Strict Positive Definiteness under Axial Symmetry on the Sphere

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Abstract

Axial symmetry for covariance functions defined over spheres has been a very popular assumption for climate, atmospheric, and environmental modeling. For Gaussian random fields defined over spheres embedded in a three-dimensional Euclidean space, maximum likelihood estimation techiques as well kriging interpolation rely on the inverse of the covariance matrix. For any collection of points where data are observed, the covariance matrix is determined through the realizations of the covariance function associated with the underlying Gaussian random field. If the covariance function is not strictly positive definite, then the associated covariance matrix might be singular.

We provide conditions for strict positive definiteness of any axially symmetric covariance function. Furthermore, we find conditions for reducibility of an axially symmetric covariance function into a geodesically isotropic covariance. Finally, we provide conditions that legitimate Fourier inversion in the series expansion associated with an axially symmetric covariance function.

Keywords: `Axial Symmetry`, `Covariance Function`, `Fourier Inversion`, `Reducibility`.

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1 Introduction

1.1 Context

The last few years have seen an increasing interest in modeling data on a global scale, both from climate model simulations and from satellite observations (Porcu et al., 2019). Very often, data located over large portions of the planet are not isotropic, so that their covariance function does not depend exclusively on the distance between any two points of the spatial domain. Indeed, the assumption of isotropy might be suitable for microscale meteorology, but at least questionable for mesoscale and synoptic scale meteorology, or for instance for total columne ozone modeling (Stein, 2007; Porcu et al., 2019).

Apparently, any climate or meteorological model must account for the physical principles underlying the phenomena. Yet, modeling second order properties of random fields defined on a global scale is crucial to both estimation and prediction. Specifically, Stein (2007) advocates the use of covariance functions that are axially symmetric, in the sense that heterogeneity (nonstationarity) along latitudes, as well as homogeneity (stationarity) along longitudes, are assumed. The literature on axially symmetric covariance functions has been elusive so far, with the exceptions of Porcu et al. (2019) who recently proposed parametric classes of covariance functions obtained from the Matérn (Stein, 1999) and $\mathcal{F}$ (Alegria et al., 2018) classes of isotropic covariance functions. Alternative approaches have been proposed via partial derivatives (Jun and Stein, 2007, 2008). Spectral characterizations have been provided by Jones (1963) and more recently by Hitczenko and Stein (2012). Spectral conditions in concert with Fast Fourier Transform techniques have been proposed by Castruccio and Stein (2013). Alternative conditions for spectral representations under axial symmetry have been provided by Huang et al. (2012). Recently, Emery et al. (2019) have obtained axial symmetry from longitudinal integration of a Gaussian field having isotropic covariance function.

1.2 The Problem

Both maximum likelihood estimation techniques and kriging predictors rely on the inverse of the covariance matrix (Stein, 1999), having entries that are normally generated through some parametric family of covariance functions. If the covariance function is positive definite only (and not strictly positive definite), the associated covariance matrix might be singular. This problem has been extensively noted as being crucial to kriging procedures, and the reader is referred to Myers (1992), and the references therein, for a thorough account on the implications of strict positive definiteness to both geostatistics and numerical analysis. A recent contribution, with new results on product spaces, can be found in De Iaco and Posa (2018).

Stein (2007) proposes to model axial symmetry through spectral approaches and by truncating the series in Jones spectral expansion (Jones, 1963) of any axially symmetric covariance function. Truncation in such a series expansion does not necessarily ensure the covariance function obtained after truncation to be strictly positive definite.

Strict positive definiteness on d-dimensional spheres embedded in a $(d+1)$-dimensional Euclidean space has been studied by Chen et al. (2003); Menegatto (1994, 1995); Menegatto et al. (2006); Guella et al. (2016b,a, 2017); Beatson and zu Castell (2017) and Barbosa and Menegatto (2017). This part of the literature covers the problem of strict positive definiteness under the assumption of geodesic isotropy (Porcu et al., 2018), *i.e.*, the covariance function depends exclusively on the geodesic distance, being the length of the arc merging any two points located over the spherical shell.

