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# Estimation of the covariance function of Gaussian isotropic random fields on spheres, related Rosenblatt-type distributions and the cosmic variance problem

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# Estimation of the covariance function of Gaussian isotropic random fields on spheres, related Rosenblatt-type distributions and the cosmic variance problem

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**Abstract:** We consider the problem of estimating the covariance function of an isotropic Gaussian stochastic field on the unit sphere using a single observation at each point of the discretized sphere. The spatial estimator of the covariance function is expressed in a new form which provides, on one hand a way to derive the characteristic function of the estimator, and on the other hand a computationally efficient method to do so. We also describe a methodology for handling the presence of the cosmic variance which can impair the results. In simulation, we use the pixelization scheme HEALPix.

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**1. Introduction**

This paper is about the statistical analysis of a Gaussian isotropic spherical random field  $T(x)$  on the unit sphere  $\mathbb{S}_2 = \{x \in \mathbb{R}^3 : \|x\| = 1\}$  in Euclidean space  $\mathbb{R}^3$ , when only one observation of the field is available. This perspective is relevant for the analysis of the Cosmic Microwave Background Radiation (CMBR) discovered by the astronomers Arno Penzias and Robert Wilson in 1964. It is due to the emission of black body thermal energy originating from the big bang. The spectral radiation is measured at different angles of observation of the sky, see [65]. It is apparently almost isotropic.

Our goal is to estimate the covariance function of the random field  $T(x)$ ,  $x \in \mathbb{S}_2$ , in a parametric setting, given a single observation at each point of the discretized sphere. As application, using a result of Veillette-Taquq [61], we present a methodology for handling the problem of *cosmic variance* in this framework. The cosmic variance is defined in (5.1) below. It results from uncertainty due to the fact that one has only a single observation.

It is well known that the second order structure, i.e., either covariance or spectrum completely characterize a centered Gaussian random field. Therefore the estimation of these quantities is of primary importance. The estimation of the spectrum is a well-studied subject [41], [14], [13] and so is the estimation of the covariance. If the estimation is non-parametric then the cosmic variance, defined in (5.1), will prevent us in getting a good estimator unless the spectrum at low frequencies vanishes, which would be unusual. If we are dealing with a parametric problem, however, that is, if the covariance function depends on some unknown parameters, then there is a chance of getting a reasonable estimator, see [40] as well. The method would be as follows. Given observations of the random field  $T$ , estimate its covariance function non-parametrically and then its spectrum. Set the low frequencies to zero. This yields a modified estimated spectrum. Then estimate the unknown parameters by minimizing the sum of squares of the difference between the theoretical form of the spectrum and the modified estimated spectrum. As indicated below, one can alleviate in this way the cosmic variance problem. On the other hand the theory underlying the estimation of the parameters of the angular spectrum using wavelets in a framework of higher frequency asymptotics can be found a number of papers, see [12], [16], [17], [15], [11], [25], [5], [5], [39], see also their references.

Important areas of applications include modeling global atmosphere's dynamics [7], cosmic microwave background (CMB) [14], [13], temperature and polarization fluctuations [64] among others.

The paper is organized as follows. In Section 2, we review some basic notions related to isotropic random fields. In Section 3 we focus on the covariance function  $\mathcal{C}(\cos \gamma)$  which is a function of the angle  $\gamma$  between two points on the sphere. We estimate this covariance function using empirical covariances  $\widehat{\mathcal{C}}(\cos \gamma)$  based on a single observation at each point of the discretized sphere. The characteristic function of these empirical covariances is given in terms of cumulants. It turns out that our estimator follows a Rosenblatt type distribution for each given single angle  $\gamma$ . In Section 4 we focus on the difference  $R = \widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma)$ . Following results of [61], we obtain the distribution of  $R$  and related properties. In Section 5 we discuss the problem of *cosmic variance*, namely the effects of the uncertainty due to the fact that only one realization is observed. To alleviate this effect one can approximate  $R$  by  $R_M$  which does not involve the low frequencies and for which the cosmic variance is negligible. We show that  $R_M$  tends to a Gaussian distribution as  $M \rightarrow \infty$ . In Section 6 we provide simulations using HEALPix which is a high level pixelization of the sphere  $\mathbb{S}_2$  and show that  $M$  as low as 4 can suffice. Our results can be generalized to higher dimensions  $d \geq 3$ , by using Gegenbauer (ultraspherical) polynomials ( $C_n^\alpha$ ) instead of the Legendre ones ( $C_\ell^{1/2} = P_\ell$ ).

Theorems 3.2 and 5.1 are of particular interest. Theorem 3.2 provides the characteristic function of  $\widehat{\mathcal{C}}(\cos \gamma)$ . It is a theoretical result, but with a clear statistical meaning, since it specifies the distribution of the empirical covariance. For example, one could estimate the unknown parameters of the covariance function of a spherical random field using nonlinear regression, and thus having information about errors is useful when applying the existing methodology. Such information would also be needed when testing hypothesis on the unknown parameters of the nonlinear regression. Theorem 5.1 is important because it gives a normal approximation for the tail  $R_M$ .

Section 7 contains a conclusion. An appendix contains examples (Appendix A), a brief description of white noise analysis on the sphere (Appendix B), the Thorin class and measure (Appendix C) and formulae (Appendix D) used in the paper.

## 2. Preliminaries

Let  $(\Xi, F, \mathbb{P})$  be a probability space, and  $\mathbb{S}_2 = \{x \in \mathbb{R}^3 : \|x\| = 1\}$  be the unit sphere centered at the origin. We consider a real-valued random field  $T(\omega, x) = T(x)$ ,  $\omega \in \Xi$ ,  $x \in \mathbb{S}_2$ , with  $\mathbb{E}T(x) = 0$ . This random field is said to be second-order weakly isotropic or (simply) isotropic, if  $\mathbb{E}T(x)^2 < \infty$ , and  $\mathbb{E}T(x)T(y) = \mathbb{E}T(gx)T(gy)$  for any  $g \in SO(3)$ ,  $x, y \in \mathbb{S}_2$ , where  $SO(3)$  denotes the three dimensional rotational group under composition. The orthogonal system on  $\mathbb{S}_2$  is given by the complex-valued spherical harmonics  $Y_\ell^m$ , where  $\ell = 0, 1, 2, \dots$ , and  $m = -\ell, -\ell + 1, \dots, -1, 0, 1, \dots, \ell - 1, \ell$ . Their expression is given in (D.7). The

Euler angles  $(\vartheta, \varphi)$  define the position  $x(\vartheta, \varphi) = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta)$  of a point on the sphere with colatitude<sup>1</sup>  $\vartheta \in [0, \pi]$  and longitude  $\varphi \in [0, 2\pi]$ . The colatitude measures the north-south position and the longitude the east-west position. We suppose that  $T(x)$  is mean square continuous, and hence it admits a series expansion ([41]),

$$T(x) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell}^m(x), \tag{2.1}$$

in terms of the complex-valued spherical harmonics  $Y_{\ell}^m$ , with coefficients given by

$$a_{\ell m} = \int_{\mathbb{S}_2} T(x) Y_{\ell}^{m*}(x) \Omega(dx), \tag{2.2}$$

where  $\Omega(dx) = \sin \vartheta d\vartheta d\varphi$  is the Lebesgue measure of surface area on  $\mathbb{S}_2$ , and where star denotes the complex conjugate. The series (2.1) converges in  $\mathbb{L}_2(\Omega, \mathbb{R})$  for all  $x \in \mathbb{S}_2$ .

If the coefficients  $a_{\ell m}$  are independent and for fixed  $\ell$  are identically distributed then the covariance function  $\mathcal{C}_2(x_1, x_2) = \mathbb{E}T(x_1)T(x_2)$ , ( $\mathbb{E}T(x) = 0$ ) depends on the *angular distance*  $\gamma$  between  $x_1$  and  $x_2$  only. This angle  $\gamma$  results from the inner product  $x_1 \cdot x_2 = \cos \gamma$ . The covariance function depends on this central angle  $\gamma$  between locations and has the form

$$\mathcal{C}_2(x_1, x_2) = \mathcal{C}(\cos \gamma) = \sum_{\ell=0}^{\infty} f_{\ell} \frac{2\ell + 1}{4\pi} P_{\ell}(\cos \gamma), \tag{2.3}$$

where  $P_{\ell}$  denotes the Legendre polynomial, see (D.6) The coefficient  $f_{\ell}$  in (2.3) defines the *angular spectrum* and satisfies  $f_{\ell} \geq 0$ , see [41], [66]. We assume finite variance, and since the Legendre polynomials are bounded,  $|P_{\ell}(y)| \leq 1$ , and  $P_{\ell}(1) = 1$ , we get

$$\sum_{\ell=0}^{\infty} (2\ell + 1) f_{\ell} < \infty. \tag{2.4}$$

The fact that  $\mathcal{C}_2(x_1, x_2) = \mathcal{C}(\cos \gamma)$  indicates that  $\mathcal{C}_2(x_1, x_2)$  is invariant under the group of rotations. The random field  $T(x)$  said to be *linear* if  $a_{\ell m}$  are independent and if for fixed  $\ell$ , they are identically distributed. We work with Gaussian random fields, they happen to be linear and linear fields are automatically Gaussian, see [6], [58].

From now on we assume

**Assumption:**  $T(x)$  is Gaussian, with finite variance.

We can obtain the angular spectrum  $f_{\ell}$  from the covariance through the relation

$$f_{\ell} = 2\pi \int_0^{\pi} \mathcal{C}(\cos \gamma) P_{\ell}(\cos \gamma) \sin \gamma d\gamma. \tag{2.5}$$

---

<sup>1</sup>The *colatitude* is used when the North pole is at 0 degree, and *latitude* when the equator is at 0 degree. In this paper we use colatitude.

For a given  $T(x)$  we have the inversion (2.2) and  $a_{\ell,-m} = (-1)^m a_{\ell m}^*$ , since the field  $T(x)$  is real-valued and since  $Y_\ell^{m*} = (-1)^m Y_\ell^{-m}$ . The orthogonal random 'measure'  $a_{\ell m}$  is a triangular array, we have  $m = -\ell, -\ell+1, \dots, \ell-1, \ell$ , i.e. rows contain  $2\ell+1$ , i.i.d Gaussian random variables  $a_{\ell m}$  with

$$\mathbb{E}a_{\ell m} = 0, \mathbb{E}a_{\ell m}a_{kn}^* = f_\ell \delta_{\ell,k} \delta_{m,n}. \quad (2.6)$$

In particular  $a_{\ell m}$  is normal with mean 0 and variance  $\mathbb{E}|a_{\ell m}|^2 = f_\ell$ .

Characterization, construction, classes and examples of isotropic positive definite functions on spheres, i.e. covariance functions, is an interesting problem and the interested reader may consult [23], [28], [63], [36], [35], [26], [29], [22].

