Characterization Theorems for Covariance Functions on the n–Dimensional Sphere Across Time

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Abstract

This paper provides representation theorems for classes of nonstationary covariance functions on spheres across time. Isotropy on spheres comes out naturally in virtue of the addition theorem, and we show how to escape from this assumption, in order to obtain anisotropic kernels. The same criterion is used to escape from stationarity in the temporal component. An algorithm for the simulation of Gaussian processes with nonstationary and anisotropic covariances is provided.

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

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); Guella and Menegatto (2016) are apparent indications that there are some important branches of the mathematical community devoted to studying such constructions.
Recently, Porcu, Alegría and Furrer (2017) 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 the seminal paper by Schoenberg (1942). Then, Berg and Porcu (2016) 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. Jun and Stein (2007, 2008) emphasize that global data are affected by anisotropy and nonstationarity. This idea is pursued, albeit with different approaches, by Castruccio and Guinness (2016). The key argument by this group of authors is that statistical models on a spherical domain could be nonstationary for different latitudes, but stationary at the same latitude.

Our paper considers the problem of covariance functions that are anisotropic with respect to space and nonstationary with respect to time. Schoenberg's representation (Schoenberg, 1942), in concert with the addition theorem for spherical harmonics (Marinucci and Peccati, 2011), imply that the spherical isotropy is a natural assumption for the construction of covariances over spheres. Thus, the crux for generalizing the classical representation theorems to the anisotropic and nonstationary case is to evade from the addition theorem for spherical harmonics and use a different mathematical machinery. This paper puts some effort into this direction.

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.

2 Background

This section is largely expository and contains basic material that will be useful for a neater 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 symmetric mapping $k : M \times M \to \mathbb{R}$. 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 $c_1, \ldots, c_m \in \mathbb{R}$,

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

Kolmogorov's existence theorem implies that 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 $k_1 \otimes k_2((p_1, p_2), (t_1, t_2)) := k_1(p_1, t_1)k_2(p_2, t_2)$ 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 $\mathbb{S}^n \times \mathbb{R}$. It extends the special case given by Lemma 4.3 in Berg and Porcu (2016). 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 $c : \mathbb{S}^n \times \mathbb{R} \to \mathbb{R}$ with compact support,

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

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 (2005) and Dai and Xu (2013) for more details.

Let $\Delta_{\mathbb{S}^n}$ denotes the Laplace-Beltrami operator on $\mathbb{S}^n$. Introducing $\lambda_\ell = \ell(\ell + n - 1)$ with $\ell = 0, 1, \ldots$, the sequence $\{\lambda_\ell : \ell \in \mathbb{N}_0\}$ is called the spectrum of $\Delta_{\mathbb{S}^n}$. For each eigenvalue λ_ℓ, the associated eigenspace in $\mathcal{L}^2(\mathbb{S}^n, \mathrm{d}\sigma_n)$, *i.e.* the set of functions Y that satisfy the equation

$$\Delta_{\mathbb{S}^n} Y - \lambda_\ell Y = 0, \tag{2.3}$$

has uniquely determined dimension $d_{n,\ell}$, where

$$d_{n,\ell} = \begin{cases} \frac{(2\ell+n-1)(\ell+n-2)!}{\ell!(n-1)!} & if \quad \ell \in \mathbb{N}, \\ 1 & if \quad \ell = 0. \end{cases} \tag{2.4}$$

One can choose a complete orthonormal system in $\mathcal{L}^2(\mathbb{S}^n, \mathrm{d}\sigma_n)$, $\{Y_{\ell,j} : \ell \in \mathbb{N}_0,\ j = 1, \ldots, d_{n,\ell}\}$ such that each $Y_{\ell,j}$ satisfies the eigenproblem in Equation (2.3). The functions $\{Y_{\ell,j} : j = 1, \ldots, d_{n,\ell}\}$ are called spherical harmonics of order ℓ. For any $f \in \mathcal{L}^2(\mathbb{S}^n, \mathrm{d}\sigma_n)$, let us introduce

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

Thus, we have

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

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

$$X(p) = \sum_{\ell=0}^{\infty} \sum_{j=1}^{d_{n,\ell}} b_{\ell,j} Y_{\ell,j}(p), \qquad p \in \mathbb{S}^n, \tag{2.5}$$

with the coefficients $\{b_{\ell,j}\}_{\ell,j}$ being real-valued uncorrelated zero-mean random variables with variance depending on ℓ only. Specifically, we have

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

The representation in Equation (2.5) is also known as Karhunen-Loève expansion and the associated covariance kernel admits the expression

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

where the sequence $\{a_\ell\}_{\ell\in\mathbb{N}_0}$ is called angular power spectrum and is identified through the relation

$$\mathbb{E}[b_{\ell_1,j_1} b_{\ell_2,j_2}] = a_{\ell_1}\delta_{\ell_1,\ell_2}\delta_{j_1,j_2} \ , \tag{2.7}$$

where δ is the Kronecker delta function.