The problem of strict positive definiteness for axially symmetric covariance functions on spheres embedded in $\mathbb{R}^3$ has not been studied so far.

1.3 Our Contribution

We dig into the problem of strict positive definiteness under axial symmetry. We start by providing conditions for reducibility of an axially symmetric covariance function to a geodesically isotropic covariance. Then, we provide a criterion for strict positive definiteness, which requires a technical and long proof. Finally, we find sufficient conditions that ensure Fourier inversion under axial symmetry. The layout of the paper is as follows: Section 2 provides the mathematical notation and machinery needed to understand the rest of the paper. Section 3 deals with the main results of the paper. We also discuss a practical example to illustrate strict positive definiteness on the sphere for a class of axiallly symmetric covariance functions. Section 4 concludes the paper with a short discussion. Mathematical proofs and technical lemmas are deferred to the Appendix A.

2 Background Material

2.1 Spheres and Covariance Functions

We consider the unit sphere $\mathbb{S}^2 = \{\boldsymbol{s} \in \mathbb{R}^3, \|\boldsymbol{s}\| = 1\}$, where $\|\cdot\|$ denotes the Euclidean norm. We write a point $\boldsymbol{s}$ on the sphere through its spherical coordinates $\boldsymbol{s} = (L, \ell)$, with $L \in [0, \pi]$ and $\ell \in [0, 2\pi)$ being respectively the latitude and longitude (or what is equivalent, polar and the azimuthal angles).

Distances on spheres are represented through arcs joining any two points on the spherical shell.

The geodesic distance is defined as the mapping $\theta : \mathbb{S}^2 \times \mathbb{S}^2 \to [0, \pi]$ so that

$$\theta(\boldsymbol{s}, \boldsymbol{s}') = \arccos\big(\langle \boldsymbol{s}, \boldsymbol{s}' \rangle\big) = \arccos\big(\sin L \sin L' + \cos L \cos L' \cos \Delta\ell\big),$$

with $\boldsymbol{s} = (L, \ell)$, $\boldsymbol{s}' = (L', \ell')$, with $\langle \cdot, \cdot \rangle$ denoting the Euclidean dot product in $\mathbb{R}^3$, and where $\Delta\ell = \ell - \ell'$. Henceforth, we shall equivalently use $\theta(\boldsymbol{s}, \boldsymbol{s}')$ or the shortcut θ to denote the geodesic distance, whenever there is no confusion.

In this paper we consider positive definite functions in distinct contexts: a function $f : X \times X \to \mathbb{C}$ is definite positive when $\sum_{i=1}^{\kappa} \sum_{j=1}^{\kappa} c_i f\,(x_i, x_j)\, \bar{c}_j \geq 0$ for any κ dimensional collection of points $\{x_i\}_{i=1}^{\kappa} \subset X$ and constants $c_1, \ldots, c_\kappa \in \mathbb{C}$. If such inequality is strict when $\sum_{i=1}^{\kappa} c_i^2 \neq 0$, then f is called strict positive definite. We observe that when the function f is symmetric and to real-valued then the constants c_i can be considered in $\mathbb{R}$ (see (Berg et al., 1984, p. 68)).

If $\{Z(\boldsymbol{s}),\ \boldsymbol{s} \in \mathbb{S}^2\}$ is a zero mean Gaussian random fields defined over the sphere, with finite second order moment, the finite dimensional distributions are completely specified by the covariance function $C : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$, defined by

$$C(\boldsymbol{s}, \boldsymbol{s}') = \mathbb{C}\mathrm{ov}\big(Z(\boldsymbol{s}), Z(\boldsymbol{s}')\big), \qquad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{S}^2.$$

Porcu et al. (2018) call C geodesically isotropic if

$$C(\boldsymbol{s}, \boldsymbol{s}') = \psi(\theta(\boldsymbol{s}, \boldsymbol{s}')), \tag{1}$$

for particular choices of $\psi : [0, \pi] \to \mathbb{R}$ (for continuous functions, ψ, see Gneiting, 2013). The function ψ is called the geodesically isotropic part of C (Daley and Porcu, 2013). For a characterization of geodesic isotropy, the reader is referred to Schoenberg (1942).

