

Spectral Simulation of Isotropic Gaussian Random Fields on a Sphere

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Abstract A spectral algorithm is proposed to simulate an isotropic Gaussian random field on a sphere equipped with a geodesic metric. This algorithm supposes that the angular power spectrum of the covariance function is explicitly known. Direct analytic calculations are performed for exponential and linear covariance functions. In addition, three families of covariance functions are presented where the calculation of the angular power spectrum is simplified (shot-noise random fields, Yadrenko covariance functions and solutions of certain stochastic partial differential equations). Numerous illustrative examples are given.

Keywords Spherical harmonics · Angular power spectrum · Yadrenko covariance functions · Shot-noise random fields · Chentsov model

1 Introduction

In several domains of the geosciences (e.g., geodesy, paleomagnetism, climatology, and oceanology), data are supported by spheres. As the data are often spatially structured, it may be interesting to examine them using geostatistical methods. Compared to Euclidean space, a spherical space possesses two distinctive features. Firstly, a sphere is compact, which precludes any nonlocal form of ergodicity. Secondly, the group

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of motions used to define stationarity is the group of rotations, and this group is not commutative. This tends to make statistical inference, estimation and simulation more complicated (Marinucci and Peccati 2011).

This paper is devoted to the simulation of isotropic Gaussian random fields on a sphere. The statistical properties of such random fields are characterized by their mean and their covariance function. Their mean is constant, and their covariance at two points of the sphere does not depend explicitly on either point, but only on the geodesic distance between them. Whereas Porcu et al. (2018) refer to this property as geodesic isotropy, one can simply use isotropy for short.

The literature on the simulation of isotropic Gaussian random fields on a sphere is rather limited [Emery et al. (2018) and the references therein]. This probably stems from the fact that a simple algorithm based on a truncated Karhunen–Loève expansion of a Gaussian random field provides reasonably satisfactory simulations (Sect. 3). Among the most recent publications, let us mention the iterative algorithm proposed by Creasey and Lang (2018) to simulate Gauss–Markov random fields. They used a grid to benefit from FFT techniques. Emery et al. (2018) devised an ingenious construction to extend a Gaussian random field on a sphere to a (non-stationary) 3-dimensional random field that can be simulated using a turning bands algorithm. Additionally, recent publications by Lang and Schwab (2015), Clarke et al. (2018) clearly express a need for simulating Gaussian random fields on the sphere cross time.

In this paper, a novel algorithm is proposed to simulate Gaussian random fields using a spectral method, thus extending the work on spheres by Shinozuka and Jan (1972). This algorithm is continuous in the sense that it can assign a value at any point of the sphere from preliminarily simulated basic ingredients.

The paper is organized as follows. Section 2 gives some background on spherical harmonics and Schoenberg's theorem that characterizes isotropic covariance functions via their spectral measure (angular power spectrum). Section 3 presents a spectral algorithm along with numerous examples. To implement this algorithm, the spectral measure of the covariance function is required. It turns out that very little attention has been paid to its analytical determination [only the paper by Terdik (2015) was found in the literature]. Whereas direct calculations are sometimes possible (Appendix B), Sect. 4 considers three situations where an explicit assessment of the spectral measure could be considered (shot-noise random fields, Yadrenko covariance functions and solutions of certain stochastic partial differential equations).

2 Notation and Background on Spheres

Throughout this paper, the workspace is the unit sphere $\mathbb{S}^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$ centered at the origin, say o. Each point $x \in \mathbb{S}^2$ is specified by its polar coordinates (θ, ϕ) , namely its colatitude $0 \le \theta \le \pi$ and its longitude $0 \le \phi < 2\pi$. \mathbb{S}^2 is equipped with a metric that is the geodesic distance: the distance $\alpha(x, y)$ between points x and y is the angle separating both points when seen from the origin. Explicitly

$$\alpha(x, y) = \arccos(x \cdot y),$$



where $x \cdot y$ is the scalar product between vectors \overrightarrow{ox} and \overrightarrow{oy} . Let $\mathcal{B}(\mathbb{S}^2)$ be the Borel σ -algebra associated with the geodesic metric. On $(\mathbb{S}^2, \mathcal{B}(\mathbb{S}^2))$, a rotation invariant measure is defined

$$d\sigma(x) = d\sigma(\theta, \phi) = \sin\theta d\theta d\phi.$$

This measure is normalized in such a way that its integral over \mathbb{S}^2 is equal to 4π .

2.1 Spherical Harmonics

Acting on the sphere exactly like trigonometric functions on the unit circle, spherical harmonics are defined as

$$Y_{n,k}(\theta,\varphi) = \sqrt{\frac{2n+1}{4\pi} \frac{(n-k)!}{(n+k)!}} P_{n,k}(\cos\theta) e^{ik\varphi}.$$

In this formula, $n \ge 0$ is a degree, $-n \le k \le +n$ is an order, and $P_{n,k}$ are associated Legendre functions ("Appendix A"). A spherical harmonic is a complex-valued function that separates colatitudes and longitudes. When k = 0, $Y_{n,0}$ is proportional to the Legendre polynomial P_n . It may be surprising to represent a countable family of functions using a pair of indices. As a matter of fact, an order is introduced so that two harmonic functions with the same degree and opposite orders are complex conjugates, up to a possible change of sign

$$Y_{n,-k}(\theta,\varphi) = (-1)^k \, \bar{Y}_{n,k}(\theta,\varphi). \tag{1}$$

Figure 1 shows spherical harmonics (their real part) of degrees n=1,2,3 and orders k ranging from 0 to n. It can be noticed that their texture becomes more and more complicated as n increases (Fig. 2). For $k=0, Y_{n,0}(\theta,\phi)$ does not depend on ϕ , which explains the horizontal zonalities that are observed. When k=n, it can be shown that $Y_{n,n}(\theta,\phi)$ is proportional to $\sin^n\theta \ e^{in\phi}$. The dominant structure is the periodicity of the longitude, which gives rise to a sectorial structure. When k increases from 0 to n, the texture gradually evolves from zonal to sectorial.

Spherical harmonics satisfy three properties that are essential in this paper (Marinucci and Peccati 2011; Dym and McKean 2016).