**Remark 2.1.** *A function defined by (2.3) with the coefficients  $f_\ell$  is strictly positive definite if and only if  $f_\ell$  is strictly positive for infinitely many even and infinitely many odd integers  $\ell$ , see [26] for details.*

For instance a class of covariance functions on spheres can originate from covariance functions of some homogenous and isotropic random fields on Euclidean spaces since the restriction of the field to the sphere yields an isotropic field on the sphere. In this case consider two locations  $x_1$  and  $x_2$  on the sphere with angle  $\gamma \in [0, \pi]$ . Then the distance  $r = \|x_1 - x_2\|$  between them expressed in terms of the angle  $\gamma$  is  $2 \sin(\gamma/2)$ , see Figure 1, and the inner product is  $x_1 \cdot x_2 = \cos \gamma$ , which gives a direct correspondence between the original covariance function  $\mathcal{C}_0(r)$ , in the Euclidean space and the covariance function

$$\mathcal{C}_2(x_1, x_2) = \mathcal{C}(\cos \gamma) = \mathcal{C}_0(2 \sin(\gamma/2)),$$

on the sphere. This holds for any dimension of the Euclidean space. The disadvantage of using  $\mathcal{C}_0$  is that it depends on the chordal distance between two points on the sphere instead of the grand-circle (spherical or geodesic) distance, which is not practical.

One can consider a more natural Laplacian model defined directly on the sphere  $\mathbb{S}_2$  when the distance is measured using the grand-circle distance.

**Example 2.1. Laplace-Beltrami model** on  $\mathbb{S}_2$ . *We consider the stochastic model on the sphere  $\mathbb{S}_2$  for an isotropic random field  $T_B$  on  $\mathbb{S}_2$ , (the index  $B$  is for "Beltrami") satisfying the equation*

$$(\Delta_B - c^2)T_B = \partial W_B,$$

in the  $L_2$  sense, where  $\partial W_B$  denotes the white noise with variance  $\sigma^2$ , see the Appendix B for the definition of  $\partial W_B$ . The Laplace-Beltrami operator is

$$\Delta_B = \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}.$$

A direct calculation leads to the spectrum

$$f_\ell = \frac{1}{(\ell(\ell+1) + c^2)^2}, \quad (2.7)$$

for  $T_B$ , and the covariance function

$$\mathcal{C}(\cos \gamma) = \frac{\sigma^2}{4\pi} \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{(\ell(\ell + 1) + c^2)^2} P_{\ell}(\cos \gamma),$$

is given by formula (2.3). This form of covariance function obtained via white-noise-driven damped diffusion equations for modeling global temperature fields by [43], see also [31]. The rigorous theory can be developed in the same line as it is done in [32] see again Appendix B for more details and references.

The methodology described in this paper applies to some more examples, see the Appendix A.

### 3. Empirical covariances

We have defined  $\mathcal{C}(\cos \gamma)$  in (2.3), and now we suppose that an observation of the field  $T(x)$ , is given on the whole unit sphere  $\mathbb{S}_2$  and  $\mathbb{E}T(x) = 0$ .

Consider a location  $x$  on the sphere  $\mathbb{S}_2$  and let an angle  $\gamma \in [0, \pi]$  be given. Consider all locations  $y_{\gamma}$  with angular distance  $\gamma$  to  $x$ , so that  $x \cdot y_{\gamma} = \cos \gamma$ . Locations  $y_{\gamma}$  form a circle  $C(x, \gamma)$  with center  $x$  and radius  $\sin \gamma$ , see Figure 1. Now define a rotation  $g(x, \psi) \in SO(3)$  which rotates the sphere  $\mathbb{S}_2$  around  $x$  by an angle  $\psi$ . The point  $x$  being the center will not be moved but any location  $y_{\gamma}$  on the circle  $C(x, \gamma)$  will be moved to some new location denoted  $y_{\gamma}(x, \psi) = g(x, \psi) \tilde{y}_{\gamma}$ . The  $y_{\gamma}(x, \psi)$  has the property  $x \cdot y_{\gamma}(x, \psi) = \cos \gamma$  since the rotation preserves the angular distance between two points.

The empirical covariance  $\hat{\mathcal{C}}(\cos \gamma)$  for an angular distance  $\gamma$  will be given in two steps. First we fix a location  $x$  and superpose  $T(x)T(y_{\gamma}(x, \psi)) d\psi/2\pi$  over all  $y_{\gamma}(x, \psi)$  on the circle  $C(x, \gamma)$  by varying  $\psi$ , then secondly, we integrate over

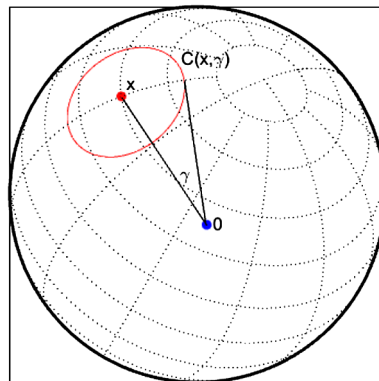


FIG 1. The sphere  $\mathbb{S}_2$  with the circle  $C(x, \gamma)$

all  $x$  on the sphere  $\mathbb{S}_2$ , yielding

$$\widehat{C}(\cos \gamma) = \int_{\mathbb{S}_2} \int_{C(x, \gamma)} T(x) T(y_\gamma(x, \psi)) \frac{d\psi}{2\pi} \frac{\Omega(dx)}{4\pi}. \quad (3.1)$$

In practice the data  $T(x)$  is discretized, for instance when  $T(x)$  measures the Cosmic Microwave Background anisotropies, the measurements are given on a high resolution pixel structure called HEALPix of the sphere  $\mathbb{S}_2$  and therefore (3.1) can be approximated with high precision. The calculation of (3.1) involves summation of products of the data as is the usual case for covariance estimators. The usual estimator of the covariances used in cosmology, due to [48], involves estimating the spectrum (through  $\mathbb{E}a_{\ell m}^2 = f_\ell$ ) first, then using (2.3) next.

We shall use a discretized version of (3.1) for actual computation of the estimate but formula (3.2) in the next Theorem will be used to obtain the distribution of the estimator.

**Theorem 3.1.** *If  $T(x)$  is Gaussian then*

$$\widehat{C}(\cos \gamma) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left( |\widehat{a}_{\ell 0}|^2 + 2 \sum_{m=1}^{\ell} |\widehat{a}_{\ell m}|^2 \right) P_\ell(\cos \gamma), \quad (3.2)$$

where  $\widehat{a}_{\ell m}$  are independent and identically distributed normal random variables with

$$\mathbb{E}\widehat{a}_{\ell m} = 0, \text{ and } \mathbb{E}|\widehat{a}_{\ell m}|^2 = f_\ell.$$

*Proof.* We denote the North pole  $N = (0, 0, 1)$  since it is at colatitude  $\vartheta = 0$  and longitude  $\varphi = 0$  and since the radius equals 1. For each location  $x$  one can find a rotation  $g$  such that  $x = gN$ , that is it maps the North pole to  $x$ . The inverse  $g^{-1}$  of the rotation  $g$  does not change the angular distance between two points hence  $g^{-1}x \cdot g^{-1}y_\gamma(x, \psi) = \cos \gamma$ . The rotation  $g^{-1}$  maps  $x$  to the North pole  $g^{-1}x = N$ , and the circle  $C(x, \gamma)$  to the circle  $C(N, \gamma)$ . The points on that circle are  $g^{-1}y_\gamma(x, \psi) = z_\gamma(N, \psi) = (\sin \gamma \cos \psi, \sin \gamma \sin \psi, \cos \gamma)$ ,  $\psi \in [0, 2\pi]$ . Now in (3.1), the integral on  $C(x, \gamma)$  becomes an integral from 0 to  $2\pi$  and the integral on  $\mathbb{S}_2$  becomes to the integral on  $SO(3)$  according to the Haar measure, see (D.3), so

$$\widehat{C}(\cos \gamma) = \int_{SO(3)} \int_0^{2\pi} T(gN) T(gz_\gamma(N, \psi)) \frac{d\psi}{2\pi} dg.$$

We apply the series expansion (2.1) to both  $T(x) = T(gN)$  and  $T(gz_\gamma(N, \psi))$ ,

$$T(gz_\gamma(N, \psi)) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \widehat{a}_{\ell m}^* \sum_{k=-\ell}^{\ell} D_{k,m}^{(\ell)*}(g) Y_\ell^{k*}(z_\gamma(N, \psi)),$$

where  $\widehat{a}_{\ell m} = a_{\ell m}$ , are calculated in (2.2), they are independent and identically distributed normal random variables with

$$\mathbb{E}\widehat{a}_{\ell m} = 0, \quad \mathbb{E}|\widehat{a}_{\ell m}|^2 = f_\ell, \quad (3.3)$$

and  $D_{k,m}^{(\ell)}$  denotes the Wigner D-matrix, see (D.4). We integrate first term by term from 0 to  $2\pi$  and get by (D.7)

$$\begin{aligned} \int_0^{2\pi} Y_\ell^{k*}(z_\gamma(N, \psi)) \frac{d\psi}{2\pi} &= \int_0^{2\pi} (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-k)!}{(\ell+k)!}} P_\ell^k(\cos \gamma) e^{-ik\psi} \frac{d\psi}{2\pi} \\ &= (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-k)!}{(\ell+k)!}} P_\ell^k(\cos \gamma) \int_0^{2\pi} e^{-ik\psi} \frac{d\psi}{2\pi} \\ &= \delta_{0,k} Y_\ell^{k*}(z_\gamma(N, \psi)). \end{aligned}$$

Then we continue the integration using the Haar measure

$$\begin{aligned} \widehat{\mathcal{C}}(\cos \gamma) &= \int_{SO(3)} \int_0^{2\pi} T(gN) T(gz_\gamma(N, \psi)) \frac{d\psi}{2\pi} dg \\ &= \sum_{\ell, \ell_1=0}^{\infty} \sqrt{\frac{2\ell_1+1}{4\pi}} \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \gamma) \\ &\quad \times \sum_{m_1=-\ell_1}^{\ell_1} \sum_{m=-\ell}^{\ell} \widehat{a}_{\ell m}^* \widehat{a}_{\ell_1 m_1} \int_{SO(3)} D_{0,m}^{(\ell)*}(g) D_{0,m_1}^{(\ell_1)}(g) dg \\ &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |\widehat{a}_{\ell m}|^2 P_\ell(\cos \gamma), \end{aligned} \tag{3.4}$$

see (D.3), (D.5). Notice  $|\widehat{a}_{\ell m}|^2 = |\widehat{a}_{\ell, -m}|^2$ , hence (3.2) follows.  $\square$

The next Theorem gives the marginal and joint characteristic function of  $\widehat{\mathcal{C}}(\cos \gamma)$ . See also [48].

