}(t_i) : i = 1, 2\}_{\ell,j}$ in such a way that the time covariance is given by formula (4.3).

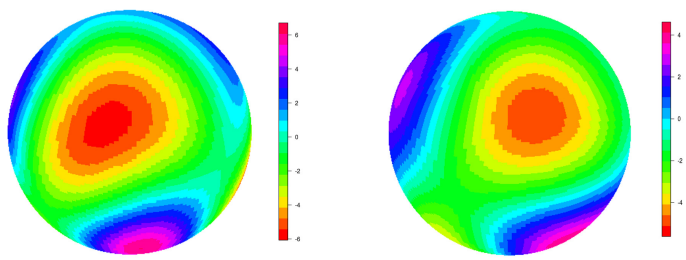

Figure 4. Anisotropic nonstationary Gaussian random field simulated at time instants $t_1 = 0.2$, $t_2 = 0.4$ respectively, with $N = 10$ over a mesh in $\mathbb{S}^2$ with 40.000 points.

In order to better appreciate the anisotropy, we plot the field at $t_2 = 0.4$ from different viewing directions, which are obtained varying the azimuthal angle or rotating the sphere.

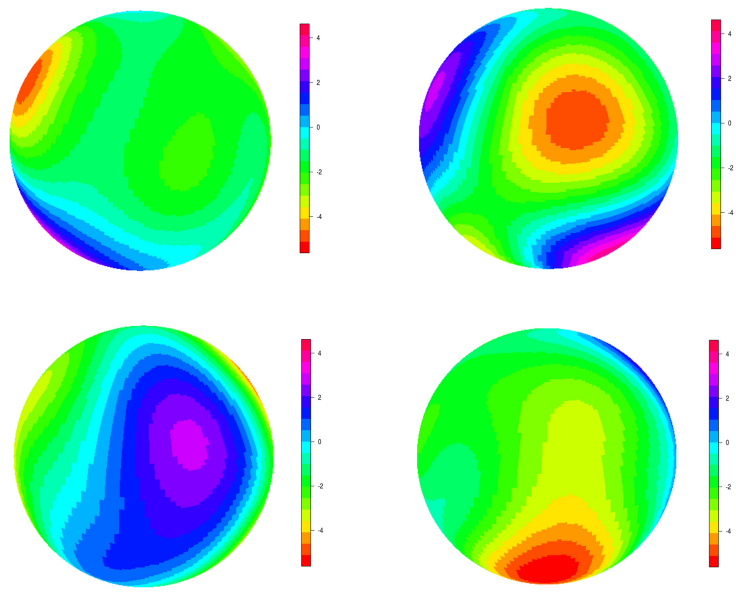

Figure 5. Anisotropic nonstationary Gaussian random field simulated at $t_2 = 0.4$ with viewing directions given by the azimuthal angles 0°, 90°, 180° and 270° respectively.

In Figure 5, we can see the field in the instant t_2 from four different directions, in order to observe changes in the appearance according to the zone of the sphere, which may reflect the anisotropy.

Appendix: Proofs

Proof of Theorem 3.1

a) For any positive integer N, let us define

$$k_N(p_1, t_1, p_2, t_2) := \sum_{\ell=0}^{N} \sum_{j=1}^{d_{n,\ell}} \varphi^n_{\ell,j}(t_1, t_2) Y_{\ell,j}(p_1) \overline{Y_{\ell,j}}(p_2). \tag{4.4}$$

For every t_1 and t_2 in T, $k_N(\cdot, t_1, \cdot, t_2)$ converges to $k(\cdot, t_1, \cdot, t_2)$ as $N \to \infty$ uniformly on $\mathbb{S}^n \times \mathbb{S}^n$, and hence in $\mathcal{L}^2(\mathbb{S}^n \times \mathbb{S}^n, \mathrm{d}\sigma_n \otimes \mathrm{d}\sigma_n)$, *i.e.*

$$\|k(\cdot, t_1, \cdot, t_2) - k_N(\cdot, t_1, \cdot, t_2)\|^2_{\mathcal{L}^2(\mathbb{S}^n \times \mathbb{S}^n)} \underset{N\to\infty}{\longrightarrow} 0. \tag{4.5}$$

The left-hand side in (4.5) is equal to

$$\int_{\mathbb{S}^n} \int_{\mathbb{S}^n} \left| \sum_{\ell=N+1}^{\infty} \sum_{j=1}^{d_{n,\ell}} \varphi^n_{\ell,j}(t_1, t_2) Y_{\ell,j}(p_1) \overline{Y_{\ell,j}}(p_2) \right|^2 \mathrm{d}\sigma_n(p_1) \mathrm{d}\sigma_n(p_2)$$

$$= \sum_{\ell=N+1}^{\infty} \sum_{j=1}^{d_{n,\ell}} \sum_{\ell'=N+1}^{\infty} \sum_{j'=1}^{d_{n,\ell}} \varphi^n_{\ell,j}(t_1, t_2) \overline{\varphi^n_{\ell',j'}}(t_1, t_2) \int_{\mathbb{S}^n} \int_{\mathbb{S}^n} Y_{\ell,j}(p_1) \overline{Y_{\ell',j'}}(p_1)\, \overline{Y_{\ell,j}}(p_2) Y_{\ell',j'}(p_2) \mathrm{d}\sigma_n(p_1) \mathrm{d}\sigma_n(p_2)$$

$$= \sum_{\ell=N+1}^{\infty} \sum_{j=1}^{d_{n,\ell}} |\varphi^n_{\ell,j}(t_1, t_2)|^2 \ .$$