Property 1 *Spherical harmonics form an orthonormal basis of the complex Hilbert space* $L^2(\mathbb{S}^2, \mathbb{C}, \sigma)$ *endowed with the inner product*

$$\langle f, g \rangle = \int_{\mathbb{S}^2} f(x) \, \bar{g}(x) \, d\sigma(x).$$

This means (i) that spherical harmonics are orthonormal

$$\int_{\mathbb{S}^2} Y_{n,k}(x) \, \bar{Y}_{n',k'}(x) \, \mathrm{d}\sigma(x) = \delta_{n,n'} \, \delta_{k,k'},$$



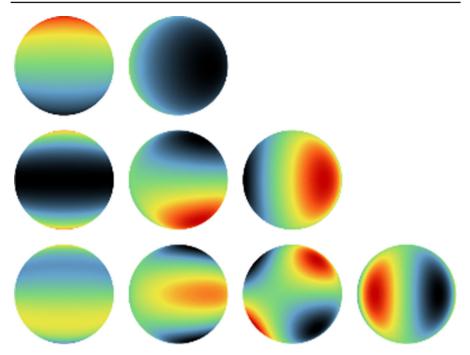


Fig. 1 Spherical harmonics. Top: $Y_{1,0}$ and $Y_{1,1}$. Middle: $Y_{2,0}$, $Y_{2,1}$ and $Y_{2,2}$. Bottom: $Y_{3,0}$, $Y_{3,1}$, $Y_{3,2}$ and $Y_{3,3}$

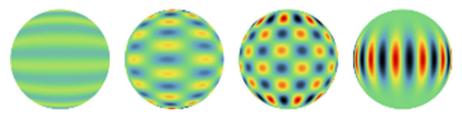


Fig. 2 Spherical harmonics of degree 15 and orders 0, 5, 10 and 15

and (ii), that any function $f \in L^2(\mathbb{S}^2,\mathbb{C},\sigma)$ can be expanded into spherical harmonics

$$f(x) = \sum_{n=0}^{\infty} \sum_{k=-n}^{+n} f_{n,k} Y_{n,k}(x).$$

Moreover, this expansion is unique (because of the orthogonality), and the coefficients $f_{n,k}$ are given by the formula

$$f_{n,k} = \langle f, Y_{n,k} \rangle = \int_{\mathbb{S}^2} f(x) \, \bar{Y}_{n,k}(x) \, d\sigma(x) \qquad n \ge 0, \ -n \le k \le +n.$$

If f is real-valued, then formula (1) implies $f_{n,-k} = (-1)^k \bar{f}_{n,k}$.



Property 2 Spherical harmonics satisfy the additivity formula

$$\frac{4\pi}{2n+1} \sum_{k=-n}^{+n} Y_{n,k}(x) \bar{Y}_{n,k}(y) = P_n(x \cdot y) \quad x, y \in \mathbb{S}^2,$$
 (2)

where P_n denotes a Legendre polynomial of degree n (cf. "Appendix A").

This property is simply a spherical version of the additivity formula for trigonometric functions. For a proof, see Marinucci and Peccati (2011), Dym and McKean (2016).

Property 3 Spherical harmonics are eigenfunctions of the Laplacian operator on a sphere (Laplace–Beltrami operator)

$$\Delta_{\mathbb{S}^2} Y_{n,k}(x) = -n(n+1) Y_{n,k}(x) \qquad x \in \mathbb{S}^2.$$

The spherical Laplacian $\Delta_{\mathbb{S}^2}$ is defined as a restriction to the unit sphere of the 3-dimensional Euclidean Laplacian (expressed in polar coordinates). This explicitly gives

$$\Delta_{\mathbb{S}^2} = \sin^{-1}\theta \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \sin^{-2}\theta \frac{\partial^2}{\partial \phi^2}.$$

It should be pointed out that all eigenvalues depend on the degree of the spherical harmonics but not their order.

2.2 Schoenberg's Theorem

Let Z be a real random field on \mathbb{S}^2 . Z is isotropic if it has a finite mean that is constant over \mathbb{S}^2 , and if the covariance at two points is finite and does not explicitly depend on either point but only on the geodesic distance between them. In other words, there exists a function $C: [0,\pi] \to \mathbb{R}$ such that

$$Cov{Z(x), Z(y)} = C(\alpha(x, y))$$
 $x, y \in \mathbb{S}^2$.

Since a covariance function is of positive type, the function C cannot be arbitrary. The following theorem by Schoenberg (1942) provides a complete characterization of such C functions.

Theorem 1 The function $(x, y) \mapsto C(\alpha(x, y))$ is of positive type on \mathbb{S}^2 if and only if there exists a summable series of nonnegative coefficients (a_n) such that

$$C(t) = \sum_{n=0}^{\infty} a_n P_n(\cos t) \quad t \in [0, \pi].$$
(3)



A geometric interpretation of this theorem is that the functions C form a convex cone, the extremal elements of which are the functions $t \mapsto P_n(\cos t)$. Note also that $C(0) = \sum_{n=0}^{\infty} a_n$.

Starting from C, the coefficients a_n can be retrieved by using the orthogonality property of the Legendre polynomials

$$a_n = \frac{2n+1}{2} \int_{-1}^{+1} C(\operatorname{arccos} t) P_n(t) dt \qquad n \in \mathbb{N}.$$
 (4)

Combined with Dirac measures, these coefficients form a positive measure

$$\mu_C = \sum_{n=0}^{\infty} a_n \delta_n,$$

usually called the angular power spectrum of C. Since Schoenberg's theorem plays the same role on \mathbb{S}^2 as Bochner's theorem on Euclidean space, it is also natural to call μ_C the spectral measure of C. It is discrete because \mathbb{S}^2 is compact.

Let Z be an isotropic random field on \mathbb{S}^2 . Z is Gaussian if any finite linear combination of its variables is a Gaussian variable. Its spatial distribution is completely characterized by its mean m and covariance function C (or, equivalently, its spectral measure μ_C).

3 Simulation of an Isotropic Gaussian Random Field on \mathbb{S}^2

The question precisely addressed in this section is: how can one produce simulations of an isotropic Gaussian random field on \mathbb{S}^2 with mean m = 0 and covariance function C?