For quantities observed on a global scale, isotropy is not tenable. While processes at small scale (micro-scale, turbulence scale) might be approximately regarded as isotropic, large-scale meteorological patterns have preferred directions driven by general circulation (Porcu et al., 2019). Indeed, Stein (2007) showed that total column ozone data show significant changes over latitudes. Castruccio and Stein (2013) argued that both the inter- and intra-annual variability for surface temperature are dependent on latitude. The covariance function, C, is called *axially symmetric* when it depends on the latitudes and the difference of the longitudes, that is,

$$C\left(\boldsymbol{s}, \boldsymbol{s}'\right) = K(L_1, L_2, \Delta\ell), \tag{2}$$

for particular choices of the function $K : [0, \pi]^2 \times [-2\pi, 2\pi] \to \mathbb{R}$.

2.2 Legendre polynomials

Let P_n be the normalized ordinary Legendre polynomial of degree n, and let P_n^m be the associated Legendre polynomial of degree n and order m (for both, see Abramowitz and Stegun, 1964). By the addition theorem for spherical harmonics (Marinucci and Peccati, 2011), we have

$$P_n(\langle \boldsymbol{s}, \boldsymbol{s}' \rangle) = \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n^m(\sin(L)) P_n^m(\sin(L')) \cos(m\Delta\ell) \tag{3}$$

where $\boldsymbol{s}, \boldsymbol{s}'$ belong to $\mathbb{S}^2$. Recall that (Abramowitz and Stegun, 1964, formulas (8.14.11) and (8.14.13))

$$\int_{-1}^{1} P_n^m(x) P_\ell^m(x) \, \mathrm{d}x = 0 \qquad \text{if } \ell \neq m, \quad \text{and} \tag{4}$$

$$\int_{-1}^{1} (P_n^m(x))^2 \, \mathrm{d}x = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!}, \tag{5}$$

for which a change of variable implies

$$\int_{-\pi/2}^{\pi/2} P_n^m(\sin t) P_\ell^m(\sin t) \cos t \, \mathrm{d}t = 0 \qquad \text{if } \ell \neq m, \quad \text{and} \tag{6}$$

$$\int_{-\pi/2}^{\pi/2} (P_n^m(\sin t))^2 \cos t \, \mathrm{d}t = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!}, \tag{7}$$

respectively. Let $\bar{P}_n^m$ stand for the normalized version of the associated Legendre polynomial of degree n and order m (so that its squared integral on $[-1, 1]$ is identically equal to 1). Hence, by (5), we have:

$$\bar{P}_n^m = \sqrt{\frac{(2n+1)(n-m)!}{2(n+m)!}} P_n^m, \tag{8}$$

for $m \geq 0, n \geq |m|$. Moreover, recall that:

$$P_n^{-m} = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m, \quad m \geq 0, n \geq |m|, \tag{9}$$

whereas $P_n^m = 0$ if $|m| > n$. Equations (8) and (9) imply that

$$\bar{P}_n^{-m} = (-1)^m \bar{P}_n^m, \tag{10}$$

and that (3) can be rewritten as

$$P_n(\langle \boldsymbol{s}, \boldsymbol{s}' \rangle) = \frac{2}{2n+1} \sum_{m=-n}^{n} \bar{P}_n^m(\sin(L)) \bar{P}_n^m(\sin(L')) \cos(m\Delta\ell). \tag{11}$$

If $\boldsymbol{s} = \boldsymbol{s}'$ then (11) yields:

$$n + \frac{1}{2} = \left(n + \frac{1}{2}\right) P_n(\langle \boldsymbol{s}, \boldsymbol{s} \rangle) = \sum_{m=-n}^{n} (\bar{P}_n^m(\sin(L)))^2. \tag{12}$$