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 $\mathcal{L}^2([-1,1],(1-z^2)^{\nu-1/2}\mathrm{d}z)$.

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) and (Lemma 17.3 in Wendland, 2005):

$$C_\ell^{(n-1)/2}(\langle p_1, p_2\rangle) = \omega_n \frac{n-1}{2\ell+n-1} \sum_{j=1}^{d_{n,\ell}} Y_{\ell,j}(p_1)Y_{\ell,j}(p_2), \qquad p_1, p_2 \in \mathbb{S}^n, \tag{2.8}$$

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 $\mathbb{S}^n$. Besides, for all $\ell \in \mathbb{N}_0$,

$$|C_\ell^{(n-1)/2}(z)| \leq C_\ell^{(n-1)/2}(1) = \binom{\ell+n-2}{\ell}, \qquad \forall\, z \in [-1,1], \tag{2.9}$$

and

$$\begin{aligned} \|C_\ell^{(n-1)/2}\|^2_{\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)} &= \int_0^\pi \left(C_\ell^{(n-1)/2}(\cos\theta)\right)^2 \sin\theta^{n-1}\mathrm{d}\theta \\ &= \frac{\omega_n}{\omega_{n-1}} \frac{\binom{\ell+n-2}{\ell}}{(1+\frac{2\ell}{n-1})}. \end{aligned} \tag{2.10}$$

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

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

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 (2.7) 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 on $\mathbb{S}^n \times \mathbb{S}^n$ is positive definite and isotropic if and only if

$$k(p_1, p_2) = \psi(\theta(p_1, p_2)) = \sum_{\ell=0}^{\infty} \alpha_\ell^n C_\ell^{(n-1)/2}(\cos(\theta(p_1, p_2))), \qquad p_1, p_2 \in \mathbb{S}^n, \tag{2.11}$$

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 coeficients with respect to the dimension of the sphere $\mathbb{S}^n$.

3 Results

Throughout, T denotes either any compact interval in $\mathbb{R}$ or $\mathbb{R}$ itself. We are concerned with the representation of real-valued positive definite kernels on $\mathbb{S}^n \times T$. At this point, 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

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

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 $\{\varphi_{\ell,j}^n(t_1, t_2)\}_{\ell,j}$ of real numbers such that

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

where the convergence holds uniformly with respect to (p_1, p_2) in $\mathbb{S}^n \times \mathbb{S}^n$.

An example of a kernel k belonging to $\mathcal{E}(\mathbb{S}^n, T)$ is given by the covariance kernel of a random field X on $\mathbb{S}^n \times T$ such that

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

with $\{b_{\ell,j}(t) : \ell \in \mathbb{N}_0, \ j = 1, \ldots, d_{n,\ell}\}$ a sequence of independent centered random processes on T such that $\mathbb{E}\left(\sum_{\ell=0}^\infty \sum_{j=1}^{d_{n,\ell}} b_{\ell,j}(t)^2\right) < \infty$, for all $t \in T$. In that case, the covariance function associated with X satisfies Equation (3.1) with

$$\varphi_{\ell,j}^n(t_1, t_2) = \operatorname{cov}(b_{\ell,j}(t_1), b_{\ell,j}(t_2)), \qquad t_1, t_2 \in T.$$

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 $j \in \{1,\dots,d_{n,\ell}\}$,

$$\varphi^n_{\ell,j}(t_1,t_2) = \int_{\mathbb{S}^n}\int_{\mathbb{S}^n} k(p_1,t_1,p_2,t_2)Y_{\ell,j}(p_1)Y_{\ell,j}(p_2)\mathrm{d}\sigma_n(p_1)\mathrm{d}\sigma_n(p_2). \tag{3.3}$$

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

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 $j \in \{1,\dots,d_{n,\ell}\}$, $\varphi^n_{\ell,j}$ is a positive definite kernel on T.