3.1 Karhunen-Loève Expansion

There exists a spherical version to this well-known result in Euclidean space (Marinucci and Peccati 2011; Lang and Schwab 2015):

Theorem 2 Let Z be an isotropic Gaussian random field on \mathbb{S}^2 , with zero mean and spectral measure $\mu_C = \sum_{n=0}^{\infty} a_n \delta_n$. The following statements hold true:

(1) Z satisfies almost surely

$$\int_{\mathbb{S}^2} Z^2(x) \, \mathrm{d}\sigma(x) < \infty.$$

(2) Z admits a Karhunen-Loève expansion

$$Z(x) = \sum_{n=0}^{\infty} \sum_{k=-n}^{+n} A_{n,k} Y_{n,k}(x),$$



and the random complex coefficients $A_{n,k}$ satisfy

$$A_{n,k} = \int_{\mathbb{S}^2} Z(x) \, \bar{Y}_{n,k}(x) \, \mathrm{d}\sigma(x).$$

(3) The previous series expansion converges in the quadratic mean for all $x \in \mathbb{S}^2$

$$\lim_{n_0 \to \infty} E\left[\left(Z(x) - \sum_{n=0}^{n_0} \sum_{k=-n}^{+n} A_{n,k} Y_{n,k}(x) \right)^2 \right] = 0.$$

More can be said about the random coefficients $A_{n,k}$ (Lang and Schwab 2015). For $0 \le k \le n$, $A_{n,k}$ are centered and independent. For k > 0, $Re A_{n,k}$ and $Im A_{n,k}$ are independent and normally distributed with variance $a_n/2$. For k=0, $A_{n,0}$ is real-valued and normally distributed with variance a_n . Finally, for k < 0, $A_{n,k} =$ $(-1)^k \bar{A}_{n,-k}$.

Theorem 2 suggests the following algorithm to simulate a Gaussian random field on a sphere:

Algorithm 1 (Truncated Karhunen–Loève)

- (1) *choose* $n_0 > 0$;
- (2) for each $0 \le n \le n_0$, generate $A_{n,0} \sim \mathcal{N}(0, a_n)$;
- (3) for each $1 \le k \le n \le n_0$, generate $Re A_{n,k}$, $Im A_{n,k} \sim \mathcal{N}(0, a_n/2)$;
- (4) for each $1 \le k \le n \le n_0$, set $A_{n,-k} = (-1)^k \bar{A}_{n,k}$; (5) for each $x \in \mathbb{S}^2$, return $\sum_{n=0}^{n_0} \sum_{k=-n}^{+n} A_{n,k} Y_{n,k}(x)$.

Accordingly, one simulation is completely specified by $(n_0 + 1)^2$ normal values. These values ensure that the simulated random field is exactly Gaussian. Now, it must be mentioned that Algorithm 1 raises two difficulties. The first difficulty concerns the determination of the spectral measure. Its coefficients are required, analytically or numerically, to simulate $A_{n,k}$. The second difficulty is in regards to the truncation, which only approximately reproduces the covariance function. In addition, as the highest frequencies are discarded, the realizations produced are smoother than expected.

A spectral method is now presented to overcome this latter difficulty.

3.2 Spectral Method

There is no inconvenience in assuming that the target random field has unit variance, that is, $\sum_{n=0}^{\infty} a_n = 1$. In such a case, μ_C is a probability measure.

The spectral method is based on the following result. Let N be a random degree distributed like μ_C (in short, $N \sim \mu_C$). Given N, let also K be a uniform order (in short, $K|N \sim \mathcal{U}(\{-N, \dots, +N\})$. Finally, let Φ be a uniform phase over $[0, 2\pi[$, independent of N and K. Then, the following proposition holds true.

Proposition 1 The random field defined by $Z(x) = 2\sqrt{2\pi} Re(Y_{N,K}(x) e^{i\Phi})$ is standardized with covariance function C.



The proof is as follows. The random phase implies that *Z* is centered. To calculate its covariance function, the random field is rewritten as

$$Z(x) = \sqrt{2\pi} (Y_{N,K}(x) e^{i\Phi} + \bar{Y}_{N,K}(x) e^{-i\Phi}),$$

from which one derives at once

$$\begin{aligned} &\text{Cov}\{Z(x), Z(y)\} \\ &= 2\pi \, \text{E}\Big\{ \big(Y_{N,K}(x)e^{i\Phi} + \bar{Y}_{N,K}(x)e^{-i\Phi}\big) \, \big(Y_{N,K}(y)e^{i\Phi} + \bar{Y}_{N,K}(y)e^{-i\Phi}\big) \Big\}. \end{aligned}$$

Firstly, expectation is taken with respect to (w.r.t.) Φ . The previous formula becomes

$$Cov\{Z(x), Z(y)\} = 2\pi E\{Y_{N,K}(x)\bar{Y}_{N,K}(y) + \bar{Y}_{N,K}(x)Y_{N,K}(y)\}.$$

Secondly, expectation is taken w.r.t. K. The additivity formula (2) can be applied, and the formula simplifies to

$$Cov{Z(x), Z(y)} = E\{P_N(x \cdot y)\}.$$

Thirdly, expectation is taken w.r.t. N. Owing to Schoenberg's theorem, this finally gives

$$Cov\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} a_n P_n(x \cdot y) = C(\alpha(x, y)).$$

However, the random field Z that is built is not Gaussian. Then, consider independent copies $(Z_p, p \ge 1)$ of Z. By the central limit theorem, the spatial distribution of the random field $Z^{(p)} = (Z_1 + \cdots + Z_p)/\sqrt{p}$ tends to become Gaussian when p becomes very large. This leads to the following algorithm:

Algorithm 2 (Spectral method)

- (1) choose p;
- (2) generate $n_1, \ldots, n_p \sim \mu_C$;
- (3) for each i = 1, ..., p, generate $k_i \sim \mathcal{U}(\{-n_i, ..., +n_i\})$;
- (4) for each i = 1, ..., p, generate $\phi_i \sim \mathcal{U}([0, 2\pi])$;
- (5) for any $x \in \mathbb{S}^2$, return $(z_1(x) + \cdots + z_p(x))/\sqrt{p}$.

Once p has been chosen, p degrees, p orders and p phases are simulated, which makes it subsequently possible to assign a value at any point of the sphere. The criteria for choosing p are exactly the same as those for the spectral method (or the turning bands method) in Euclidean space [for more information, the reader can consult Lantuéjoul (2002) or Emery and Lantuéjoul (2006)]. The simulated random field is only approximately Gaussian, but it has the exact covariance function. Exactly as for the Karhunen–Loève algorithm, the spectral measure is required.