2.3 Expansions for Random Fields on Spheres

We can now come back to random fields $\{Z(\boldsymbol{s}) : \boldsymbol{s} \in \mathbb{S}^2\}$, as already defined, with finite first- and second-order moments. The stochastic expansion theorem provided by Marinucci and Peccati (2011) shows that Z admits a uniquely determined expansion of the type

$$Z(\boldsymbol{s}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} A_{n,m} \mathcal{Y}_{n,m}(\boldsymbol{s}), \qquad \boldsymbol{s} \in \mathbb{S}^2, \tag{13}$$

where $\mathcal{Y}_{n,m}$ denote the complex-valued spherical harmonic of degree n and order m. Spherical harmonics constitute an orthonormal basis of the space of square integrable functions with respect to the Lebesgue measure on $\mathbb{S}^2$, and are defined through the identity

$$\mathcal{Y}_{n,m}(\boldsymbol{s}) = \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_n^m(\cos L) \mathrm{e}^{\mathrm{i} m \ell}, \qquad L \in [0, \pi], \quad \ell \in [0, 2\pi), \tag{14}$$

with i denoting the imaginary unit. The sequence $\{A_{n,m}\}_{n,m}$ of complex-valued random variables is crucial to determine the second-order properties of Z in (13). If $A_{n,m} = A^*_{n,-m}$, with $*$ denoting the complex conjugate, then Z is real-valued. As it will be clear from Proposition 1, if $\mathrm{cov}\left(A_{n,m}, A_{n',m'}\right) = \delta_{nn'}\delta_{mm'} 2b_n/(2n+1)$, with δ being the Kronecker delta function and $\{b_n\}_{n=0}^{\infty}$ a summable sequence of nonnegative coefficients, then the covariance function associated with Z is geodesically isotropic. Precisely, Schoenberg's theorem (Schoenberg, 1942) shows that

$$\mathrm{cov}\left(Z(\boldsymbol{s}), Z(\boldsymbol{s}')\right) = \sum_{n=0}^{\infty} b_n P_n(\cos\theta(\boldsymbol{s}, \boldsymbol{s}')) =: \psi(\theta(\boldsymbol{s}, \boldsymbol{s}')), \qquad \text{where} \quad \psi : [0, \pi] \to \mathbb{R}. \tag{15}$$

We follow Daley and Porcu (2013) and call the sequence $\{b_n\}_{n=0}^{\infty}$ a Schoenberg sequence. Classical Fourier inversion shows that, for each $n = 0, 1 \ldots,$ the coefficients b_n can be attained through

$$b_n = \int_0^{\pi} \psi(\theta) P_n(\cos\theta) \sin\theta \mathrm{d}\theta. \tag{16}$$

Arguments in Jones (1963) show that an axially symmetric covariance function admits an expansion of the type

$$\operatorname{cov}\left(Z(\boldsymbol{s}), Z(\boldsymbol{s}')\right) = K(L, L', \Delta\ell) = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} \sum_{n'=|m|}^{\infty} \mathrm{e}^{\mathrm{i}m\Delta\ell} \overline{P}_n^m(\sin L) \overline{P}_{n'}^m(\sin L') c_m(n, n'), \quad (17)$$

and such an expansion is attained provided $c_{-m}(n, n') = c_m(n, n')^*$, where * indicates complex conjugate for scalars or conjugate transpose for matrices. Also, for each $m \geq 0$, $c_m(n, n')$ is positive definite as a function from $\{m, m+1, \dots\} \times \{m, m+1, \dots\}$ into $\mathbb{C}$. Moreover, such functions must guarantee that the series (17) pointwise converges. The expression (17) can be obtained from (13) if $\operatorname{cov}\left(A_{n,m}, A_{n',m'}\right) = \delta_{mm'} c_m(n, n')$.

3 Results

The following result provides conditions for an axially symmetric covariance function to reduce to a geodesically isotropic covariance (see Stein (2007)) and it provides an explicit expression for the associated Schoenberg sequence $\{b_n\}$ in (16) which is related to the sequence of the covariance functions $c_m(n, n')$ in (17). Even if part of it is not new, we provide a complete proof in order to make the paper self–contained.