**Theorem 3.2.** *Let  $\gamma \in [0, \pi]$  be given. The empirical covariance function  $\widehat{\mathcal{C}}(\cos \gamma)$  in (3.1) has the form (3.2) with characteristic function*

$$\varphi(z) = \prod_{\ell=0}^{\infty} \frac{1}{(1 - iz f_\ell P_\ell(\cos \gamma) / 2\pi)^{\ell+1/2}}. \tag{3.5}$$

Let  $\gamma_m \in [0, \pi]$ ,  $m = 1, 2, \dots, j$ , be given angles, then the joint characteristic function of  $\widehat{\mathcal{C}}(\cos \gamma_1), \widehat{\mathcal{C}}(\cos \gamma_2), \dots, \widehat{\mathcal{C}}(\cos \gamma_j)$  is

$$\varphi((z_1, z_2, \dots, z_j)) = \prod_{\ell=0}^{\infty} \frac{1}{\left(1 - i f_\ell \left(\sum_{m=1}^j z_m P_\ell(\cos \gamma_m)\right) / 2\pi\right)^{\ell+1/2}}.$$

*Proof.*  $\widehat{\mathcal{C}}$  is unbiased since (3.4) implies

$$\mathbb{E} \widehat{\mathcal{C}}(\cos \gamma) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} f_\ell (2\ell+1) P_\ell(\cos \gamma)$$

$$= \mathcal{C}(\cos \gamma). \quad (3.6)$$

Consider the difference

$$\begin{aligned} \widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma) &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left( |\widehat{a}_{\ell m}|^2 - f_{\ell} \right) P_{\ell}(\cos \gamma) \\ &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left( |\widehat{a}_{\ell 0}|^2 - f_0 + 2 \sum_{m=1}^{\ell} \left( |\widehat{a}_{\ell m}|^2 - f_{\ell} \right) \right) P_{\ell}(\cos \gamma), \end{aligned} \quad (3.7)$$

and notice that the coefficients  $|\widehat{a}_{\ell m}|^2 - f_{\ell}$  are Hermite polynomials of degree 2, see Appendix, D for details. Let  $H_2(\widehat{a}_{\ell m})$  denote  $|\widehat{a}_{\ell m}|^2 - f_{\ell} = |\widehat{a}_{\ell m}|^2 - \mathbb{E}|\widehat{a}_{\ell m}|^2$ , for simplicity and rewrite (3.7) in terms of Hermite polynomials

$$\widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left( H_2(\widehat{a}_{\ell 0}) + 2 \sum_{m=1}^{\ell} H_2(\widehat{a}_{\ell m}) \right) P_{\ell}(\cos \gamma). \quad (3.8)$$

We now use the cumulants of the Hermite polynomials (see (D.1) and (D.2)), in particular the variance  $\text{Var}(\widehat{\mathcal{C}}(\cos \gamma)) = \text{Cum}_2(\widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma))$ . In formula (3.8), all  $H_2(\widehat{a}_{\ell m})$  are independent for all  $\ell = 0, 1, 2, \dots$ , and  $m = 0, 1, \dots, \ell - 1, \ell$ . Moreover  $\text{Cum}_2(H_2(\widehat{a}_{\ell-m})) = \text{Cum}_2(H_2(\widehat{a}_{\ell m})) = f_{\ell}^2$ , hence we obtain from (3.8)

$$\begin{aligned} \text{Var}(\widehat{\mathcal{C}}(\cos \gamma)) &= \frac{1}{(4\pi)^2} \sum_{\ell=0}^{\infty} \left( \text{Cum}_2(H_2(\widehat{a}_{\ell 0})) + 4 \sum_{m=1}^{\ell} \text{Cum}_2(H_2(\widehat{a}_{\ell m})) \right) P_{\ell}^2(\cos \gamma) \\ &= \frac{1}{(4\pi)^2} \sum_{\ell=0}^{\infty} \left( 2f_{\ell}^2 + 4 \sum_{m=1}^{\ell} f_{\ell}^2 \right) P_{\ell}^2(\cos \gamma) \\ &= \frac{2}{(4\pi)^2} \sum_{\ell=0}^{\infty} (2\ell + 1) f_{\ell}^2 P_{\ell}^2(\cos \gamma) < \infty. \end{aligned} \quad (3.9)$$

The convergence of (3.9) follows from (2.4), i.e.  $f_{\ell} < o(\ell^{-1})$ , and from the fact that  $P_{\ell}$  is bounded by one for any  $\ell$ . Similarly for general  $k$ , we use the higher order cumulants (D.1) and (D.2) of the Hermite polynomials and obtain

$$\begin{aligned} \text{Cum}_k \left( H_2(\widehat{a}_{\ell 0}) + 2 \sum_{m=1}^{\ell} H_2(\widehat{a}_{\ell m}) \right) &= \text{Cum}_k H_2(\widehat{a}_{\ell 0}) + 2^k \sum_{m=1}^{\ell} \text{Cum}_k H_2(\widehat{a}_{\ell m}) \\ &= (2^{k-1} (k-1)! + \ell 2^k (k-1)!) f_{\ell}^k \\ &= 2^{k-1} (k-1)! (2\ell + 1) f_{\ell}^k. \end{aligned}$$

Hence by (3.8)

$$\text{Cum}_k(\widehat{\mathcal{C}}(\cos \gamma)) = \frac{(k-1)!}{(4\pi)^k} \sum_{\ell=0}^{\infty} 2^{k-1} (2\ell + 1) f_{\ell}^k P_{\ell}^k(\cos \gamma) \quad (3.10)$$

$$= \frac{(k-1)!}{2(2\pi)^k} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}^k P_{\ell}^k(\cos \gamma).$$

The cumulant characteristic function of  $\widehat{\mathcal{C}}(\cos \gamma)$  follows:

$$\begin{aligned} \ln \varphi(z) &= \sum_{k=1}^{\infty} \frac{i^k}{k!} z^k \text{Cum}_k(\widehat{\mathcal{C}}(\cos \gamma)) \\ &= \sum_{k=1}^{\infty} \frac{i^k z^k}{2k(2\pi)^k} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}^k P_{\ell}^k(\cos \gamma) \\ &= \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{k=1}^{\infty} \frac{i^k z^k}{2k(2\pi)^k} f_{\ell}^k P_{\ell}^k(\cos \gamma). \end{aligned} \tag{3.11}$$

Now, from the identity

$$\sum_{k=1}^{\infty} \frac{x^k}{k} = -\ln(1-x), \quad |x| < 1,$$

we obtain

$$\ln \varphi(z) = -\frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) \ln(1 - iz f_{\ell} P_{\ell}(\cos \gamma) / 2\pi),$$

which leads to

$$\varphi(z) = \prod_{\ell=0}^{\infty} \frac{1}{(1 - iz f_{\ell} P_{\ell}(\cos \gamma) / 2\pi)^{\ell+1/2}}.$$

Consider now the joint cumulant. Using the relation  $\text{Cum}_2(aX, bY) = ab \text{Cum}_2(X, Y)$  and (3.10), we get

$$\text{Cum}_2(\widehat{\mathcal{C}}(\cos \gamma_1), \widehat{\mathcal{C}}(\cos \gamma_2)) = \frac{2}{(4\pi)^2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}^2 P_{\ell}(\cos \gamma_1) P_{\ell}(\cos \gamma_2).$$

Therefore, with  $k = k_1 + k_2$ ,

$$\begin{aligned} \ln \varphi(z_1, z_2) &= \mathbb{E} e^{i(z_1 \widehat{\mathcal{C}}(\cos \gamma_1) + z_2 \widehat{\mathcal{C}}(\cos \gamma_2))} \\ &= \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{k_1+k_2 \geq 1} \frac{(k-1)! i^k z_1^{k_1} z_2^{k_2}}{2(2\pi)^k k_1! k_2!} f_{\ell}^k P_{\ell}^{k_1}(\cos \gamma_1) P_{\ell}^{k_2}(\cos \gamma_2) \\ &= \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{k=1}^{\infty} \frac{i^k f_{\ell}^k}{2k(2\pi)^k} (z_1 P_{\ell}(\cos \gamma_1) + z_2 P_{\ell}(\cos \gamma_2))^k, \\ \varphi(z_1, z_2) &= \prod_{\ell=0}^{\infty} \frac{1}{(1 - i f_{\ell} (z_1 P_{\ell}(\cos \gamma_1) + z_2 P_{\ell}(\cos \gamma_2)) / 2\pi)^{\ell+1/2}}. \end{aligned}$$

In general the joint cumulant is given by

$$\begin{aligned} \text{Cum}_k \left( \widehat{\mathcal{C}}(\cos \gamma_1), \widehat{\mathcal{C}}(\cos \gamma_2), \dots, \widehat{\mathcal{C}}(\cos \gamma_k) \right) \\ = \frac{(k-1)!}{2(2\pi)^k} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}^k \prod_{j=0}^k P_{\ell}(\cos \gamma_j). \end{aligned} \quad (3.12)$$

hence the characteristic function is

$$\varphi(z_1, z_2, \dots, z_j) = \prod_{\ell=0}^{\infty} \frac{1}{\left(1 - i f_{\ell} \left(\sum_{m=1}^j z_m P_{\ell}(\cos \gamma_m)\right) / 2\pi\right)^{\ell+1/2}}. \quad \square$$

#### 4. Distribution of the error

We shall focus here on

$$R = \widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma). \quad (4.1)$$

This is the error we make by using  $\widehat{\mathcal{C}}(\cos \gamma)$  instead of  $\mathcal{C}(\cos \gamma)$ . Recall that  $\mathbb{E}\widehat{\mathcal{C}}(\cos \gamma) = \mathcal{C}(\cos \gamma)$  by (3.6).

**Theorem 4.1.** *The random variable  $R$  in (4.1) can be represented as*

$$R \stackrel{d}{=} \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} P_{\ell}(\cos \gamma) \left( \frac{U_{2\ell+1}}{2\ell+1} - 1 \right), \quad (4.2)$$

where  $\stackrel{d}{=}$  means equality in distribution and where  $U_{2\ell+1}/(2\ell+1)$  is Gamma distributed with parameters  $(2\ell+1)/2$  and  $2/(2\ell+1)$ . The characteristic function of  $R$  is

$$\varphi(z) = e^{-iz\mathcal{C}(\cos \gamma)} \prod_{\ell=0}^{\infty} \frac{1}{\left(1 - iz f_{\ell} P_{\ell}(\cos \gamma) / 2\pi\right)^{\ell+1/2}} \quad (4.3)$$

$$= \exp \left( \sum_{k=2}^{\infty} \left( \frac{iz}{2\pi} \right)^k \frac{1}{2k} \sum_{\ell=0}^{\infty} (2\ell+1) (f_{\ell} P_{\ell}(\cos \gamma))^k \right), \quad (4.4)$$

which is a Rosenblatt type characteristic function. It is infinitely divisible and selfdecomposable

$$\varphi(z) = \exp \left( \int_0^{\infty} [e^{izx} - 1 - izx] \nu(x) dx \right),$$

with Lévy density

$$\nu(x) = \frac{1}{2x} \sum_{\ell=0}^{\infty} (2\ell+1) \exp \left( -\frac{x}{8\pi f_{\ell} P_{\ell}(\cos \gamma)} \right).$$

Moreover  $\varphi(z)$  belongs to the Thorin class  $T(\mathbb{R})$ , with Thorin measure given by

$$U(dx) = \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell + 1) \delta_{1/b_\ell}(x),$$

where  $b_\ell = 8\pi f_\ell P_\ell(\cos \gamma)$ .