3.3 Examples

It turns out that spectral measures of standard covariance functions are not always standard probability distributions. For this reason, two different types of examples are considered, depending on whether the spatial distribution of the Gaussian random field is specified by its spectral measure or by its covariance function.

In the following examples, all simulations are performed using p = 20,000 basic random fields.

Example 1 Let $0 < \rho < 1$. If $a_n = (1 - \rho) \rho^n$ (geometric distribution), then the generating function of the Legendre polynomials (11) in "Appendix A" shows at once that

$$C(\alpha) = \frac{1 - \rho}{\sqrt{1 - 2\rho \cos \alpha + \rho^2}}.$$

The geometric distribution tends to scatter as ρ decreases. In this case, higher degrees are generated, which makes the simulation less regular (Figs. 3, 4).

Example 2 Let $\lambda > 0$. If $a_n = \exp(-\lambda)\lambda^n/n!$ (Poisson distribution), then formula (12) in "Appendix A" shows that $C(\alpha) = \exp(\lambda(\cos\alpha - 1)) J_0(\lambda \sin\alpha)$. Figure 5 shows an example with $\lambda = 10$.

Example 3 Let $\lambda > 0$. If $a_n = \sqrt{\pi} (2n+1) \exp(-\lambda) I_{n+1/2}(\lambda) / \sqrt{2\lambda}$ where $I_{n+1/2}$ denotes the modified Bessel function of order n+1/2, then formula (13) in "Appendix A" shows that $C(\alpha) = \exp(\lambda(\cos \alpha - 1))$. Figure 6 shows an example with $\lambda = 40$.

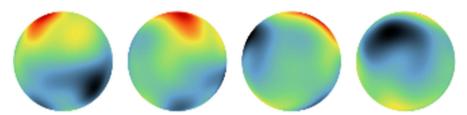


Fig. 3 Four views at 90° angles of a Gaussian random field with a geometric spectral measure ($\rho = 0.5$)

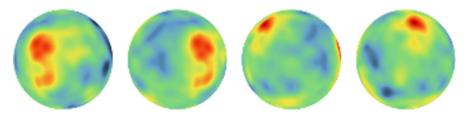


Fig. 4 Four views at 90° angles of a Gaussian random field with a geometric spectral measure ($\rho = 0.2$)



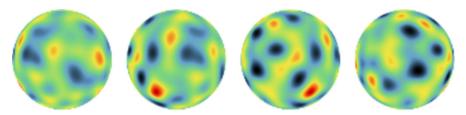


Fig. 5 Four views at 90° angles of a Gaussian random field with a Poisson spectral measure ($\lambda = 10$)

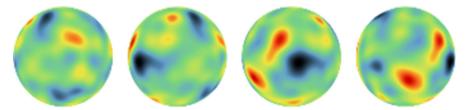


Fig. 6 Four views at 90° angles of a Gaussian random field with a discrete Bessel spectral measure ($\lambda = 40$)

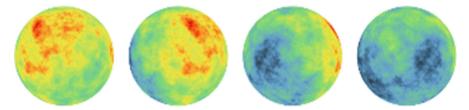


Fig. 7 Four views at 90° angles of a Gaussian random field with a linear covariance function

Example 4 Consider the linear covariance function $C(\alpha) = 1 - 2\alpha/\pi$. Because $t \mapsto C(\arccos t)$ is an odd function, the even coefficients of the spectral measure vanish. The values of the odd coefficients are (Abramovitz and Stegun 1964)

$$a_{2n+1} = \frac{4n+3}{4\pi} \frac{\Gamma^2(n+1/2)}{\Gamma^2(n+2)}.$$

They are related by the induction formula

$$a_n = \frac{2n+1}{2n-3} \frac{(n-2)^2}{(n+1)^2} a_{n-2},$$

starting from $a_0 = 0$ and $a_1 = 3/4$. It can be noted that $C(\pi) = -1$, which requires that antipodal points take opposite values. This explains the diurnal-nocturnal effect observed in the simulation of Fig. 7.

Example 5 The exponential function $C(\alpha) = e^{-\nu \alpha}$ is a standard covariance function in Euclidean space. It is also a function of positive type on the sphere. Its spectral measure can be analytically derived ("Appendix B"). One explicitly finds



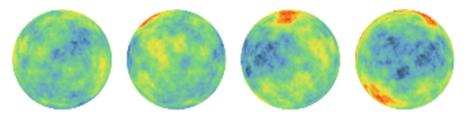


Fig. 8 Four views at 90° angles of a Gaussian random field with an exponential covariance function ($\nu = 1$)

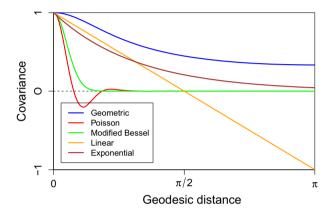


Fig. 9 Covariance functions of the simulated models

$$a_{2n} = \frac{(4n+1)\left(1 + \exp(-\nu\pi)\right)}{2(1+\nu^2)} \prod_{k=0}^{n-1} \frac{(2k)^2 + \nu^2}{(2k+3)^2 + \nu^2},$$

$$a_{2n+1} = \frac{(4n+3)\left(1 - \exp(-\nu\pi)\right)}{2(4+\nu^2)} \prod_{k=0}^{n-1} \frac{(2k+1)^2 + \nu^2}{(2k+4)^2 + \nu^2},$$

that the product over k is equal to 1 when n = 0. These coefficients can be computed using the induction formula

$$a_n = \frac{2n+1}{2n-3} \frac{v^2 + (n-2)^2}{v^2 + (n+1)^2} a_{n-2},$$

with $a_0 = 1/2 (1 + e^{-\nu \pi})/(1 + \nu^2)$ and $a_1 = 3/2 (1 - e^{-\nu \pi})/(4 + \nu^2)$. A simulation of this model with $\nu = 1$ is reproduced in Fig. 8.

To summarize, the covariance functions of all the simulated models presented in this section are depicted in Fig. 9.

Remark 1 It is sometimes possible to build simple isotropic random fields on a sphere with prespecified covariance functions. In such a case, spectral measures do not need to be determined. For instance, Chentsov's construction used to simulate intrinsic random fields in Euclidean space (Chentsov 1957) can be adapted to simulate a model



with a linear covariance function on a sphere. In addition, by making Chentsov's construction multiplicative rather than additive, a new random field model is obtained with an exponential covariance function. For more details, the reader is referred to "Appendix C".