Proposition 1. *Let K be the function defined through (17). If $c_m(n, n') = c(n)\delta_{nn'}$ where $c(n) \geq 0$ for every $n \geq 0$ and $\sum_{n=0}^{\infty} n c(n) < \infty$, then*

$$K(L, L', \Delta\ell) = \psi(\theta(\boldsymbol{s}, \boldsymbol{s}')), \qquad \boldsymbol{s} = (L, \ell), \quad \boldsymbol{s}' = (L', \ell'),$$

for some continuous function $\psi : [0, \pi] \to \mathbb{R}$ that admits a uniquely determined expansion (15) with Schoenberg sequence $\{b_n\}$ having elements defined through

$$b_n = (n + 1/2)c(n), \qquad n = 0, 1, \dots.$$

Proposition 1 is not only of independent interest: in view of it, Theorem 2 below generalizes Corollary 1 in Xu and Cheney (1992). Specifically, Theorem 2 provides conditions for strict positive definiteness of a given covariance function that is axially symmetric on the sphere, while Xu and Cheney's result gives conditions for strict positive definiteness of an isotropic covariance function.

Theorem 2. *Let $\{c_m(\cdot, \cdot)\}_{m=0}^{\infty}$ be a sequence of mappings such that, for each fixed $m \geq 0$, $c_m : \{m, m+1, \dots\} \times \{m, m+1, \dots\} \to \mathbb{C}$ is strictly positive definite. Then, the mapping K defined through (17) is strictly positive definite as well.*

3.1 Fourier inversions for Axially Symmetric covariance functions

We now show that, under some additional conditions on the sequences $\{c_m(\cdot,\cdot)\}$, it is possible to specify the analogue of the Fourier inversion formula (16) obtained under the simpler case of isotropy.

Theorem 3. *Let K be the function defined through (17). If*

$$\sum_{n,n'=0}^{\infty} \sqrt{\left(n+\frac{1}{2}\right)\left(n'+\frac{1}{2}\right)} \sup_{m\in\{-(n\wedge n'),\dots,n\wedge n'\}} \left|c_m(n,n')\right| < \infty, \tag{18}$$

then, for each $m = 0, 1, \dots,$ the functions $c_m : \{m, m+1, \dots\} \times \{m, m+1, \dots\} \to \mathbb{C}$ in (17) are uniquely determined through

$$c_m(n,n') = \frac{1}{2\pi}\int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2}\int_{-\pi}^{\pi} K(L,L',\Delta\ell)e^{-\mathrm{i}m\Delta\ell}\bar{P}_{n'}^{m}(\sin L')\bar{P}_{n}^{m}(\sin L)\cos L\cos L'\mathrm{d}\Delta\ell\mathrm{d}L\mathrm{d}L'. \tag{19}$$

We conclude this section with an example. Emery et al. (2019) consider the following axially symmetric covariance function:

$$K_\Lambda(L,L',\Delta\ell) = \sum_{n=0}^{\infty} b_n \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n^m(\sin L)P_n^m(\sin L')\cos(m\Delta\ell)\mathrm{sinc}^2(m\Lambda), \tag{20}$$

where $\{b_n\}_{n=0}^{\infty}$ is a sequence of non negative numbers that sum up to one, $\Lambda \in [0,\pi]$ and sinc denotes the cardinal sine function, namely $\mathrm{sinc}(x) = \sin(x)/x$ for every $x \in \mathbb{R}\setminus\{0\}$ and $\mathrm{sinc}(0) = 1$. Since (10), $\cos(m\Delta\ell) = (e^{\mathrm{i}m\Delta\ell} + e^{-\mathrm{i}m\Delta\ell})/2$ and sinc is an even function, it is not difficult to verify that (20) becomes

$$K_\Lambda(L,L',\Delta\ell) = \sum_{n=0}^{\infty} b_n \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n^m(\sin L)P_n^m(\sin L')e^{\mathrm{i}m\Delta\ell}\mathrm{sinc}^2(m\Lambda). \tag{21}$$

Thanks to (25) in Appendix A, we can swap the two series in (21) obtaining:

$$K_\Lambda(L,L',\Delta\ell) = \sum_{m=-\infty}^{\infty}\sum_{n=|m|}^{\infty} b_n \frac{(n-m)!}{(n+m)!} P_n^m(\sin L)P_n^m(\sin L')e^{\mathrm{i}m\Delta\ell}\mathrm{sinc}^2(m\Lambda). \tag{22}$$

We can now see that K_Λ satisfies the representation given by (17) if we take:

$$c_m(n,n') = \frac{b_n}{2n+1}\mathrm{sinc}^2(m\Lambda)\delta_{nn'},$$

for every $n, n' \geq |m|$ and every $m \in \mathbb{Z}$, and, by Theorem 2, K_Λ is strictly positive definite if $b_n > 0$, for every $n \geq 0$, and $\Lambda/\pi \notin \mathbb{Q}$.