*Proof.* The characteristic function (4.3) and (4.4) of  $R$  follows from (3.11) and (3.5). Now, rewrite  $R$  given in (3.7) in the following form

$$\begin{aligned} R &= \widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma) \\ &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} f_\ell P_\ell(\cos \gamma) \left( \left( \frac{|\widehat{a}_{\ell 0}|^2}{f_\ell} - 1 \right) + \sum_{m=1}^{\ell} \left( \frac{|\widehat{a}_{\ell m}|^2}{f_\ell/2} - 1 \right) \right). \end{aligned} \tag{4.5}$$

Since  $\widehat{a}_{\ell 0}$  is real therefore  $|\widehat{a}_{\ell 0}|^2/f_\ell$  has  $\chi_1^2$  distribution  $2|\widehat{a}_{\ell m}|^2/f_\ell$  has  $\chi_2^2$  distribution and they are independent. A simple consequence of this is that the random variables

$$\sum_{m=-\ell}^{\ell} \left( \frac{|\widehat{a}_{\ell m}|^2}{f_\ell} - 1 \right),$$

are  $\chi_{2\ell+1}^2 - (2\ell + 1)$  distributed and independent. Hence the characteristic function of  $R$  can be expressed as

$$\varphi(z) = \mathbb{E}e^{izR} = \exp \left( \sum_{k=2}^{\infty} \left( \frac{iz}{2\pi} \right)^k \frac{1}{2k} \sum_{\ell=0}^{\infty} (2\ell + 1) (f_\ell P_\ell(\cos \gamma))^k \right).$$

Hence a Rosenblatt type characteristic function [46], [47] shows up, see also [62] and [34].

The expression (4.5) can be rewritten as

$$R = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell P_\ell(\cos \gamma) \left( \frac{U_{2\ell+1}}{2\ell + 1} - 1 \right),$$

by setting

$$U_{2\ell+1} - (2\ell + 1) = \sum_{m=-\ell}^{\ell} \left( \frac{|\widehat{a}_{\ell m}|^2}{f_\ell} - 1 \right). \tag{4.6}$$

This last expression is  $\chi_{2\ell+1}^2 - (2\ell + 1)$ , distributed and hence  $U_{2\ell+1}/(2\ell + 1)$  is Gamma distributed with parameters  $(2\ell + 1)/2$  and  $2/(2\ell + 1)$ .

The Veillette-Taqu [61] result on Lévy–Khintchine representation of variables with a similar form to  $R$  can now be applied. The Veillette-Taqu’s result concerns a random variable of the form

$$\sum_{\ell=0}^{\infty} \lambda_\ell (\eta_\ell - 1),$$

where  $\eta_\ell$  are independent  $\text{Gamma}(r_\ell, 1/r_\ell)$  random variables. Hence we identify

$$\begin{aligned}\lambda_\ell &= (2\ell + 1) f_\ell P_\ell(\cos \gamma) / 4\pi, \\ r_\ell &= (2\ell + 1) / 2,\end{aligned}\tag{4.7}$$

and

$$\eta_\ell = U_{2\ell+1} / (2\ell + 1).$$

The assumption in Proposition 2.1 of [61] to be checked is

$$\sum_{\ell=0}^{\infty} \frac{\lambda_\ell^2}{r_\ell} = \frac{2}{(4\pi)^2} \sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell^2 P_\ell^2(\cos \gamma) < \infty.\tag{4.8}$$

But this holds because this quantity coincides with  $\text{Var}(R) = \text{Var}(\widehat{\mathcal{C}}(\cos \gamma))$  given in (3.9), and for each  $\gamma \in [0, \pi]$ ,

$$\sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell^2 P_\ell^2(\cos \gamma) < \infty,$$

see (3.9). Therefore it follows, (see Veillette-Taquq, [61], [62], Leonenko et al. [34]) that the distribution with characteristic function (4.4) is *infinitely divisible*:

$$\varphi(z) = \exp\left(\int_0^\infty [e^{izx} - 1 - izx]\nu(x) dx\right),$$

with Lévy density

$$\nu(x) = \frac{1}{2x} \sum_{\ell=0}^{\infty} (2\ell + 1) \exp\left(-\frac{x}{8\pi f_\ell P_\ell(\cos \gamma)}\right).$$

It is *selfdecomposable* (see [50], p.95, Corollary 15.11) since its Lévy measure has a density  $\nu$  satisfying:  $\nu(x) = h(x)/|x|, x > 0$ , with  $h(x)$  decreasing on  $(0, \infty)$ .

Let  $\mathcal{ID}(\mathbb{R}), \mathcal{SD}(\mathbb{R})$  be the classes of *infinitely divisible* and *selfdecomposable* distributions correspondingly. We next define the *Thorin class* on  $\mathbb{R}$  (see [59], [9], [30], [37], Appendix C) as follows: We refer to the product  $\gamma u$  as an *elementary gamma random variable* if  $u$  is nonrandom non-zero vector in  $\mathbb{R}$ , and  $\gamma$  is a gamma random variable on  $\mathbb{R}_+$ . Then, the *Thorin class* on  $\mathbb{R}$  (or the class of extended generalized gamma convolutions), denoted by  $T(\mathbb{R})$ , is defined as the smallest class of distributions that contains all elementary gamma distributions on  $\mathbb{R}$ , and is closed under convolution and weak convergence. It is known that

$$T(\mathbb{R}) \subset \mathcal{SD}(\mathbb{R}) \subset \mathcal{ID}(\mathbb{R}),$$

and inclusions are strict, [30]. Since any selfdecomposable distribution on  $\mathbb{R}$  is absolutely continuous (see, for instance, Example 27.8 of [50]) and is unimodal (by [67], see also Theorem 53.1 of [50]), then, any selfdecomposable distribution has a bounded density function. Thus the distribution with characteristic function (4.4) has a bounded unimodal density.

Also (see Leonenko et al.[34] for details ) that the distribution with characteristic function (4.4) belongs to the Thorin class  $T(\mathbb{R})$ , with Thorin measure given by

$$U(d\omega) = \frac{1}{2} \sum_{l=0}^{\infty} (2l + 1) \delta_{1/b_l}(\omega),$$

where  $b_l$  is given in the statement of the theorem. □

**Remark 4.1.** *Theorem 4.1 shows the similarities and differences between the behavior of the estimation errors of an unknown covariance function for isotropic random field and the results for stochastic processes or time series, in which only asymptotic distributions are known. Surprisingly in our case we can obtain the explicit distribution, in terms of characteristic function, of the approximation error and even the rate of convergence.*

### 5. Dealing with the cosmic variance problem

Consider a sample path of the field

$$T(x) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell}^m(x).$$

All information contained in this single sample path about the coefficients  $f_{\ell}$  in the series expansion of the covariance function  $\mathcal{C}(\cos \gamma)$ , see (2.3), is expressed through the random variables  $a_{\ell m}$ . Although  $a_{\ell m}$  can be inverted with high precision for every indices  $\ell, m$ , see (2.2), for small ‘frequencies’  $\ell$ ,  $a_{\ell m}$  has little information useful for estimation. For instance if  $\ell = 0$ ,  $\hat{f}_0 = |\hat{a}_{00}|^2$  is a single value realization of  $a_{00}$  which tells almost nothing about  $f_0 = \mathbb{E} |a_{00}|^2$ . If  $\ell$  is large then we have  $\hat{a}_{\ell m}$ ,  $m = -\ell, -\ell + 1, \dots, \ell - 1, \ell$ , i.e. a  $2\ell + 1$  ‘sample’ for estimating  $f_{\ell} = \mathbb{E} \hat{f}_{\ell} = \mathbb{E} |\hat{a}_{\ell m}|^2$ . By introducing

$$\hat{f}_{\ell} = \frac{1}{2\ell + 1} \left( \sum_{m=-\ell}^{\ell} |\hat{a}_{\ell m}|^2 \right),$$

which has the property

$$\mathbb{E} \hat{f}_{\ell} = \frac{1}{2\ell + 1} (2\ell + 1) \mathbb{E} |\hat{a}_{\ell m}|^2 = f_{\ell},$$

and

$$\begin{aligned} \text{Var}(\hat{f}_{\ell}) &= \frac{1}{(2\ell + 1)^2} \left( \text{Var} \sum_{m=-\ell}^{\ell} |\hat{a}_{\ell m}|^2 \right) \\ &= \frac{1}{(2\ell + 1)^2} (2\ell + 1) \left( \sum_{m=-\ell}^{\ell} \text{Var} |\hat{a}_{\ell m}|^2 \right) \end{aligned}$$

$$= \frac{2f_\ell^2}{2\ell + 1},$$

since  $\widehat{a}_{\ell m}$  is normal with mean 0 and variance  $f_\ell$ . We can now define the *cosmic variance* as

$$\mathbb{E} \left( \frac{f_\ell - \widehat{f}_\ell}{f_\ell} \right)^2 = \frac{2}{2\ell + 1}, \quad (5.1)$$

see [64], p. 138. This quantity does not depend on the actual values of the spectrum and is decreasing with  $\ell$ . It underlines the uncertainty of statistical methods associated with the estimation of either the spectrum or the covariance function. Therefore reducing the cosmic variance is of primary importance.

How to decrease the influence of the cosmic variance? Since the main contribution to that variance comes from  $f_\ell$  with small values of  $\ell$ , we should try to ignore these  $f_\ell$  by truncating the difference  $R = \widehat{\mathcal{C}}(\cos \gamma) - \mathcal{C}(\cos \gamma)$ , given in (4.1) and (4.2).

Consider then the case when  $f_\ell = 0$ ,  $\ell = 0, 1, \dots, M - 1$ , in  $R$ , see (4.5), i.e. the remainder

$$R_M = \frac{1}{4\pi} \sum_{\ell=M}^{\infty} (2\ell + 1) f_\ell P_\ell(\cos \gamma) \left( \frac{U_{2\ell+1}}{2\ell + 1} - 1 \right),$$

where the sum starts at  $\ell = M$ . Since  $R_M$  is associated to the sample path  $T_M(x)$  defined as

$$T_M(x) = T(x) - \sum_{\ell=0}^{M-1} \sum_{m=-\ell}^{\ell} \widehat{a}_{\ell m} Y_\ell^m(x), \quad (5.2)$$

and since  $\widehat{a}_{\ell m}$  are good approximations of the current values which are generating the observed random field  $T(x)$ , see (2.2), (not like the estimation of  $f_\ell$ ), therefore  $T_M(x)$  is a good approximation to the remainder field with  $f_\ell = 0$ ,  $\ell = 0, 1, \dots, M - 1$ , and with covariance function

$$\mathcal{C}_M(\cos \gamma) = \mathcal{C}(\cos \gamma) - \frac{1}{4\pi} \sum_{\ell=0}^{M-1} f_\ell (2\ell + 1) P_\ell(\cos \gamma).$$

The asymptotic distribution and Berry–Esseen bound for the remainder  $R_M$  given in the next Theorem can be obtained as in Theorem 3.1 of [61].