4 Three Families of Covariance Functions on Spheres

To be applicable, the spectral simulation algorithm requires the spectral measure to be available, either analytically or numerically. Of course, an analytical calculation should be preferred to a numerical computation because it gives a better understanding of the distribution of the high frequencies. Spectral measures may have rather intricate analytical expression, which indicates that their calculation might not be quite straightforward. However, there are three situations where this calculation can be considered. These situations are addressed in turn.

4.1 Covariance Function of a Shot-Noise Process

The ingredients of this model are (i) a homogeneous Poisson point process \mathscr{P} on \mathbb{S}^2 (λ points on average), (ii) independent copies (F_p , $p \in \mathscr{P}$) of a stochastic process F on $[0, \pi]$ that is real- or complex-valued and square-integrable, and (iii) independent sign variables (ϵ_p , $p \in \mathscr{P}$). The shot-noise model is defined as

$$Z(x) = \sum_{p \in \mathcal{P}} \epsilon_p F_p \big(\alpha(x, p) \big) \quad x \in \mathbb{S}^2.$$

This random field is clearly centered. Regarding its covariance function, it is not difficult to establish

$$\operatorname{Cov}\{Z(x), Z(y)\} = \frac{\lambda}{4\pi} \int_{\mathbb{S}^2} \operatorname{E}\left\{F(\alpha(x, p) \,\bar{F}(\alpha(y, p)) \,d\sigma(p).\right\} (5)$$

Further, set $G(t) = F(\arccos t)$. Then, G is square-integrable on [-1, +1], and thus can be expanded into Legendre polynomials. It is shown in "Appendix E" that Z is an isotropic random field with the Schoenberg representation

$$Cov\{Z(x), Z(y)\} = \lambda \sum_{n=0}^{\infty} \frac{E\{|G_n|^2\}}{2n+1} P_n(x \cdot y),$$
 (6)

that involves the coefficients G_n of the Legendre expansion of G. The associated spectral measure is

$$a_n = \lambda \frac{E\{|G_n|^2\}}{2n+1}$$
 $n \in \mathbb{N}$.



For instance, the additive Chentsov model is a shot-noise random field with $F(\alpha) = 1$ if $0 \le \alpha \le \pi/2$ and -1 otherwise.

4.2 Yadrenko's Covariance Function

Let C_e be an isotropic function of positive type in \mathbb{R}^3 , and let R be its radial part $(C_e(h) = R(|h|))$. Yadrenko (1983) showed that

$$C(\alpha) = R\left(2\sin\frac{\alpha}{2}\right) \tag{7}$$

is a valid model of covariance on \mathbb{S}^2 .

An interesting feature of the Yadrenko's construction is that it is possible to relate the spectral measures of C and C_e . More precisely, let d be an integer such that $1 \le d \le 3$. R can be seen as a radial covariance function in d = 1, 2 or 3 dimensions. In \mathbb{R}^d , the spectral measure of R is given by its Hankel transform (Gneiting 1999)

$$R(t) = \Gamma(\nu+1) \int_0^\infty \left(\frac{2}{rt}\right)^{\nu} J_{\nu}(rt) dF_d(r), \tag{8}$$

where J_{ν} is the Bessel function of order $\nu = d/2 - 1$. "Appendix D" shows that

$$a_n = (2n+1)\frac{\pi}{2} \int_0^\infty \frac{J_{n+1/2}^2(r)}{r} dF_3(r),$$

$$a_n = (2n+1) \int_0^\infty \frac{J_{2n+1}(2r)}{r} dF_2(r),$$

$$a_n = \frac{\pi}{2} \int_0^\infty r \left[J_{n-1/2}^2(r) - J_{n+3/2}^2(r) \right] dF_1(r).$$

Using standard properties of Bessel functions, it is not difficult to check that these coefficients add up to 1. A direct proof of their positivity when d = 1 or 2 is more problematic. The integration measures dF_1 and dF_2 are not arbitrary positive measures on $[0, \infty[$ since they derive from dF_3 , and this must definitely play an important role.

For instance, the covariance function with the modified Bessel spectral measure of example 3 can be written $C(\alpha) = \exp(-2\lambda \sin^2(\alpha/2))$. This Yadrenko covariance function is associated with the Euclidean covariance function $C_e(h) = \exp(-\lambda |h|^2/2)$. Note that the Gaussian covariance function is not of positive type on the sphere (Gneiting 2013).

4.3 Covariance Function of a Stochastic Partial Differential Equation (SPDE)

Since the publication of the paper by Lindgren et al. (2011), there has been a considerable surge of interest concerning the specification of Gaussian random fields using SPDEs. The present paper deals with the SPDE



$$\left(\kappa^2 - \Delta_{\mathbb{S}^2}\right)^{\mu} Z = W_{\mathbb{S}^2},\tag{9}$$

where κ and μ are positive constants, $\Delta_{\mathbb{S}^2}$ is the spherical Laplacian and $W_{\mathbb{S}^2}$ is white noise on the sphere. Specifically, $W_{\mathbb{S}^2}$ is an orthogonal Gaussian random measure on \mathbb{S}^2 . On the other hand, the operator $(\kappa^2 - \Delta_{\mathbb{S}^2})^{\mu}$ is defined on $L^2(\mathbb{S}^2; \mathbb{C}, d\sigma)$ by its spectrum

$$(\kappa^2 - \Delta_{\mathbb{S}^2})^{\mu} Y_{n,k} = (\kappa^2 + n(n+1))^{\mu} Y_{n,k},$$

thus extending the case where μ is an integer.