Hence, $\sum_{\ell=0}^{\infty}\sum_{j=1}^{d_{n,\ell}}|\varphi_{\ell,j}^n(t_1,t_2)|^2<\infty$. By the orthonormality of the spherical harmonics, for any $t_1,t_2\in T$, we can thus prove that

$$\int_{\mathbb{S}^n}\int_{\mathbb{S}^n}k(p_1,t_1,p_2,t_2)\overline{Y_{\ell,j}}(p_1)Y_{\ell,j}(p_2)\mathrm{d}\sigma_n(p_1)\mathrm{d}\sigma_n(p_2)=\varphi_{\ell,j}^n(t_1,t_2).$$

Application of Lebesgue's Theorem to the above integral shows continuity of $\varphi_{\ell,j}^n$ on $T\times T$ for all ℓ and j.

b) Suppose that k is a positive definite kernel on $\mathbb{S}^n\times T$. For any fixed ℓ and j, and any compactly supported function q on T, we apply Lemma 2.1 with $c(p,t)=Y_{\ell,j}(p)\,q(t)$ for $(p,t)\in\mathbb{S}^n\times T$, and obtain

$$\int_{\mathbb{S}^n\times T}\int_{\mathbb{S}^n\times T}k(p_1,t_1,p_2,t_2)\,Y_{\ell,j}(p_1)\,q(t_1)\,\overline{Y_{\ell,j}}(p_2)\,\overline{q(t_2)}\,\mathrm{d}\sigma_n(p_1)\mathrm{d}\sigma_n(p_2)\mathrm{d}t_1\mathrm{d}t_2\ \geq 0.$$

Direct application of Fubini's Theorem yields

$$\int_T\int_T q(t_1)\,\overline{q(t_2)}\left(\int_{\mathbb{S}^n}\int_{\mathbb{S}^n}k(p_1,t_1,p_2,t_2)\,Y_{\ell,j}(p_1)\,\overline{Y_{\ell,j}}(p_2)\,\mathrm{d}\sigma_n(p_1)\mathrm{d}\sigma_n(p_2)\right)\mathrm{d}t_1\mathrm{d}t_2\ \geq 0.$$

The fact that the inner integral is equal to $\varphi_{\ell,j}^n(t_1,t_2)$ proves that $\varphi_{\ell,j}^n$ is a positive definite kernel on T.

Conversely, suppose that $\varphi_{\ell,j}^n$ is a positive definite kernel on T for all ℓ and j. Then, for $a_1,\dots,a_m$ in $\mathbb{C}$ and $(p_1,t_1),\dots,(p_m,t_m)$ in $\mathbb{S}^n\times T$, we have

$$\begin{aligned}\sum_{i,i'=1}^{m}a_i\overline{a_{i'}}k(p_i,t_i,p_{i'},t_{i'})&=\sum_{i,i'=1}^{m}a_i\overline{a_{i'}}\lim_{N\to\infty}\sum_{\ell=0}^{N}\sum_{j=1}^{d_{n,\ell}}\varphi_{\ell,j}^n(t_i,t_{i'})Y_{\ell,j}(p_i)\overline{Y_{\ell,j}}(p_{i'})\\&=\lim_{N\to\infty}\sum_{\ell=0}^{N}\sum_{j=1}^{d_{n,\ell}}\sum_{i,i'=1}^{m}a_i\overline{a_{i'}}\varphi_{\ell,j}^n(t_i,t_{i'})Y_{\ell,j}(p_i)\overline{Y_{\ell,j}}(p_{i'})\geq 0,\end{aligned}$$

since $\varphi_{\ell,j}^n(t_i,t_{i'})Y_{\ell,j}(p_i)\overline{Y_{\ell,j}}(p_{i'})$ is a positive definite kernel on $\mathbb{S}^n\times T$, being the tensor product of positive definite kernels on T and $\mathbb{S}^n$ respectively, for every ℓ and j. ■