**Theorem 5.1.** *Let*

$$\sigma_M^2 = \frac{2}{(4\pi)^2} \sum_{\ell=M}^{\infty} (2\ell + 1) f_\ell^2 P_\ell^2(\cos \gamma),$$

*then  $R_M/\sigma_M$  is asymptotically standard normal distributed as  $M \rightarrow \infty$ . In addition there is a Berry–Esseen bound*

$$\sup_{x \in \mathbb{R}} |P(R_M/\sigma_M \leq x) - \Phi(x)| \leq 0.7056\kappa_{3,M},$$

where  $\Phi$  is the standard normal CDF, and  $\kappa_{3,M}$  denotes the third cumulant (skewness) of  $R_M$

$$\kappa_{3,M} = \frac{1}{(2\pi)^3 \sigma_M^3} \sum_{\ell=M}^{\infty} (2\ell + 1) f_{\ell}^3 P_{\ell}^3(\cos \gamma).$$

*Proof.* The theorem follows from the Theorem 3.1 of [61], provided one has

$$\frac{\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^3}{r_{\ell}^2}}{\left(\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^2}{r_{\ell}}\right)^{3/2}} \rightarrow 0, \text{ as } M \rightarrow \infty,$$

where  $\lambda_{\ell}$  and  $r_{\ell}$  are defined in (4.7). Consider

$$\begin{aligned} \frac{\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^3}{r_{\ell}^2}}{\left(\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^2}{r_{\ell}}\right)^{3/2}} &= \frac{\sqrt{2} \sum_{\ell=M}^{\infty} (2\ell + 1)^{-1/2} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^3}{\left(\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2\right)^{3/2}} \\ &< \frac{\sqrt{2}}{\sqrt{2M + 1}} \frac{\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^3}{\left(\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2\right)^{3/2}}. \end{aligned}$$

The series  $\sum_{\ell=0}^{\infty} (2\ell + 1) f_{\ell}^2 P_{\ell}^2(\cos \gamma)$  converges by (4.8) hence  $\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2 < 1$ , if  $M$  sufficiently large, therefore

$$\left(\frac{\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^3}{\left(\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2\right)^{3/2}}\right)^{2/3} \leq \frac{\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2}{\sum_{\ell=M}^{\infty} (\sqrt{2\ell + 1} f_{\ell} P_{\ell}(\cos \gamma))^2} = 1,$$

where in the nominator we applied the inequality  $(x + y)^a \leq x^a + y^a$ . valid for any  $0 \leq x, y \leq 1$ , and any  $0 < a < 1$ . Summarizing these we obtain

$$\left(\frac{\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^3}{r_{\ell}^2}}{\left(\sum_{\ell=M}^{\infty} \frac{\lambda_{\ell}^2}{r_{\ell}}\right)^{3/2}}\right)^{2/3} \leq \left(\frac{\sqrt{2}}{\sqrt{2M + 1}}\right)^{2/3} \rightarrow 0, \text{ as } M \rightarrow \infty. \quad \square$$

Edgeworth expansion for the distribution function of  $R_M$  is also given in [61] and the assumptions are satisfied in our case as well. We will not include them here. Our simulation and the numerical example of [61] show that the speed of convergence is really fast and  $M$  can be chosen to be larger than 5, which is satisfactory for cosmology ([64], p. 138) and as we shall see in the next section our estimator of the covariance function gives very good results even when  $M = 4$ . An earlier attempt in this direction has been made in [8].

## 6. Simulations

When dealing in practice with random fields, we do not use for  $\widehat{\mathcal{C}}(\cos \gamma)$  its expression (3.1) or equivalently (3.2) instead we use a discretization of integral (3.1), namely (6.2) below, which corresponds to the time domain estimator of covariances in time series analysis. We consider a discretized unit sphere  $\mathbb{S}_2$ . The discretization, called HEALPix (Hierarchical, Equal Area and iso Latitude Pixelization), is applied. For a detailed description see [27]. This pixelization of the sphere contains quadrilaterals (pixels), in our case the total number of equal-area spherical pixels equals to  $N_{pix} = 49152$ , with area  $\Omega_{pix} = 4\pi/N_{pix}$ , since  $4\pi$  is the surface of the unit sphere.

The integral for fixed angle  $\gamma$

$$\widehat{\mathcal{C}}(\cos \gamma) = \int_{\mathbb{S}_2} \int_{C(x,\gamma)} T(x) T(x_\gamma(\varphi, x)) \frac{d\varphi}{2\pi} \frac{\Omega(dx)}{4\pi},$$

is discretized, as follows

$$\int_{C(x,\gamma)} T(x) T(x_\gamma(\varphi, x)) \frac{d\varphi}{2\pi} \sim \frac{1}{n_x} (T(x) - \bar{T}) \sum_{x \cdot x_j = \cos \gamma} (T(x_j) - \bar{T}), \quad (6.1)$$

where  $x_j$  denote locations of pixel centers,  $\bar{T} = (1/N_{pix}) \sum_x T(x)$ , is the mean and  $n_x$  is the number of all possible pairs of  $x$  and  $x_j$ , such that  $x \cdot x_j = \cos \gamma$ . Hence the covariance estimator is

$$\widehat{\mathcal{C}}(\cos \gamma) = \frac{1}{N_{pix}} \sum_i \frac{1}{n_{x_i}} \sum_{j: x_i \cdot x_j = \cos \gamma} (T(x_i) - \bar{T}) (T(x_j) - \bar{T}). \quad (6.2)$$

Since  $\gamma$  is the angular distance and for a given location  $x$  all the locations with angular distance  $\gamma$  constitute a circle, in practice instead of a circle we considered a ring with a very narrow belt so that (6.1) contains all the pixel centers from this belt. The reason is that the pixel structure provides some specific angular distances only and we collect all the pixel centers having angular distance close enough to  $\gamma$ . One may consult with [4], [33] for properties of the above approximation.

From now on we shall scale the covariance function such that  $\mathcal{C}(\cos 0) = \mathcal{C}(1) = 1$  resulting in the correlation function. We do so because the parameter estimation requires that there be a unique correspondence between the model and its parameters. Thus no multiplicative constant will appear in the parameter estimation.

For simulation purposes, following (2.1), we generated a truncated field

$$T_{(K)}(x) = \sum_{\ell=0}^K \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell}^m(x), \quad (6.3)$$

where  $K = 42$ , and  $a_{\ell m}$ ,  $\ell = 0, 1, 2, \dots, K$ ,  $m = 0, \pm 1, \pm 2, \dots, \pm \ell$ , complex-valued Gaussian random numbers  $\mathbb{E}a_{\ell m} = 0$ ,  $\mathbb{E}a_{\ell m} a_{kn}^* = f_{\ell} \delta_{\ell, k} \delta_{m, n}$ , such

that  $a_{\ell,-m} = (-1)^m a_{\ell m}^*$ . The spectrum  $f_\ell$ ,  $\ell = 0, 1, 2, \dots, K$ , is calculated using the Laplace-Beltrami model (Example 2.1), with parameters  $\sigma^2 = 2$ ,  $c = 2$ . We get  $f_\ell$  by applying (2.7).

For all pixel centers  $x_i$  on the sphere we generated the field  $T_{(K)}(x_i)$ ,  $i = 1, 2, \dots, N_{pix}$  using (6.3).

Now we consider the covariance function of the model with the values of  $f_\ell$  truncated up to  $L$ ,

$$\mathcal{C}_{(L)}(\cos \gamma) = \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} f_\ell P_\ell(\cos \gamma), \quad \gamma \in [0, \pi], \tag{6.4}$$

and we are going to estimate  $\mathcal{C}_{(L)}(\cos \gamma)$  using  $T_{(K)}(x)$ . The correspondence between the function  $\mathcal{C}_{(L)}(\cos \gamma)$  and the spectrum  $\{f_\ell\}_0^L$  is given by the integral

$$\begin{aligned} f_\ell &= 2\pi \int_0^\pi \mathcal{C}_{(L)}(\cos \gamma) P_\ell(\cos \gamma) \sin \gamma d\gamma \\ &= 2\pi \int_{-1}^1 \mathcal{C}_{(L)}(y) P_\ell(y) dy. \end{aligned} \tag{6.5}$$

The exact value of that integral can be calculated via the Gauss-Legendre quadrature, as follows

$$f_\ell = 2\pi \sum_{i=1}^{L+1} w_i \mathcal{C}_{(L)}(y_i) P_\ell(y_i), \tag{6.6}$$

where the nodes  $y_1, \dots, y_{L+1}$  are the roots of the Legendre polynomial  $P_{L+1}(x)$ , while  $w_1, \dots, w_{L+1}$  are the corresponding weights of the formula. In this case the quadrature is exact for polynomials up to order  $2L + 1$ , [44], [56]. Note that the order (highest degree of the polynomial) of  $\mathcal{C}_{(L)}(y) P_\ell(y)$  is not larger than  $2L$ , for any  $\ell$ .

Given real data,  $L$  is not known, one chooses  $L$  and  $L + 1$  angles  $\gamma_1, \dots, \gamma_{L+1}$ , with  $L$  large enough so as to ensure that the estimator  $\widehat{\mathcal{C}}(\cos \gamma)$  in (6.2) provides good results. The number of terms in the second summation of (6.2) depends on the angular distance and if this number of terms is too small, one may end up with a bad estimate for  $\mathcal{C}(\cos \gamma)$ . The number  $L$  can therefore be considered as a bandwidth in this estimation. We used here angles  $\gamma_1, \dots, \gamma_{L+1}$  corresponding to the roots of the Legendre polynomial  $P_{L+1}(x)$ . Here we set  $L = 42$ .

After estimating the covariance function  $\mathcal{C}_{(L)}(\cos \gamma_i) = \mathcal{C}_{(L)}(y_i)$  via (6.2), one can then estimate the spectrum  $f_\ell$  by

$$\widehat{f}_\ell = 2\pi \sum_{i=1}^{L+1} w_i \widehat{\mathcal{C}}(y_i) P_\ell(y_i), \tag{6.7}$$

namely, by replacing  $\mathcal{C}_{(L)}$  in (6.6) by  $\widehat{\mathcal{C}}(y_i)$  obtained by using (6.2).

The Laplace-Beltrami model with given  $\sigma^2$  depends on an unknown parameter  $c$ , see Example 2.1 and has spectrum  $f_\ell(c)$  given in (2.7). We estimated the parameter  $c$  in two steps.

First we used the estimated covariance function  $\widehat{C}(\cos \gamma)$  in (6.2) to estimate the spectra  $\widehat{f}_\ell$  by (6.7). Then we fitted  $f_\ell = f_\ell(c)$  to  $\widehat{f}_\ell$ ,  $\ell = 1, 2, \dots, L = 42$ , by the nonlinear least squares method, i.e. minimizing the

$$\sum_{\ell=1}^{42} \left( f_\ell(c) - \widehat{f}_\ell \right)^2, \quad (6.8)$$

and derived the estimate  $\widehat{c}$ .