Following Lang and Schwab (2015), we are looking for a solution of (9) that admits the Karhunen–Loève expansion

$$Z(x) = \sum_{n=0}^{\infty} \sum_{k=-n}^{+n} A_{n,k} Y_{n,k}(x) \qquad x \in \mathbb{S}^2.$$

Owing to the orthonormality of spherical harmonics, the random coefficient $A_{n,k}$ is found to be equal to $W(\bar{Y}_{n,k})/(\kappa^2 + n(n+1))^{\mu}$. Setting $W_{n,k} = W(\bar{Y}_{n,k})$ for short, the tentative SPDE solution takes the form

$$Z(x) = \sum_{n=0}^{\infty} \sum_{k=-n}^{+n} \frac{W_{n,k}}{(\kappa^2 + n(n+1))^{\mu}} Y_{n,k}(x) \qquad x \in \mathbb{S}^2.$$

From this solution, resorting to the additivity property and the independence of $W_{n,k}$, we finally obtain

$$Cov\{Z(x), Z(y)\} = \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{2n+1}{(\kappa^2 + n(n+1))^{2\mu}} P_n(x \cdot y).$$
 (10)

In particular, $\text{Var}\{Z(x)\} \propto \sum_{n=0}^{\infty} (2n+1)/(\kappa^2 + n(n+1))^{2\mu}$. Z is isotropic only if $\mu > 0.5$. In this case, its spectral measure is

$$a_n = \frac{1}{4\pi} \frac{2n+1}{(\kappa^2 + n(n+1))^{2\mu}} \quad n \in \mathbb{N}.$$

5 Conclusions

A spectral method has been proposed to perform continuous simulations of isotropic Gaussian random fields on a sphere. This method relies on knowledge of the angular power spectrum of the covariance function. Although little attention has been paid hitherto to its determination, this present paper demonstrates that its explicit calculation is possible in a large number of situations.



The range of applicability of isotropic random fields may seem rather limited, but it is perfectly appropriate when the physical phenomenon under study can be modeled as a sum of a drift and an isotropic residual. In this case, conditional simulations can be performed using the standard algorithm (kriging plus simulated residual) developed for Euclidean space.

Nonetheless, there is clearly a need for models with axial symmetry and more general nonisotropic models. In this case, the covariance function is a bivariate function, and there may not be a corresponding angular power spectrum unless the random field is harmonizable.

The spectral simulation algorithm was implemented in the R package RGeostats. Interested readers can consult the vignette (RGeostats 2019) corresponding to the routine simsph in the site given in reference.

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Appendix A: Legendre Polynomials and Associated Functions

Legendre polynomials are defined by Rodrigues' formula

$$P_n(x) = \frac{(-1)^n}{2^n n!} \frac{\partial^n}{\partial x^n} (1 - x^2)^n - 1 \le x \le +1.$$

They form an orthogonal family in $L^2([-1, +1])$

$$\int_{-1}^{+1} P_m(x) P_n(x) dx = \frac{2}{2n+1} \delta_{m,n}.$$

Typical examples of expansions into Legendre polynomials are

$$\sum_{n=0}^{\infty} P_n(x) t^n = \frac{1}{\sqrt{1 - 2xt + t^2}},$$
(11)

$$\sum_{n=0}^{\infty} P_n(x) \, \frac{t^n}{n!} = e^{t \cos \alpha} J_0 \left(t \sqrt{1 - x^2} \right), \tag{12}$$

$$\sum_{n=0}^{\infty} P_n(x) (2n+1) I_{n+1/2}(t) = \sqrt{\frac{2t}{\pi}} e^{tx}.$$
 (13)

The first example is the generating function of Legendre polynomials (Gradshteyn and Ryshik 1994). The second example can be found in Olver et al. (2010), and the third one in Abramovitz and Stegun (1964) and Terdik (2015).

More generally, for $n \ge 0$ and $-n \le k \le +n$, the associated Legendre function of degree n and order k is defined by

$$P_{n,k}(t) = \frac{(-1)^{n+k}}{2^n n!} (1 - t^2)^{k/2} \frac{\partial^{n+k}}{\partial t^{n+k}} (1 - t^2)^n - 1 \le t \le +1.$$



Only functions of even order are polynomials (in particular, $P_{n,0} = P_n$). The associated Legendre functions of the same degree and opposite orders are proportional

$$P_{n,-k}(t) = (-1)^k \frac{(n-k)!}{(n+k)!} P_{n,k}(t).$$

Appendix B: Spectral Measure of the Exponential Covariance Function on \mathbb{S}^2

The function $t \in [-1, +1] \mapsto F(t) = \exp(-\nu \arccos t)$ is the solution of a second-order differential equation $(1 - t^2) F''(t) - t F'(t) - \nu^2 F(t) = 0$ with the initial conditions $F(0) = \exp(-\nu \pi/2)$ and $F'(0) = \nu \exp(-\nu \pi/2)$. Let $F(t) = \sum_{k=0}^{\infty} \alpha_k t^k$ be its series expansion. The coefficients α_k are related by the induction formula

$$\alpha_{k+2} = \alpha_k \frac{v^2 + k^2}{(k+1)(k+2)}$$
 $k \in \mathbb{N}$.

This gives

$$\alpha_{2k} = \frac{\exp(-\nu\pi/2)}{(2k)!} \prod_{\ell=0}^{k-1} (\nu^2 + (2\ell)^2),$$

$$\alpha_{2k+1} = \frac{\nu \exp(-\nu\pi/2)}{(2k+1)!} \prod_{\ell=0}^{k-1} (\nu^2 + (2\ell+1)^2).$$

These two formulae can be condensed into a single formula that is expressed in terms of gamma functions of complex variables

$$\alpha_k = \frac{\nu \left(1 - \exp(-\nu \pi) (-1)^k\right)}{4\pi} \frac{2^k \Gamma\left((k + i\nu)/2\right) \Gamma\left((k - i\nu)/2\right)}{k!}.$$
 (14)

Now, let us more explicitly turn to a calculation of the spectral measure of the exponential covariance. According to (4), it can be written as

$$a_n = \frac{2n+1}{2} \int_{-1}^{+1} F(t) P_n(t) dt = \frac{2n+1}{2} \sum_{k=0}^{\infty} \alpha_k \int_{-1}^{+1} t^k P_n(t) dt.$$

The expression involves integrals that vanish if t < n or if k and n do not have the same parity. Accordingly, we have

$$a_n = \frac{2n+1}{2} \sum_{k=0}^{\infty} \alpha_{n+2k} \int_{-1}^{+1} t^{n+2k} P_n(t) dt.$$



In addition, such integrals are analytically tractable (Rainville 1960)

$$\int_{-1}^{+1} t^{n+2k} P_n(t) dt = \frac{\Gamma(k+n/2+1/2) \Gamma(k+n/2+1)}{k! \Gamma(k+n+3/2)}.$$
 (15)