Proof of Theorem 3.2

Suppose that k is a positive definite kernel on $\mathbb{S}^n\times T$ and additionnaly spatially isotropic.
First, by Definition 1, there exists a function $\widetilde{k}_S:[0,\pi]\times T\times T\to\mathbb{R}$ such that for every $t_1,t_2\in T$ and $p_1,p_2\in\mathbb{S}^n$,

$$k(p_1,t_1,p_2,t_2)=\widetilde{k}_S(\theta(p_1,p_2),t_1,t_2).$$

Let us fix t_1 and t_2 in T. Since the map $\widetilde{k}_S(\arccos(\cdot),t_1,t_2)$ belongs to $\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)$, it admits an expansion in terms of the Gegenbauer polynomials, *i.e.* there exists a sequence of real numbers $\{\alpha_\ell^n(t_1,t_2)\}_{\ell\in\mathbb{N}_0}$ such that

$$\widetilde{k}_S(\arccos(\cdot),t_1,t_2)=\sum_{\ell=0}^{\infty}\alpha_\ell^n(t_1,t_2)\,C_\ell^{(n-1)/2}(\cdot),\tag{4.6}$$

where the convergence holds in $\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)$. Using (2.7), we see that k satisfies Equation (3.1) with, for $n=2,3,\ldots$,

$$\varphi^n_{\ell,j}(t_1,t_2)=\frac{\omega_n\,(n-1)}{2\ell+n-1}\,\alpha^n_\ell(t_1,t_2),\qquad \ell\in\mathbb{N}_0,\ j=1,\ldots,d_{n,\ell},$$

and $\varphi^1_{\ell,j}(t_1,t_2)=\pi\,\alpha^1_\ell(t_1,t_2)$ for $\ell\in\mathbb{N}_0$, $j=1,2$. Hence, k belongs to $\mathcal{E}(\mathbb{S}^n,T)$. Then, Theorem 3.1 applies and shows that $\{\alpha^n_\ell\}_{\ell\in\mathbb{N}_0}$ is a sequence of continuous positive definite kernels on T. Point $i)$ is thus established.

We now focus on point $ii)$. Let $t\in T$ be fixed and let us recall that Expansion (4.6) holds in $\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)$ for $t_1=t_2=t$. Moreover, since $\widetilde{k}_S(\arccos(\cdot),t,t)$ is continuous on $[-1,1]$, we have that the series in (4.6) is Abel summable on $[0,1)$ for any $z\in[-1,1]$ (see Theorem 9 in Müller, 1966), *i.e.* the limit $\lim_{r\to1^-}\sum_{\ell=0}^\infty(\alpha^n_\ell(t,t)\,C^{(n-1)/2}_\ell(z)\,r^\ell)$ exists. For $z=1$, since $\alpha^n_\ell(t,t)\,C^{(n-1)/2}_\ell(1)\geq 0$ for all $\ell\in\mathbb{N}_0$, it implies that the series $\sum_{\ell=0}^\infty(\alpha^n_\ell(t,t)\,C^{(n-1)/2}_\ell(1))$ is finite. Noting that, for $n=2,3,\ldots$, $C^{(n-1)/2}_\ell(1)=\binom{\ell+n-2}{\ell}\sim\frac{\ell^{n-2}}{(n-2)!}$ and $C^0_\ell(1)\sim 2\ell^{-1}$ when $\ell\to\infty$. Then, the convergence of the series is equivalent to

$$\sum_{\ell=1}^\infty\alpha^n_\ell(t,t)\ell^{n-2}<\infty.$$

Hence, we get $ii)$.

Finally, it remains to establish assertion $iii)$. We consider Expansion (4.6) for fixed $t_1,t_2\in T$. By Cauchy-Schwarz inequality and by (2.8), we can see that for $z\in[-1,1]$ and for all $\ell\in\mathbb{N}_0$,

$$|\alpha^n_\ell(t_1,t_2)C^{(n-1)/2}_\ell(z)|\leq\frac{1}{2}\,(\alpha^n_\ell(t_1,t_1)+\alpha^n_\ell(t_2,t_2))\binom{\ell+n-2}{\ell},$$

with $\sum_{\ell=1}^\infty\alpha^n_\ell(t_i,t_i)\ell^{n-2}<\infty$ for $i=1,2$. Then, by the M-test of Weierstrass, the series in (4.6) converges uniformly to a continuous function, being precisely the function $\widetilde{k}_S(\arccos(\cdot),t_1,t_2)$. This proves the uniform convergence of the series in (3.5) for fixed $(t_1,t_2)\in T\times T$.

At last, Equation (3.6) follows directly from the orthogonality of the Gegenbauer polynomials and (2.9).

Let us prove now the converse part of Theorem 3.2. If k is a kernel that satisfies Expansion (4.6) with $i),ii),iii)$ then, using the addition formula (2.7), it is easy to see that k belongs to $\mathcal{E}(\mathbb{S}^n,T)$. The converse part of Theorem 3.1 allows us to state that k is a positive definite kernel on $\mathbb{S}^n\times T$. The isotropy property is clear from (4.6) since the right-hand side only depends on the inner product of p_1 and p_2 in $\mathbb{S}^n$. ■

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