Proof. a) For any positive integer N, let us define

$$k_N(p_1,t_1,p_2,t_2) := \sum_{\ell=0}^{N}\sum_{j=1}^{d_{n,\ell}} \varphi^n_{\ell,j}(t_1,t_2)Y_{\ell,j}(p_1)Y_{\ell,j}(p_2). \tag{3.4}$$

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.*

$$\|k(\cdot,t_1,\cdot,t_2) - k_N(\cdot,t_1,\cdot,t_2)\|^2_{\mathcal{L}^2(\mathbb{S}^n\times\mathbb{S}^n)} \underset{N\to\infty}{\longrightarrow} 0. \tag{3.5}$$

The left-hand side in (3.5) is equal to

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

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

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

Application of Lebesgue's Theorem to the above integral shows continuity of $\varphi^n_{\ell,j}$ 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

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

Direct application of Fubini's Theorem yields

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

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

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

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

since $\varphi^n_{\ell,j}(t_i, t_{i'}) Y_{\ell,j}(p_i) Y_{\ell,j}(p_{i'})$ is positive definite on $(\mathbb{S}^n \times T)^2$ being the tensor product of positive definite kernels on T and $\mathbb{S}^n$ repectively, for every ℓ and j. Then, the limit of a sequence of positive definite kernels on $\mathbb{S}^n \times T$ is also a positive definite kernel on $\mathbb{S}^n \times T$. □

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 (2016), 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 $(p_i, t_i) \in \mathbb{S}^n \times T, \quad i = 1, 2,$

$$k(p_1, t_1, p_2, t_2) = \sum_{\ell=0}^{\infty} \alpha^n_\ell(t_1, t_2) C^{(n-1)/2}_\ell(\cos(\theta(p_1, p_2))), \tag{3.6}$$

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 (3.6) is uniform with respect to $\theta \in [0, \pi]$.*

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

$$\alpha^n_\ell(t_1, t_2) = \frac{\omega_{n-1}}{\omega_n} \frac{(1 + \frac{2\ell}{n-1})}{\binom{\ell+n-2}{\ell}} \int_0^\pi \widetilde{k}_S(\theta, t_1, t_2) C^{(n-1)/2}_\ell(\cos\theta)\, (\sin\theta)^{n-1} \mathrm{d}\theta, \quad \textit{for } n = 2, 3, \dots\ , \tag{3.7}$$

and

$$\alpha^1_\ell(t_1, t_2) = \begin{cases} \frac{\ell}{\pi} \int_0^\pi \widetilde{k}_S(\theta, t_1, t_2)\, \cos(\ell\theta)\, \mathrm{d}\theta, & \textit{for} \quad \ell = 1, 2, \dots \\ \frac{1}{\pi} \int_0^\pi \widetilde{k}_S(\theta, t_1, t_2)\, \mathrm{d}\theta, & \textit{for} \quad \ell = 0. \end{cases} \tag{3.8}$$

Proof. 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

$$\widetilde{k}_S(\arccos(\cdot), t_1, t_2) = \sum_{\ell=0}^{\infty} \alpha_\ell^n(t_1,t_2)\, C_\ell^{(n-1)/2}(\cdot), \tag{3.9}$$

where the convergence holds in $\mathcal{L}^2([-1,1],(1-z^2)^{(n-2)/2}\mathrm{d}z)$. Using (2.8), we see that k satisfies Equation (3.1) with, for $n = 2, 3, \ldots$,

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

and $\varphi_{\ell,j}^1(t_1,t_2) = \pi\,\alpha_\ell^1(t_1,t_2)$ 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 $\{\alpha_\ell^n\}_{\ell\in\mathbb{N}_0}$ 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 (3.9) 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 (3.9) is Abel summable on $[0,1)$ for any $z\in[-1,1]$ (see Theorem 9 in Müller, 1966), *i.e.* the limit $\lim_{r\to 1^-}\sum_{\ell=0}^{\infty}(\alpha_\ell^n(t,t)\,C_\ell^{(n-1)/2}(z)\,r^\ell)$ exists. For $z=1$, since $\alpha_\ell^n(t,t)\,C_\ell^{(n-1)/2}(1)\geq 0$ for all $\ell\in\mathbb{N}_0$, it implies that the series $\sum_{\ell=0}^{\infty}(\alpha_\ell^n(t,t)\,C_\ell^{(n-1)/2}(1))$ is finite. Noting that, for $n=2,3,\ldots$, $C_\ell^{(n-1)/2}(1) = \binom{\ell+n-2}{\ell} \sim \frac{\ell^{n-2}}{(n-2)!}$ and $C_\ell^0(1)\sim 2\ell^{-1}$ when $\ell\to\infty$. Then, the convergence of the series is equivalent to

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

Hence, we get *ii*).