Then, formulae (14) and (15) are combined. The duplication of the gamma function allows important simplifications in the numerator of (15) and the denominator of (14), which leads to

$$a_n = \frac{2n+1}{2} \frac{\nu \left(1 - \exp(-\nu \pi) (-1)^n\right)}{4\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{\Gamma(k + (n+i\nu)/2) \Gamma(k + (n-i\nu)/2)}{k! \Gamma(k+n+3/2)}.$$

Now, the series in the right-hand side member is proportional to a hypergeometric function, the value of which is given by formula 9.122 of Gradshteyn and Ryshik (1994). The formula for a_n simplifies to

$$a_{n} = \frac{2n+1}{2} \frac{\nu (1 - \exp(-\nu \pi) (-1)^{n})}{8} \frac{\Gamma((n+i\nu)/2) \Gamma((n-i\nu)/2)}{\Gamma((n+3+i\nu)/2) \Gamma((n+3-i\nu)/2)}.$$
(16)

Further simplifications can be made

$$R_n = \frac{\Gamma((n+i\nu)/2) \Gamma((n-i\nu)/2)}{\Gamma((n+3+i\nu)/2) \Gamma((n+3-i\nu)/2)},$$

by using the three gamma formulae $\Gamma(x+1) = x \Gamma(x)$, $\Gamma(x) \Gamma(1-x) = \pi/\sin(\pi x)$ and $\Gamma(1+ix) \Gamma(1-ix) = \pi x/\sin(\pi x)$, depending on the parity of n.

- In the even case

$$\begin{split} R_{2n} &= \frac{\Gamma(n+i\nu/2) \, \Gamma(n-i\nu/2)}{\Gamma(n+3/2+i\nu/2) \, \Gamma(n+3/2-i\nu/2)} \\ &= \prod_{k=0}^{n-1} \frac{(2k)^2 + \nu^2}{(2k+3)^2 + \nu^2} \, \frac{\Gamma(i\nu/2) \, \Gamma(-i\nu/2)}{\Gamma\left((3+i\nu)/2\right) \, \Gamma\left((3-i\nu)/2\right)} \\ &= \prod_{k=0}^{n-1} \frac{(2k)^2 + \nu^2}{(2k+3)^2 + \nu^2} \, \frac{8 \coth(\nu\pi/2)}{\nu \, (\nu^2 + 1)}. \end{split}$$



In the odd case

$$R_{2n+1} = \frac{\Gamma(n + (1+i\nu)/2) \Gamma(n + (1-i\nu)/2)}{\Gamma(n+2+i\nu/2) \Gamma(n+2-i\nu/2)}$$

$$= \prod_{k=0}^{n-1} \frac{(2k+1)^2 + \nu^2}{(2k+4)^2 + \nu^2} \frac{\Gamma((1+i\nu)/2) \Gamma((1-i\nu)/2)}{\Gamma(2+i\nu/2) \Gamma(2-i\nu/2)}$$

$$= \prod_{k=0}^{n-1} \frac{(2k+1)^2 + \nu^2}{(2k+4)^2 + \nu^2} \frac{8 \tanh(\nu\pi/2)}{\nu(\nu^2 + 4)}.$$

It remains to replace R_n by its expression in (16) to obtain

$$a_{2n} = \frac{(4n+1)\left(1 + \exp(-\nu\pi)\right)}{2(1+\nu^2)} \prod_{k=0}^{n-1} \frac{(2k)^2 + \nu^2}{(2k+3)^2 + \nu^2},$$

$$a_{2n+1} = \frac{(4n+3)\left(1 - \exp(-\nu\pi)\right)}{2(4+\nu^2)} \prod_{k=0}^{n-1} \frac{(2k+1)^2 + \nu^2}{(2k+4)^2 + \nu^2}.$$

Appendix C: Chentsov Models

The following model is a spherical transposition of an Euclidean model by Chentsov (1957) to simulate random fields with a linear variogram. Its ingredients are a homogeneous point process \mathscr{P} (λ points on average on the sphere), and an independent sign variable ϵ . The model is defined as

$$Z(x) = \epsilon \sum_{p \in \mathscr{P}} \operatorname{sign}(x \cdot p) \quad x \in \mathbb{S}^2.$$
 (17)

This random field is clearly centered. To calculate the covariance between Z(x) and Z(y), the first step is to randomize the number of Poisson points

$$\operatorname{Cov}\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \operatorname{E}\left\{\sum_{i \le n} \operatorname{sign}(x \cdot \dot{p}_i) \sum_{j \le n} \operatorname{sign}(y \cdot \dot{p}_j)\right\},\,$$

where $\dot{p}_1, \ldots, \dot{p}_n$ are n points independent and uniform over \mathbb{S}^2 . The expectation contains n^2 terms. All terms containing two independent points vanish. Consequently, the covariance reduces to

$$Cov\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} n \operatorname{E} \{\operatorname{sign}(x \cdot \dot{p}) \operatorname{sign}(y \cdot \dot{p})\},$$

where \dot{p} is a uniform point over \mathbb{S}^2 . Now, let H_x and H_y be hemispheres centered at x and y. $\mathrm{sign}(x \cdot \dot{p})$ $\mathrm{sign}(y \cdot \dot{p})$ is positive if $\dot{p} \in (H_x \cap H_y) \cup (H_{-x} \cap H_{-y})$, that is, if



 \dot{p} belongs to two disjoint spherical wedges, each with a dihedral angle $\pi - \alpha(x, y)$. Accordingly, one has

$$E\left\{\operatorname{sign}(x \cdot \dot{p}) \operatorname{sign}(y \cdot \dot{p})\right\} = (+1)\frac{4\left(\pi - \alpha(x, y)\right)}{4\pi} + (-1)\frac{4\alpha(x, y)}{4\pi}$$
$$= 1 - \frac{2\alpha(x, y)}{\pi},$$

and since the mean value of a Poisson distribution is equal to its parameter, we finally obtain

$$Cov{Z(x), Z(y)} = \lambda \left(1 - \frac{2\alpha(x, y)}{\pi}\right).$$

This shows that this model is isotropic with a linear covariance function.