Secondly, we obtained  $\widehat{c}_M$  with  $M = 4$ , in order to reduce the cosmic variance. To do so we estimate  $\widehat{a}_{\ell m}$  from  $T_{(K)}(x)$  and remove the corresponding terms by

$$T_{(K,4)}(x) = T_{(K)}(x) - \sum_{\ell=0}^4 \sum_{m=-\ell}^{\ell} \widehat{a}_{\ell m} Y_\ell^m(x).$$

We get a new model where  $a_{\ell m} = 0$ ,  $\ell = 0, 1, 2, 3$ ,  $m = 0, \pm 1, \pm 2, \dots, \pm \ell$ , without modifying the other  $a_{\ell m}$ . This yields the sample path with spectrum  $f_\ell(c) = 0$ ,  $\ell = 0, 1, 2, 3$ . Now we re-estimated the correlations  $\widehat{C}(\cos \gamma_k)$  in (6.2) replacing the field  $T$  by  $T_{(K,4)}$ . We obtain a far better estimate of  $c$  because the cosmic variance has been reduced, setting its values corresponding to  $\ell = 0, 1, 2, 3$ , to zero. To get  $\widehat{c}_M$ , we repeated the least squares estimation by setting  $f_\ell = 0$ , for  $\ell = 0, 1, 2, 3$ , and  $f_\ell = f_\ell(\widehat{c}_M)$ , for  $\ell = M, M + 1, \dots, 42$ . Putting the estimated value  $\widehat{c}_M$  in (2.7) we get new values  $f_\ell(\widehat{c}_M)$ ,  $\ell = 0, 1, 2, \dots, L$ . We use them in (6.4) to obtain a new estimated  $\widehat{C}(\cos \gamma)$ .

We did 100 iterations. In each iteration we computed  $\widehat{c}$  and  $\widehat{c}_M$ , then  $\widehat{f}_\ell$  using (2.7) and then the corresponding estimated covariance curve using (6.4). The results then were averaged including the covariance curves. Note that the displayed Figures 2, 3, 4 have different vertical scales.

The true value of  $c$  was 2 and the average of  $\widehat{c}$  over 100 iterations was 1.1866 with standard deviation 0.5329, while the average of  $\widehat{c}_M$  was 1.8063 with standard deviation 1.3672. The average of  $\widehat{c}_M$  is closer to the true value than the average of  $\widehat{c}$  though variance.

The plot in Figure 2 contains from top to bottom the following covariance functions obtained as follows:

- (a) estimated using (6.4) with  $\widehat{c}$ ,
- (b) estimated using (6.4) with  $\widehat{c}_M$ ,
- (c) theoretical using (6.4) with  $c = 2$ ,
- (d) estimated using (6.2).

Note that the curve (b) using  $\widehat{c}_M$  is the closest to the theoretical one (c).<sup>2</sup>

<sup>2</sup>Removing the sample mean from the data in (6.1) results in removing  $a_{00}Y_0^0$ . Hence the estimated covariance function does not contain  $f_0$ , that is  $\widehat{f}_0 = 0$ . It is true that  $a_{00}Y_0^0$  is

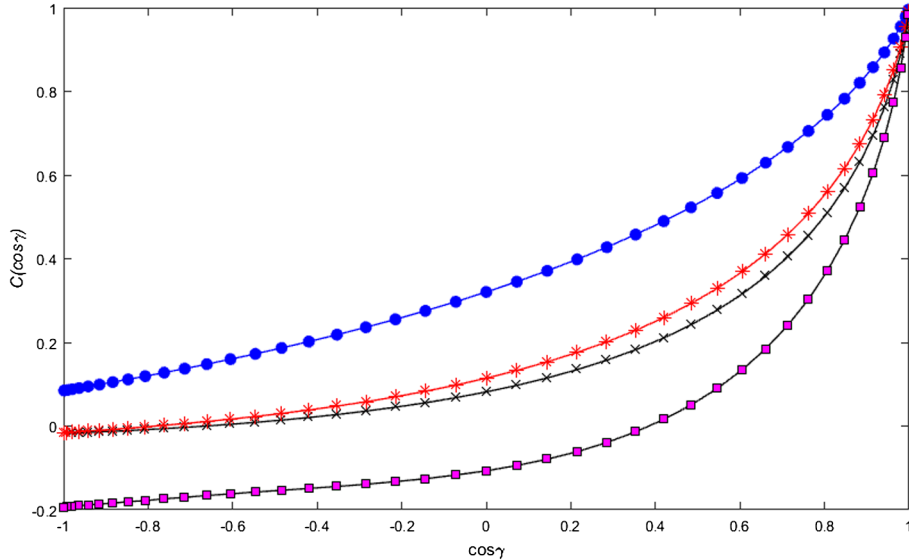


FIG 2. Correlation functions from top to bottom: (a) using (6.4) with  $\hat{c}$ ; (b) using (6.4) with  $\hat{c}_M$ ; (c) theoretical using (6.4); (d) estimated using (6.2).

The plot in Figure 3 shows the theoretical covariance function (continuous blue line with asterisks, computed from the spectrum (2.7) of the Laplace-Beltrami model using (6.4)), the average of the 100 estimations of the covariances  $\hat{C}(\cos \gamma_k)$  (red dashed line with circles), upper and lower 95% confidence intervals (red dashed line with asterisks), each of the 100 estimations  $\hat{C}(\cos \gamma_k)$  (black points). It is seen that even the average of 100 estimations is not a good estimate of the covariance function mainly because of the cosmic variance. We obtain better results using  $\hat{c}$  as seen in Figure 4.

We conclude from Figure 4 that using the model  $T_{(K,4)}(x)$  with reduced cosmic variance gives good estimates for the corresponding correlation function. As a consequence the updated estimate of the original covariance function by  $\hat{c}_M$  provides a better estimator not only for the covariance function but for the spectrum as well. Figure 2 yields the same conclusion.

**Remark 6.1.** *Figure 2 is unsurprising: It is intuitive that the covariance curve based on the correct model with a good parameter estimate is closer than a non-parametric alternative. In a sense here the message is more about the comparison of using  $\hat{c}$  vs.  $\hat{c}_M$ . Note that a comparison of Figures 3 and 4 yields information on the quality of the estimators  $\hat{c}$  vs.  $\hat{c}_M$ . In both cases, different models (with different covariance functions) are assumed and the Figures show that it is easier to estimate the covariance function if low frequencies of the spectrum are zero.*

random and not a constant, since  $a_{00}$  is Gaussian, but for real data we have only a single realization which means that we have a single value of a Gaussian variable. Thus, after estimating  $\hat{c}$  we added  $f_0(\hat{c})$  to (6.4). In other words we proceeded as in the estimation of  $\hat{c}_M$  but for  $M = 0$ .

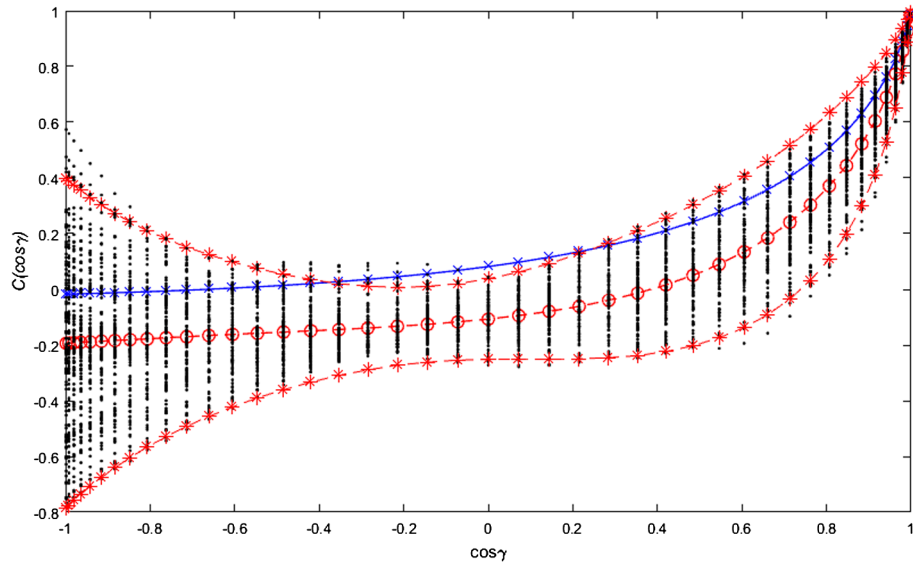


FIG 3. Listed from the middle ( $\cos \gamma = 0$ ), from top to bottom: theoretical (6.4) with  $c = 2$ ; upper confidence curve, estimated (6.2), lower confidence curve. The vertical dots are the results of the individual simulations from 1 to 100.

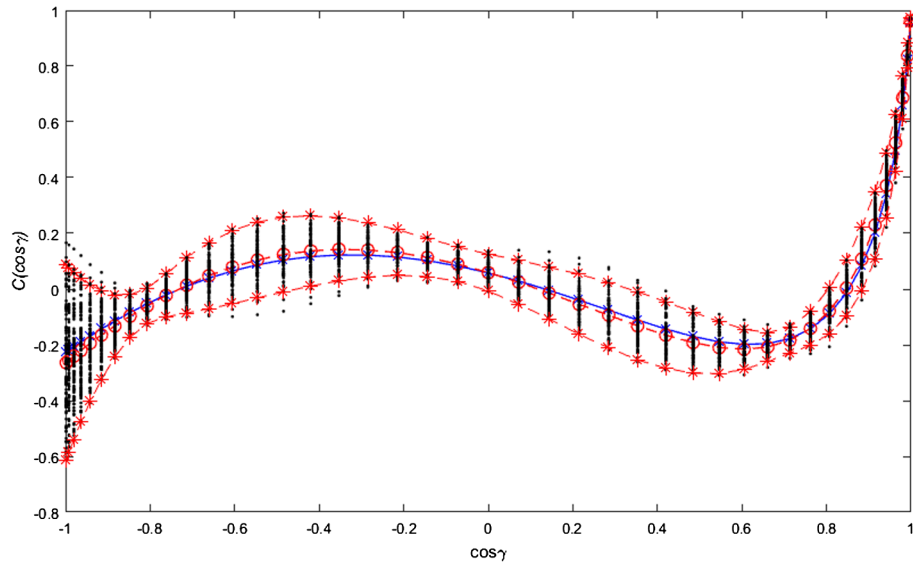


FIG 4. Estimation of the correlation function when  $f_\ell = 0$ ,  $\ell = 0, 1, 2, 3$ . The estimated (6.2) is closed to the theoretical. The vertical dots are the results of the individual simulations from 1 to 100.

## 7. Conclusion

We considered the problem of estimating the covariance function of an isotropic field on the sphere, at a fixed time as is the case of CMB data for instance. We derived the distributional properties of the nonparametric estimator of the covariance function.

The problem of estimating either the correlation function or the spectrum for the CMB data has a wide literature [18]. Most of the methods considered, like Pseudo- $C_\ell$  estimators, NRML (maximum-likelihood using Newton–Raphson algorithm), QML (quadratic ML) hybrid estimator, suffer from cosmic variance. The paper [19] considers estimates of the correlation function based on methods used in [18] paying attention to the cosmic variance as well. The aim of those investigations include checking Gaussianity, isotropy, modeling using six-parameter inflationary CDM cosmology etc. There is a common agreement that “the analytic approximations at low multipoles are useless for any quantitative application such as parameter estimation“ ([18]). One of our aims was to reduce the cosmic variance in parametric models.