Finally, it remains to establish assertion *iii*). We consider Expansion (3.9) for fixed $t_1, t_2 \in T$. By Cauchy-Schwarz inequality and by (2.9), we can see that for $z\in[-1,1]$ and for all $\ell\in\mathbb{N}_0$,

$$|\alpha_\ell^n(t_1,t_2)C_\ell^{(n-1)/2}(z)| \leq \frac{1}{2}\,(\alpha_\ell^n(t_1,t_1)+\alpha_\ell^n(t_2,t_2))\binom{\ell+n-2}{\ell},$$

with $\sum_{\ell=1}^{\infty}\alpha_\ell^n(t_i,t_i)\ell^{n-2}<\infty$ for $i=1,2$. Then, by the M-test of Weierstrass, the series in (3.9) 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 (3.6) for fixed $(t_1,t_2)\in T\times T$.

At last, Equation (3.7) follows directly from the orthogonality of the Gegenbauer polynomials and (2.10).

Let us prove now the converse part of Theorem 3.2. If k is a kernel that satisfies Expansion (3.9) with $i), ii), iii)$ then, using the addition formula (2.8), 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 (3.9) since the right-hand side only depends on the inner product of p_1 and p_2 in $\mathbb{S}^n$. □

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 $\{\varphi^n_{\ell,j}\}_{\ell,j}$ appearing in Expansion (3.1) do not depend on the j index, i.e. they are such that

$$\varphi^n_{\ell,j} \equiv \varphi^n_{\ell,j'} \ , \quad \textit{for all} \ \ j, j' \in \{1, \ldots, d_{n,\ell}\} \ , \ \ell \in \mathbb{N}_0.$$

Furthermore, the functions $\{\varphi^n_{\ell,j}\}_{\ell,j}$ are linked with the functions $\{\alpha^n_\ell\}_\ell$ in Expansion (3.6) by the following, for $n \geq 2$,

$$\varphi^n_{\ell,j}(t_1, t_2) = \frac{\omega_n \, (n-1)}{2\ell + n - 1} \, \alpha^n_\ell(t_1, t_2) \ , \ \ t_1, t_2 \in T, \tag{3.10}$$

and $\varphi^1_{\ell,j}(t_1, t_2) = \pi \, \alpha^1_\ell(t_1, t_2)$ for $n = 1$.

4 Examples of nonstationary models on $\mathbb{S}^n \times \mathbb{R}$

In this section, we will consider random fields given by expansions of the type (3.2). Our purpose, is to simulate the data with the necessary knowledge of the covariance structure of the field.

4.1 An isotropic nonstationary model on $\mathbb{S}^n \times \mathbb{R}$

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

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

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 $\{\alpha^n_\ell\}_{\ell \in \mathbb{N}_0}$ that appear in (3.6) when expanding the kernel, are given by (3.7). If $n = 2$ for every $t_1, t_2 \in \mathbb{R}$,

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

4.2 Simulation of an isotropic nonstationary Gaussian field on $\mathbb{S}^2 \times \mathbb{R}$

We simulate in R software 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 Fig. 1). Then we take four time instants $t_1 = 0.1$, $t_2 = 0.3$, $t_3 = 0.5$ and $t_4 = 0.7$, in order to observe the changes of the field realization along the time, we chose $\lambda = 2$ 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

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

In this way, it requires 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 $N = 10$, that means $\ell = 0, 1, \ldots, 10$, since in this case the decay of α_ℓ^2 is fast enough as ℓ increases.

Additionally, 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

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

where $P_{\ell,j}$ denote the associated Legendre function.