Since the number of Poisson points is almost surely finite, it is possible to replace the sum by the product in the definition (17). We then obtain what we call a multiplicative Chentsov random field

$$Z(x) = \epsilon \prod_{p \in \mathscr{P}} \operatorname{sign}(x \cdot p) \quad x \in \mathbb{S}^2.$$
 (18)

This random field is also centered, and the covariance at x and y can be written as

$$\operatorname{Cov}\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \operatorname{E} \left\{ \prod_{i < n} \operatorname{sign}(x \cdot \dot{p}_i) \prod_{j < n} \operatorname{sign}(y \cdot \dot{p}_j) \right\}.$$

Using the independence of \dot{p}_i , this covariance becomes

$$Cov\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} E^n \{ sign(x \cdot \dot{p}) \ sign(y \cdot \dot{p}) \}.$$

The expectation has just been calculated above. This finally gives

$$\operatorname{Cov}\{Z(x), Z(y)\} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \left(1 - \frac{2\alpha(x, y)}{\pi} \right)^n = \exp\left(-\frac{2\lambda\alpha(x, y)}{\pi} \right),$$

which shows that Z is isotropic with an exponential covariance function.

Appendix D: Spectral Measure of Yadrenko Covariance Functions

If $\alpha = \arccos t$, then $t = \cos \alpha = 1 - 2\sin^2(\alpha/2)$, from which it follows that $2\sin(\alpha/2) = \sqrt{2(1-t)}$. Accordingly, if $C(\alpha) = R(2\sin(\alpha/2))$, then $C(\arccos t) = R(\sqrt{2(1-t)})$. Plugging this formula into (4) gives



$$a_n = \frac{2n+1}{2} \int_{-1}^{+1} R(\sqrt{2(1-t)}) P_n(t) dt.$$

Now, to introduce the Euclidean spectral measure, R is replaced by its Hankel representation (8) in d dimensions. This gives, after permuting the integrals

$$a_n = \frac{2n+1}{2} \Gamma(\nu+1) \int_0^\infty I_d(r) \, \mathrm{d}F_d(r),$$

with v = d/2 - 1 and

$$I_d(r) = \int_{-1}^{+1} \left(\frac{2}{r\sqrt{2(1-t)}} \right)^{\nu} J_{\nu} \left(r\sqrt{2(1-t)} \right) P_n(t) dt.$$

To calculate this latter integral, a change of variables $u = \sqrt{(1-t)/2}$ is performed, which leads to

$$I_d(r) = 4 \int_0^1 \left(\frac{1}{ru}\right)^{\nu} J_{\nu}(2ru) P_n(1 - 2u^2) u \, du.$$
 (19)

At this point, three cases must be considered, depending on the d value:

– If d=3, then $\nu=1/2$ and $J_{\nu}(z)=\sqrt{2}\sin z/\sqrt{\pi z}$. Formula 7.244 of Gradshteyn and Ryshik (1994) gives

$$I_3(r) = \frac{4}{r\sqrt{\pi}} \int_0^1 \sin(2ur) P_n(1 - 2u^2) du = \frac{2\sqrt{\pi}}{r} J_{n+1/2}^2(r),$$

which leads to

$$a_n = (2n+1)\frac{\pi}{2} \int_0^\infty \frac{J_{n+1/2}^2(r)}{r} dF_3(r).$$

- If d=2, then $\nu=0$. Formula 7.251 of Gradshteyn and Ryshik (1994) gives

$$I_2(r) = 2 \int_0^1 J_0(2ru) P_n(1 - 2u^2) u \, du = \frac{2}{r} J_{2n+1}(2r).$$

Consequently

$$a_n = (2n+1) \int_0^\infty \frac{J_{2n+1}(2r)}{r} dF_2(r).$$

– If d=1, then $\nu=-1/2$ and $J_{\nu}(z)=\sqrt{2}\cos z/\sqrt{\pi z}$. This implies

$$I_1(r) = \frac{4}{\sqrt{\pi}} \int_0^1 \cos(2ur) P_n(1 - 2u^2) u \, du.$$



Compared to the formulae encountered in the case d=3, the sine has been replaced by a cosine. In addition, a new term u is present. This suggests to calculate $I_1(r)$ by taking the derivative of formula 7.244 of Gradshteyn and Ryshik (1994) w.r.t. r. This gives

$$I_1(r) = 2\sqrt{\pi} J_{2n+1}(r) J'_{2n+1}(r),$$

which yields

$$a_n = (2n+1) \pi \int_0^\infty J_{2n+1}(r) J'_{2n+1}(r) dF_1(r).$$

Additionally, further simplifications occur by using the following two standard formulae

$$(2n+1)J_{n+1/2}(r) = J_{n-1/2}(r) + J_{n+3/2}(r),$$

$$2J'_{n+1/2}(r) = J_{n-1/2}(r) - J_{n+3/2}(r),$$

The final result is

$$a_n = \frac{\pi}{2} \int_0^\infty r \left[J_{n-1/2}^2(r) - J_{n+3/2}^2(r) \right] dF_1(r).$$

Appendix E: Spectral Measure of Shot-Noise Random Fields

Let us start from formula (5), which can be rewritten as

$$\operatorname{Cov}\{Z(x), Z(y)\} = \frac{\lambda}{4\pi} \operatorname{E} \left\{ \int_{\mathbb{S}^2} G(x \cdot p) \, \bar{G}(y \cdot p) \, \mathrm{d}\sigma(p) \right\}.$$

To calculate the integral, G is first expanded into Legendre polynomials, and then the Legendre polynomials themselves are expanded into spherical harmonics using the additivity formula (2)

$$G(x \cdot p) = \sum_{n=0}^{\infty} G_n \frac{4\pi}{2n+1} \sum_{k=-n}^{+n} Y_{n,k}(x) \, \bar{Y}_{n,k}(p),$$

$$G(y \cdot p) = \sum_{n=0}^{\infty} G_n \frac{4\pi}{2n+1} \sum_{k=-n}^{+n} \bar{Y}_{n,k}(y) Y_{n,k}(p).$$

Now integrate over p. Because of the orthonormality of spherical harmonics, many terms cancel, giving

$$\operatorname{Cov}\{Z(x), Z(y)\} = \frac{\lambda}{4\pi} \operatorname{E} \left\{ \sum_{n=0}^{\infty} |G_n|^2 \left(\frac{4\pi}{2n+1} \right)^2 \sum_{k=-n}^{+n} Y_{n,k}(x) \, \bar{Y}_{n,k}(y) \right\}.$$



Finally, the additivity formula is used again, which yields

$$Cov\{Z(x), Z(y)\} = \lambda \sum_{n=0}^{\infty} \frac{E\{|G_n|^2\}}{2n+1} P_n(x \cdot y).$$

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