Theorems 3.2, 4.1 and 5.1 are connected. They describe and quantify the distribution of errors between the empirical covariance and the theoretical covariance function of spherical random fields. Theorem 5.1 is of interest in statistical inference since it quantifies the errors of approximation after truncation. It is known that the cosmic variance prevents us to getting a good estimator mainly because of the problem of estimating the spectrum  $f_\ell$  at low frequencies,  $\ell = 0, 1, \dots, M-1$ , say. Since the cosmic variance affects mainly the spectral coefficients  $f_\ell$  at low values of  $\ell$ , we ignore these  $f_\ell$  setting them to 0. We then reestimate the covariance function and use it to estimate the unknown parameters of our parametric model, for example, the parameter  $c$  in the Laplace-Beltrami model.

The steps described above change the model, but this modified model now provides better estimates of the covariance hence, better estimation of the spectrum and the unknown parameters. Using these estimated parameters we estimate  $f_\ell$  for a low  $\ell$  as well.

We carried out simulations for a Laplace-Beltrami model. In practice when a set of observations is given, we have to decide how to choose the level of truncation which we denoted by  $L$ . The truncation parameter  $L$  depends on the number of observations and is connected to the number of angles  $\gamma$  where  $C(\cos \gamma)$  will be estimated. We used the Gauss-Legendre quadrature for calculating the spectrum from the covariance and vice versa. It involves  $L+1$  angles, actually the roots of the Legendre polynomial  $P_{L+1}(x)$ . We chose the method of nonlinear least squares for estimation of the parameters  $c$  from the estimated spectra  $f_\ell(c)$ . Other methods like weighted least squares, MCMC and likelihood and noisy data are the subject of further investigations.

## Appendix A: Examples

The following are examples of homogenous and isotropic random field  $T_0(x)$ ,  $x \in \mathbb{R}^3$  restricted to the sphere  $\mathbb{S}_2$ . Then the covariance function  $\mathcal{C}(r)$  of the

stochastic field  $T(x)$  on the sphere  $\mathbb{S}_2$  equals the covariance function  $\mathcal{C}_0(r)$  of the original field  $T_0$  restricted to the sphere. At the same time the power spectrum  $f_\ell$  of the field  $T(x)$  is defined by the power spectrum of the field  $T_0(x)$  through a formula (A.1) called Poisson formula, see [55], VII. 2.

**Example A.1.** For an homogeneous isotropic random field on  $\mathbb{R}^3$  we have the spectral representation

$$\mathcal{C}_0(r) = \int_0^\infty j_0(\lambda r) \Phi(d\lambda),$$

of the covariance function, where  $\Phi(d\lambda)$  is some spectral measure, see [66], and where  $j_m$  is the Spherical Bessel function of the first kind,  $j_0(r) = \sin r/r$ , see [2]. If we consider two locations  $x_1$  and  $x_2$  on the sphere  $\mathbb{S}_2$  with angle  $\gamma \in [0, \pi]$ , then we obtain the covariance function  $C(\cos \gamma) = \mathcal{C}_0(2 \sin(\gamma/2))$  on the sphere  $\mathbb{S}_2$  with spectrum

$$f_\ell = 2\pi^2 \int_0^\infty J_{\ell+1/2}^2(\lambda) \frac{1}{\lambda} \Phi(d\lambda), \quad (\text{A.1})$$

where  $J_{\ell+1/2}$  denotes the Bessel function of the first kind, see [2]. More generally, in case of  $\mathbb{R}^d$ ,  $d \geq 3$ ,

$$\mathcal{C}_0(r) = \int_0^\infty j_{(d-3)/2}(\lambda r) \Phi(d\lambda),$$

and the corresponding spectrum on the sphere is

$$f_\ell = c_d^2 \int_0^\infty J_{\ell+(d-2)/2}^2(\lambda) \frac{1}{\lambda^{d-2}} \Phi(d\lambda).$$

**Example A.2. Laplace model restricted to the sphere.** The following covariance function corresponds to an homogeneous isotropic random field  $T$  on  $\mathbb{R}^d$  satisfying the equation

$$(\Delta - c^2)^\nu T = \partial W, \quad (\text{A.2})$$

in the  $L_2$  sense, where  $\Delta = \sum_{k=1}^d \frac{\partial^2}{\partial x_k^2}$ , denotes the Laplace operator on  $\mathbb{R}^d$ ,  $d \geq 3$ , and  $\partial W$  is the white noise in  $\mathbb{R}^d$ . The covariance function of spherical random field  $T(x)$ ,  $x \in \mathbb{S}_{d-1}$ , restriction of the homogeneous isotropic random field  $T(x)$ ,  $x \in \mathbb{R}^d$ , into the sphere  $\mathbb{S}_{d-1} = \{x \in \mathbb{R}^d; \|x\| = 1\}$ , is of the form

$$C(\cos \gamma) = \frac{\sigma^2}{(2\pi)^{\frac{d}{2}+1} 2^{2\nu-1} \Gamma(2\nu)} \left( \frac{2 \sin(\gamma/2)}{|c|} \right)^{2\nu-\frac{d}{2}} K_{2\nu-\frac{d}{2}}(2|c| \sin(\gamma/2)), \quad (\text{A.3})$$

where  $K_\nu$  is the modified Bessel (Hankel) function of the second kind. Here  $2\nu - \frac{d}{2} > 0$ , is the smoothness parameter which controls the continuity, and  $c$  controls the regularity [20], [54]. Note  $K_\nu(r) \sim \Gamma(\nu) (r/2)^{-\nu} / 2$  if  $r \rightarrow 0$ . The

correlation function on the sphere  $\mathbb{S}_{d-1}$  is

$$\rho(\cos \gamma) = \frac{(2|c|\sin(\gamma/2))^{2\nu-\frac{d}{2}}}{2^{2\nu-\frac{d}{2}-1}\Gamma(2\nu-\frac{d}{2})} K_{2\nu-\frac{d}{2}}(2|c|\sin(\gamma/2)).$$

The corresponding spectrum on  $\mathbb{S}_2$  is

$$f_\ell = 2\pi \int_0^\pi \mathcal{C}(\cos \gamma) P_\ell(\cos \gamma) \sin \gamma d\gamma.$$

Note that  $\mathcal{C}(\cos \gamma)$  belongs to the Matérn Class of Covariance Functions [42], [51]. Also in [32] one can find a proof of the form of the covariance function of Matern class from the fractional Helmholtz equation based on the theory of generalized random fields [21]. In particular for  $\nu = 1, d = 3$ , we have

$$\mathcal{C}(\cos \gamma) = \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{\sin(\gamma/2)}{2|c|}} K_{1/2}(2|c|\sin(\gamma/2)).$$

with spectrum

$$f_\ell = \int_0^\infty J_{\ell+1/2}^2(\lambda) \frac{\lambda}{(\lambda^2 + c^2)^2} d\lambda.$$

Since  $K_{1/2}(r) = \sqrt{\pi/2r}e^{-r}$ , we have

$$\mathcal{C}(\cos \gamma) = \frac{1}{8\pi|c|} e^{-2|c|\sin(\gamma/2)},$$

and the spectrum is

$$f_\ell = \frac{1}{4|c|} \int_0^\pi e^{-2|c|\sin(\gamma/2)} P_\ell(\cos \gamma) \sin \gamma d\gamma.$$

The preceding example treated an homogeneous isotropic random field on  $\mathbb{R}^d$  and then specialized it to the sphere. Another possible construction of covariance functions is based on the following. The covariance function  $\mathcal{C}_2(x_1 \cdot x_2)$  in (2.3) is strictly positive definite if all  $f_\ell$  are  $\geq 0$ , and only finitely many of them are zero ([53], [52]). Therefore if the series (2.3) is finite and only finitely many  $f_\ell = 0$ , then one can construct a Gaussian field with covariance function  $\mathcal{C}(\cos \gamma)$  which is nonnegative definite, see Remark 2.1 also. In the case where finitely many  $f_\ell > 0$ , then  $\mathcal{C}(\cos \gamma)$  is still nonnegative definite but will not be necessarily strictly positive.

**Example A.3.** The generating function of the Legendre polynomial  $P_\ell$  is

$$\sum_{\ell=0}^\infty P_\ell(y) z^\ell = (1 - 2yz + z^2)^{-1/2}, \quad y \in (-1, 1), |z| < 1. \quad (\text{A.4})$$

Let  $z$  be a fixed value ( $0 < z < 1$ ),  $\sigma^2 > 0$ , put  $y = \cos \gamma$  and

$$f_\ell = \frac{4\pi}{2\ell + 1} z^\ell,$$

then  $f_\ell > 0$ , for all  $\ell$  and from (2.3) follows that

$$\mathcal{C}(\cos \gamma) = \frac{\sigma^2}{\sqrt{1 - 2z \cos \gamma + z^2}},$$

is a covariance function. Similarly, using Gegenbauer polynomials  $C_\ell^{(d-2)/2}$  instead of  $P_\ell$  in (A.4), for any dimension  $d > 2$  we have a covariance function on  $\mathbb{S}_{d-1}$

$$\mathcal{C}(\cos \gamma) = \frac{\sigma^2}{(1 - 2z \cos \gamma + z^2)^{(d-2)/2}},$$

if  $0 < z < 1$ , (see [66]). Since it is positive definite it can be considered as a covariance function on  $\mathbb{S}_2$ , in this case the spectrum  $f_\ell$  is not given by some explicit formula. Some more examples of this type can be constructed applying formulae of series of Legendre polynomials with positive coefficients.

There is an other application of series of Legendre polynomials in probability theory, namely in directional statistics. A probability density of a rotational symmetric distribution on the sphere has a series expansion in terms of Legendre polynomials, see [45], [38]. Now if the coefficients (actually the characteristic function of the distribution) of the series expansion are positive then the same function may also serve as a covariance function. The following example is one of the basic density on the sphere.

**Example A.4.** The Fisher probability density function  $f$  on the sphere (see [45], [38], [10], [63]) is defined by

$$f(\cos \gamma) = \frac{\kappa}{4\pi \sinh(\kappa)} \exp(\kappa \cos \gamma), \quad \kappa > 0.$$

This probability density function can be considered as a covariance function. It has the series expansion

$$f(\cos \gamma) = \frac{\kappa}{\sinh(\kappa)} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \sqrt{\frac{\pi}{2\kappa}} I_{\ell+1/2}(\kappa) P_\ell(\cos \gamma),$$

where  $\sqrt{\frac{\pi}{2\kappa}} I_{\ell+1/2}(\kappa)$  is the modified spherical Bessel function of the first kind, [2]. Hence

$$\mathcal{C}(\cos \gamma) = \sigma^2 f(\cos \gamma),$$

is a covariance function with spectrum

$$f_\ell = \sigma^2 \frac{\kappa}{\sinh(\kappa)} \sqrt{\frac{\pi}{2\kappa}} I_{\ell+1/2}(\kappa) = \sigma^2 \frac{I_{\ell+1/2}(\kappa)}{I_{1/2}(\kappa)}.$$

Note  $\sinh(\kappa)/\kappa = \sqrt{\frac{\pi}{2\kappa}} I_{1/2}(\kappa)$ . We have  $I_{\ell+1/2}(\kappa) > 0$ , for all  $\ell$  see [1] §10.25(ii), 10.25.2, therefore  $f_\ell$  is a valid spectrum with strictly positive covariance function, see Remark 2.1.