4 Conclusions

This paper has provided a criterion for strict positive definiteness of covariance functions that are axially symmetric on the sphere embedded in $\mathbb{R}^3$. This work opens for other relevant questions. Given the popularity of Stein's approach (Stein, 2007), it would be relevant to explore the strict positive definiteness of the expansion (17) if truncation at a finite order is imposed. In the isotropic case, this question would have a simple solution, but under axial symmetry things become quite complicated.

The Fourier inversion provided in Theorem 3 might be very useful to explore the properties of Gaussian fields on spheres having axially symmetric covariance functions. The works of Lang and Schwab (2013) and Clarke et al. (2018) show that the rate of decay of the Schoenberg sequences are crucial to determine the regularity properties, understood in terms of interpolation spaces, of the associated Gaussian random field. The Fourier inversion provided by Theorem 3, in concert with Mercer expansion, might provide the key to extend the mentioned result to the axially symmetric case.

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A Appendix: Mathematical Proofs and Lemmas

A.1 Proof of Proposition 1

Proof. We start by making use of the assumption $c_m(n,n') = c(n)\delta_{nn'}$ to write

$$\begin{aligned} K(L,&L',\Delta\ell) \\ &= \sum_{m=-\infty}^{\infty} \sum_{n,n'=|m|}^{\infty} e^{\mathrm{i}m\Delta\ell} \bar{P}_n^m(\sin L)\bar{P}_{n'}^m(\sin L')c(n)\delta_{nn'} \\ &= \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} e^{\mathrm{i}m\Delta\ell} \bar{P}_n^m(\sin L)\bar{P}_n^m(\sin L')c(n). \end{aligned} \tag{23}$$

The two sums in (23) can be interchanged provided

$$\sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left| \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \right| c(n) < \infty. \tag{24}$$

To show it, we note that Cauchy-Schwartz inequality in concert with (12) show that, for every $n \geq 0$,

$$\sum_{m=-n}^{n} \left| \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \right| \leq \sqrt{\sum_{m=-n}^{n} (\bar{P}_n^m(\sin L))^2 \sum_{m=-n}^{n} (\bar{P}_n^m(\sin L'))^2} = n + \frac{1}{2}. \tag{25}$$

The fact that $\sum_{n=0}^{\infty}(n + 1/2)c(n) < \infty$ proves that (24) holds true, so that the interchange is legitimate. Therefore, we can swap the two sums in (23) and write:

$$K(L, L', \Delta\ell) = \sum_{n=0}^{\infty} c(n) \sum_{m=-n}^{n} e^{\mathrm{i}m\Delta\ell} \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L'). \tag{26}$$

By (10),

$$\bar{P}_n^{-m}(\sin L) \bar{P}_n^{-m}(\sin L') = \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \tag{27}$$

so that:

$$\begin{aligned} &c(n)\{e^{-\mathrm{i}m\Delta\ell} \bar{P}_n^{-m}(\sin L) \bar{P}_n^{-m}(\sin L') + e^{\mathrm{i}m\Delta\ell} \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L')\} \\ &\quad = 2c(n) \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \cos(m\Delta\ell), \end{aligned}$$

and therefore (26) yields:

$$\begin{aligned} &K(L, L', \Delta\ell) \\ &\quad = \sum_{n=0}^{\infty} c(n) \left\{ 2 \sum_{m=1}^{n} \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \cos(m\Delta\ell) + \bar{P}_n^0(\sin L) \bar{P}_n^0(\sin L') \right\}, \end{aligned}$$

which by (27) and recalling that the cosine is an even function, yields:

$$\begin{aligned} &K(L, L', \Delta\ell) \\ &\quad = \sum_{n=0}^{\infty} c(n) \sum_{m=-n}^{n} \bar{P}_n^m(\sin L) \bar{P}_n^m(\sin L') \cos(m\Delta\ell) \\ &\quad = \sum_{n=0}^{\infty} c(n)(2n+1) \frac{1}{2} \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n^m(\sin L) P_n^m(\sin L') \cos(m\Delta\ell), \end{aligned}$$

which by the spherical harmonics addition theorem (3) yields

$$K(L, L', \Delta\ell) = \sum_{n=0}^{\infty} c(n) \left(n + \frac{1}{2}\right) P_n(\langle \boldsymbol{s}, \boldsymbol{s}' \rangle), \tag{28}$$

where $\boldsymbol{s}, \boldsymbol{s}'$ belong to $\mathbb{S}^2$, so that $\boldsymbol{s} = (L, \ell)$ and $\boldsymbol{s}' = (L', \ell')$. □

A.2 Auxiliary Lemmas

To provide a constructive proof of Theorem 2, two auxiliary results are required.

Lemma 4. *Fix $m \in \mathbb{Z}$ and let $w_1, \ldots, w_h$ be h distinct points in $(-1, 1)$ such that*

$$\sum_{r=1}^{h} z_r \bar{P}_n^m(w_r) = 0 \tag{29}$$

for every $n \in \{|m|, |m| + 1, \ldots\}$ and for some complex h-ple $(z_1, \ldots, z_h)$. Then, $z_r = 0$ for every $r = 1, \ldots, h$.

Proof. The identity (29) implies that

$$\sum_{r=1}^{h} \mathrm{Re}(z_r) \bar{P}_n^m(w_r) = 0 \tag{30}$$

$$\sum_{r=1}^{h} \mathrm{Im}(z_r) \bar{P}_n^m(w_r) = 0 \tag{31}$$

for every $n \in \{|m|, |m| + 1, \ldots\}$.

At this stage, recall that

$$\bar{P}_n^m(x) = k_{m,n}(1 - x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} P_n(x)$$

where $k_{m,n}$ is a non zero constant, for each $n \in \{|m|, |m| + 1, \ldots\}$ and $x \in (-1, 1)$.

Consider now a polynomial p of degree at most $h - 1$ such that

$$p(w_r) = \mathrm{Re}(z_r)/\{(1 - w_r^2)^{|m|/2}\}, \tag{32}$$

for $r = 1, \ldots, h$, and let q be a polynomial of degree at most $h + |m| - 1$ such that the $|m|$-th partial derivative of q is p. Since the ordinary Legendre polynomials $P_0, \ldots, P_{|m|+h-2}$ are known to generate the $(|m| + h - 1)$-dimensional polynomial space, there exist $d_0, \ldots, d_{|m|+h-2} \in \mathbb{R}$ such that

$$d_0 P_0 + \ldots + d_{|m|+h-2} P_{|m|+h-2} = q,$$

which taking the $|m|$–th derivative of both sides and multiplying by $(1-x^2)^{|m|/2}$, yields that:

$$\frac{d_{|m|}}{k_{m,|m|}}\bar{P}^m_{|m|}(x)+\ldots+\frac{d_{|m|+h-2}}{k_{m,|m|+h-2}}\bar{P}^m_{|m|+h-2}(x)=(1-x^2)^{|m|/2}p(x) \tag{33}$$

for every $x\in(-1,1)$. Hence, we can consider the following function

$$f(x)=\frac{d_{|m|}}{k_{m,|m|}}P^m_{|m|}(x)+\ldots+\frac{d_{|m|+h-2}}{k_{m,|m|+h-2}}P^m_{|m|+h-2}(x)$$

knowing that by (32) and (33) we have that

$$f(w_r)=\mathrm{Re}(z_r) \tag{34}$$

as $r=1,\ldots,h$. By (30), we have that

$$\sum_{r=1}^{h}\mathrm{Re}(z_r)f(w_r)=0,$$

which by (34) yields that

$$\sum_{r=1}^{h}\mathrm{Re}(z_r)^2=0, \tag{35}$$

We have just proved that (30) implies (35). Similarly, we can prove that (31) implies