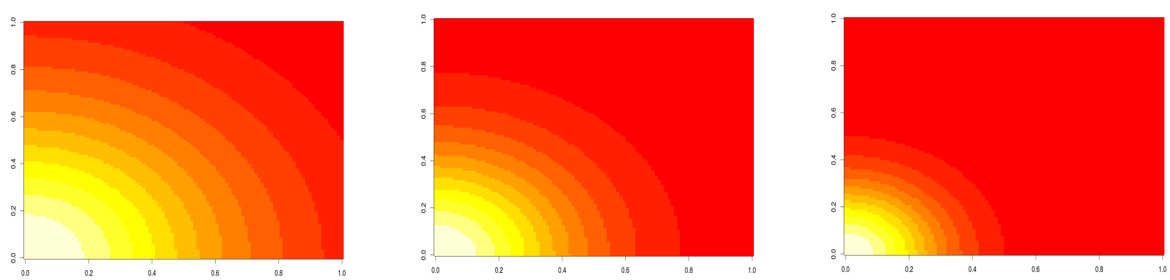

Figure 1. $\alpha_\ell^2(\cdot, \cdot)$ for $\ell = 1, 6$ and 12, with $\lambda = 2$.

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

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

with α_ℓ^2 given by (4.2). Note that the above covariance do not depend on j index. This fact induces isotropy with respect to space. Hence, $b_{\ell,j}(t_2)$ follows a conditional Gaussian distribution given $b_{\ell,j}(t_1)$, *i.e*

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

We do subsequently the same recurrence for $b_{\ell,j}(t_3)$ given $b_{\ell,j}(t_2)$ and for $b_{\ell,j}(t_4)$ given $b_{\ell,j}(t_3)$, with $j = 1,\ldots,2\ell+1$. 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 $i = 1,\ldots,4$, 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.

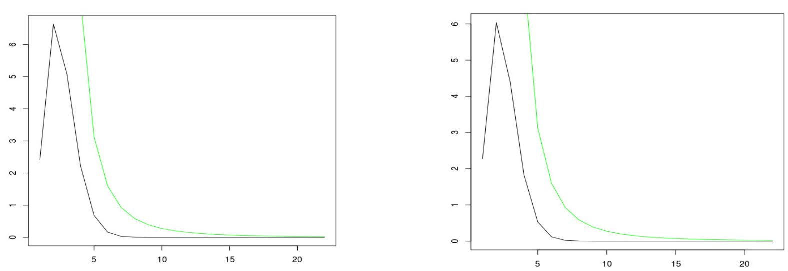

Figure 2. $\alpha_\ell^2(t_1,t_1)$ and $\alpha_\ell^2(t_2,t_2)$ respectively in color black with curves in $\mathcal{O}(\ell^{-3})$ in green, identifying the x-axis with the index ℓ.

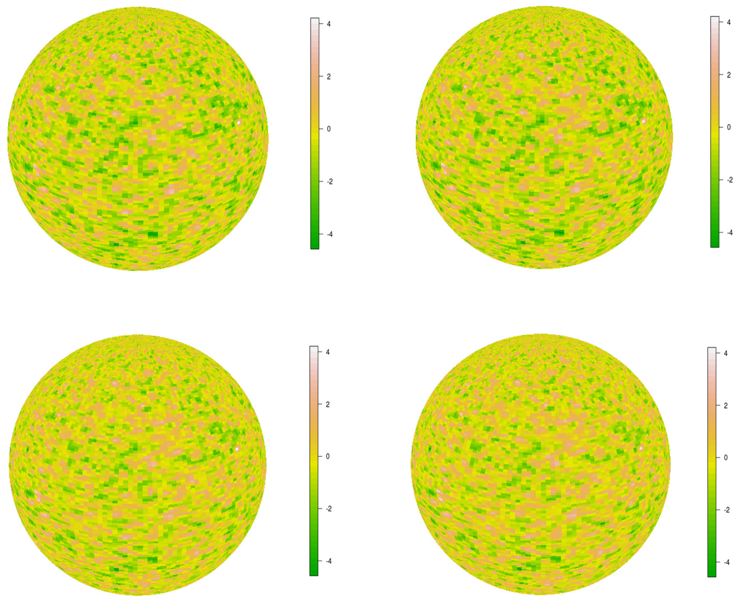

Figure 3. Isotropic nonstationary Gaussian random field simulated at time instants $t_1 = 0.1$, $t_2 = 0.3$, $t_3 = 0.5$ and $t_4 = 0.7$ respectively, with $N = 10$ over a mesh in $\mathbb{S}^2$ with 40.000 points.