The variance  $\sigma^2$  in these examples corresponds usually to some additional noise fields on top of the homogeneous isotropic field considered here. Since it is

a multiplicative constant, it will not influence our results and therefore we will set  $\sigma^2 = 1$  from now on.

**Appendix B: White noise analysis on the sphere**

Here we outline a way to make precise the derivation of the spectrum given in Example 2.1. Details will appear in a forthcoming paper. Recall the notations  $x \in \mathbb{S}_2$ ,  $x(\vartheta, \varphi) = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta)$ ,  $\Omega(dx) = \sin \vartheta d\vartheta d\varphi$ .

**Definition 1.** Let  $W_B = \{W_B(f), f \in L_2(\mathbb{S}_2, \Omega(dx))\}$ , be a generalized random field on the sphere  $\mathbb{S}_2 \subset \mathbb{R}^3$ . Then,  $W_B$  defines a white noise process on the sphere if

$$\langle f \cdot g \rangle_{L_2(\mathbb{S}_2, \Omega(dx))} = \langle W_B(f), W_B(g) \rangle_{\mathcal{L}^2(\Omega, \mathcal{A}, \mathcal{P})}.$$

Thus, the induced white noise measure  $\partial W_B$  satisfies

$$\mathbb{E} \partial W_B(x) \partial W_B(x') = \delta(x - x') \Omega(dx).$$

Now consider  $L_2(\mathbb{S}_2, \Omega(dx))$ , and the space  $H(W_B)$ , subspace of  $\mathcal{L}^2(\Omega, \mathcal{A}, \mathcal{P})$  defined as the closed span in  $\mathcal{L}^2(\Omega, \mathcal{A}, \mathcal{P})$  of  $\{W_B(f), f \in L_2(\mathbb{S}_2, \Omega(dx))\}$ . The following isometry

$$\mathcal{I} : L_2(\mathbb{S}_2, \Omega(dx)) \rightarrow H(W_B); \mathcal{I}(f) \rightarrow W_B(f), \forall f \in L_2(\mathbb{S}_2, \Omega(dx)),$$

holds between the spaces  $L_2(\mathbb{S}_2, \Omega(dx))$ , and the space  $H(W_B)$ , with

$$\langle f \cdot g \rangle_{L_2(\mathbb{S}_2, \Omega(dx))} = \langle W_B(f), W_B(g) \rangle_{\mathcal{L}^2(\Omega, \mathcal{A}, \mathcal{P})}.$$

Thus, the Reproducing Kernel Hilbert space (RKHS) of the generalized random field  $W$  can be isometrically identified with the space  $L_2(\mathbb{S}_2, \Omega(dx))$ . This corresponds to the notion of white noise in Hilbert spaces (e.g., in the sense of generalized functions, see [24]). In the Gaussian case, we have the Wiener measure on the sphere, as an example of generalized Gaussian white noise on the sphere.

Following the line of the papers [3], [32] one can obtain the angular spectrum in Example 2.1, by using the theory of generalized random fields, see [24], and also some ideas are already introduced in [21]. We can construct fractional generalized random fields in the sphere, following the methodology of the papers [32], [49], by using the covariance factorization which follows from the Karhunen-Loève representation. Using the isomorphism between the fractional Sobolev spaces related to the sphere [21] and the corresponding RKHSs of the fractional generalized spherical random fields, which is equivalent to the existence of the dual random field, one can define the solution to the fractional elliptic pseudo-differential equation on the sphere in a weak sense. Moreover, under some conditions on the non-local fractional order pseudo-differential equations, using embedding of fractional Sobolev spaces into the Hölder space related to the sphere [21], one can define the solution in the strong sense, by using the

following integral representation valid in the mean square sense of generalized random fields on the sphere:

$$T(f) \underset{m.s.}{=} \int_{\mathbb{S}_2} f(x) T(x) \Omega(dx),$$

where  $T(x)$  is an ordinary random field on the sphere.

### Appendix C: Thorin class and measure

We next define the Thorin class on  $R$  (see [59]; [9], [30]) as follows: We refer to  $\gamma x$  as an elementary gamma random variable if  $x$  is nonrandom non-zero vector in  $R$ , and  $\gamma$  is a gamma random variable on  $R_+$ . Then, the Thorin class on  $R$  (or the class of extended generalized gamma convolutions), denoted by  $T(R)$ , is defined as the smallest class of distributions that contains all elementary gamma distributions on  $R$ , and is closed under convolution and weak convergence. It is known that  $T(R) \subset SD(R) \subset ID(R)$ , and inclusions are strict. Since any selfdecomposable distribution on  $R$  is absolutely continuous (see, for instance, Example 27.8 in [50]) and is unimodal (by [67]; see also Theorem 53.1 in [50]), then, any selfdecomposable distribution has a bounded density function.

If a probability distribution function  $F$  belongs to  $T(R)$ , then, its characteristic function has the form (see [59], [9])

$$\phi(\theta) = \exp\left(i\theta a - \frac{b\theta^2}{2} - \int_{\mathbb{R}} \left[ \log\left(1 - \frac{i\theta}{u}\right) + \frac{i\theta}{1+u^2} \right] U(du)\right), \quad (\text{C.1})$$

where  $a \in R$ ,  $b \geq 0$ , and  $U(du)$  is a non-decreasing measure on  $R \setminus \{0\}$ , called Thorin measure, such that

$$U(0) = 0, \quad \int_{-1}^1 |\log|u|| U(du) < \infty, \quad \int_{-\infty}^{-1} \frac{1}{u^2} U(du) + \int_1^{\infty} \frac{1}{u^2} U(du) < \infty.$$

The Lévy density of a distribution from the Thorin class is such that

$$|u|q(u) = \begin{cases} \int_0^{\infty} \exp(-yu) U(dy), & u > 0 \\ \int_0^{\infty} \exp(yu) U(dy), & u < 0, \end{cases} \quad (\text{C.2})$$

where  $U(du)$  is the Thorin measure. In other words, the Lévy density is of the form  $h(|u|)/|u|$ , where  $h(|u|) = h_0(r)$ ,  $r \geq 0$ , is a completely monotone function over  $(0, \infty)$ .

### Appendix D: Some formulae

We list here some formulae used in the paper.

1. Let  $Z = X + iY$  be a complex Gaussian variate, then by definition  $X$  and  $Y$  are real independent Gaussian random variables with  $\text{Var } X = \text{Var } Y$ .

If  $\text{Var } Z = \sigma^2$ , then  $\text{Var } X = \sigma^2/2$ . Put  $\mathbb{E}Z = 0$ . The Hermite polynomial of degree 2 of two complex Gaussian variables  $Z_1$  and  $Z_2$ , say, is defined by  $H_2(Z_1, Z_2) = Z_1 Z_2^* - \text{cov}(Z_1, Z_2)$ . Let  $H_2(Z)$  denote  $H_2(Z, Z)$  for simplicity, i.e.  $H_2(Z) = |Z|^2 - \sigma^2 = X^2 - \sigma^2/2 + Y^2 - \sigma^2/2 = H_2(X) + H_2(Y)$ , in other words  $H_2(Z)$  is the sum of two independent real valued Hermite polynomial of degree 2. The variance of  $H_2(Z)$  is obtained as the sum of variances  $\text{Var } H_2(X) + \text{Var } H_2(Y) = 4\sigma^4/4 = \sigma^4$ . We have the higher order cumulants of Hermite polynomials (see [57], 1.4.3, Example 10), as follows,

$$\begin{aligned} \text{Cum}_k(H_2(Z)) &= \text{Cum}_k(H_2(X) + H_2(Y)) \\ &= 2 * 2^{k-1} (k-1)! (\sigma^2/2)^k = (k-1)! \sigma^{2k}. \end{aligned} \tag{D.1}$$

In case  $Z$  is real-valued we have

$$\text{Cum}_k(H_2(Y)) = 2^{k-1} (k-1)! \sigma^{2k}. \tag{D.2}$$

2. Integral using Haar measure

$$\frac{1}{4\pi} \int_{\mathbb{S}_2} U(x) \Omega(dx) = \int_{SO(3)} U(gN) dg, \tag{D.3}$$

where  $\Omega(dx) = \sin \vartheta d\vartheta d\varphi$  is the Lebesgue element of the surface area on  $\mathbb{S}_2$  and

$$dg = \sin \vartheta d\vartheta d\varphi d\gamma / 8\pi^2,$$

is the Haar measure. [55] I.4.14.

3. Wigner D-matrix. For a rotation  $g \in SO(3)$ , let  $\Lambda(g) Y_\ell^m(x) = Y_\ell^m(g^{-1}x)$ , then

$$\Lambda(g) Y_\ell^m(x) = \sum_{k=-\ell}^{\ell} D_{k,m}^{(\ell)}(g) Y_\ell^k(x), \tag{D.4}$$

and

$$\int_{SO(3)} D_{m_1,k_1}^{(\ell_1)*} D_{m_2,k_2}^{(\ell_2)} dg = \delta_{\ell_1,\ell_2} \delta_{m_1,m_2} \delta_{k_1,k_2} \frac{1}{2\ell_1 + 1}. \tag{D.5}$$

see [60], 4.11.1.

4. Standardized Legendre polynomial  $P_0(x) = 1$ ,

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell (x^2 - 1)^\ell}{dx^\ell}, \quad x \in [-1, 1], \tag{D.6}$$

$P_\ell(1) = 1$ .

5. Orthonormal spherical harmonics with complex values  $Y_\ell^m(\vartheta, \varphi)$ ,  $\ell = 0, 1, 2, \dots$ ,  $m = -\ell, -\ell + 1, \dots, -1, 0, 1, \dots, \ell - 1, \ell$  of degree  $\ell$  and order  $m$  (rank  $\ell$  and projection  $m$ ). They satisfy

$$\int_0^\pi d\vartheta \int_0^{2\pi} d\varphi Y_\ell^m(\vartheta, \varphi) Y_{\ell'}^{m'}(\vartheta, \varphi)^* = \delta_{\ell,\ell'} \delta_{m,m'},$$

and are defined as

$$Y_\ell^m(\vartheta, \varphi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(\cos \vartheta) e^{im\varphi}, \quad \varphi \in [0, 2\pi], \vartheta \in [0, \pi], \quad (\text{D.7})$$

where  $P_\ell^m$  is the *associated normalized Legendre function of the first kind* (Gegenbauer polynomial at particular indices) of degree  $\ell$  and order  $m$ , defined by

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m P_\ell(x)}{dx^m},$$

$$P_\ell^{-m}(x) = (-1)^m \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} P_\ell^m(x).$$

Note that  $P_\ell = P_\ell^0$ . We have  $Y_\ell^m(\vartheta, \varphi)^* = (-1)^m Y_\ell^{-m}(\vartheta, \varphi)$ . In particular

$$Y_\ell^0(\vartheta, \varphi) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \vartheta),$$

$$Y_\ell^m(N) = \delta_{m,0} \sqrt{\frac{2\ell+1}{4\pi}}.$$

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