In Figure 3, we can see the variation of the field along the time, there are small differences between the spheres due to the strong correlation in time.

4.3 An anisotropic nonstationary model on $\mathbb{S}^n \times \mathbb{R}$

In this section, we give an anisotropic nonstationary covariance model on $\mathbb{S}^n \times \mathbb{R}$, modifying the model given in the previous section. We still consider a random field X on $\mathbb{S}^n \times \mathbb{R}$ that admits an expansion of type (3.2),

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

We now choose a family of independent Gaussian processes $\{b_{\ell,j} : \ell \in \mathbb{N}_0,\ j = 1, \ldots, d_{n,\ell}\}$ satisfying

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

where we impose that $\varphi^n_{\ell,j}$ has dependence on the j index, in order to elude the isotropy assumption with respect to space, through the application of Corollary 3.3. In particular, when $n = 2$ we propose to use

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

where we add the j dependence through the multiplication term $\frac{2j+1}{2\ell+1}$ with α_ℓ^2 being defined as in (4.2).

4.4 Simulation of an anisotropic nonstationary Gaussian field on $\mathbb{S}^2 \times \mathbb{R}$

We simulate a Gaussian random field on $\mathbb{S}^2 \times \mathbb{R}$. The procedure to apply is analogous to the one explained in the last section, simulating in this case the $\{b_{\ell,j}(t_i) : i = 1, 2, 3, 4\}_{\ell,j}$ in such a way that the time covariance is given by formula (4.3).

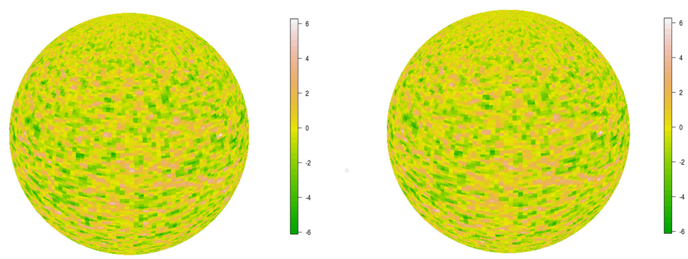

Figure 4. Anisotropic nonstationary Gaussian random field simulated at time instants $t_1 = 0.2$, $t_2 = 0.6$ respectively, with $N = 10$ over a mesh in $\mathbb{S}^2$ with 40.000 points.

In order to appreciate better the anisotropy, we plot the field at $t_1 = 0.2$ from different viewing directions, which are obtained varying the azimuthal angle or rotating the sphere.

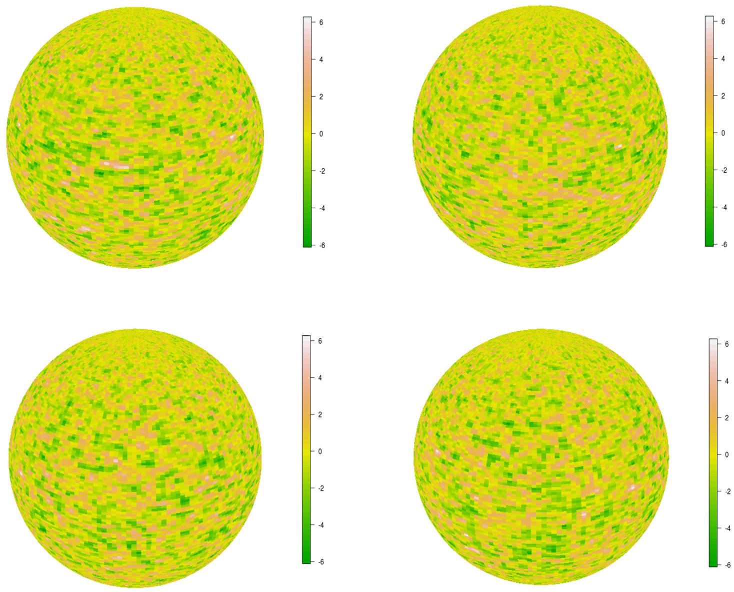

Figure 5. Anisotropic nonstationary Gaussian random field simulated at $t_1 = 0.2$ with viewing directions given by the azimuthal angles 0°, 90°, 180° and 270° respectively.

In Figure 5, we can see the field in the instant t_1 from different directions, in order to observe changes in the appearance according to the zone of the sphere, which may reflect the anisotropy.

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