$$\sum_{r=1}^{h}\mathrm{Im}(z_r)^2=0$$

and the proof is complete. □

Lemma 5. *Let K be an axially symmetric covariance function as in (17) such that for each $m\geq 0$, $c_m:\{m,m+1,\ldots\}\times\{m,m+1,\ldots\}\to\mathbb{C}$ is a strictly positive definite function. Then, for $a=(a_1,\ldots,a_k)\in\mathbb{R}^k$ and $\boldsymbol{s}_1,\ldots,\boldsymbol{s}_k$ distinct points in $\mathbb{S}^2$ such that the longitude and the latitude of $\boldsymbol{s}_j$ are $\ell_j\in(-\pi,\pi]$ and $L_j\in[-\pi/2,\pi/2]$, respectively ($j=1,\ldots,k$), the following assertions are equivalent:*

(i) $a^TKa=0$, *that is,*

$$\sum_{j,h=1}^{k}a_jK(L_j,L_h,\Delta\ell_{jh})a_h=0,\qquad(\Delta\ell_{jh}:=\ell_j-\ell_h). \tag{36}$$

(ii) The equality

$$\sum_{j=1}^{k} a_j e^{\mathrm{i}m\ell_j} \bar{P}_n^m(\sin L_j) = 0. \tag{37}$$

holds for each $m \in \mathbb{Z}$ and each $n \in \{|m|, |m|+1, \dots\}$,

Proof. Note that

$$\begin{aligned} a^T K a &:= \sum_{j,h=1}^{k} a_j K(L_j, L_h, \Delta\ell_{jh}) a_h = \\ &= \sum_{j,h=1}^{k} a_j a_h \sum_{m=-\infty}^{\infty} \sum_{n,n'=|m|}^{\infty} e^{\mathrm{i}m\Delta\ell_{jh}} \bar{P}_n^m(\sin L_j) \bar{P}_{n'}^m(\sin L_h) c_m(n,n') \\ &= \sum_{m=-\infty}^{\infty} \sum_{n,n'=|m|}^{\infty} c_m(n,n') \left\{ \sum_{j=1}^{k} a_j e^{\mathrm{i}m\ell_j} \bar{P}_n^m(\sin L_j) \right\} \left\{ \sum_{h=1}^{k} a_h e^{-\mathrm{i}m\ell_h} \bar{P}_n^m(\sin L_h) \right\}. \end{aligned} \tag{38}$$

Hence, it is clear that *(ii)* implies *(i)*. Now suppose that *(i)* holds. Combining (36) and (38), we have that:

$$\sum_{m=-\infty}^{\infty} \sum_{n,n'=|m|}^{\infty} c_m(n,n') b_{n,m} b^*_{n',m} = 0 \tag{39}$$

where

$$b_{n,m} = \sum_{j=1}^{k} a_j e^{\mathrm{i}m\ell_j} \bar{P}_n^m(\sin L_j). \tag{40}$$

Since c_m is positive definite (for every m), then

$$\sum_{n,n'=|m|}^{N} c_m(n,n') b_{n,m} b^*_{n',m} \geq 0,$$

for every N and every m. Thus, letting N diverge to infinity we have that

$$\sum_{n,n'=|m|}^{\infty} c_m(n,n') b_{n,m} b^*_{n',m} \geq 0,$$

for every m. Therefore, by (39), we have that for every $m \in \mathbb{Z}$,

$$\sum_{n,n'=|m|}^{\infty} c_m(n,n') b_{n,m} b^*_{n',m} = 0. \tag{41}$$

At this stage, for each $m, N \in \mathbb{Z}$ with $m, N > 0$, let $C_m(N)$ be the $N \times N$ matrix whose $(n-m+1, n'-m+1)$ entry is $c_m(n,n')$ $(n, n' = m, \dots, N+m-1)$.

For each $m, N \in \mathbb{Z}$ with $N, m > 0$, the matrix $C_m(N)$ must be positive definite since by assumption, for each $m \in \mathbb{Z}$, $c_m(n, n')$ is strictly positive definite. Hence, by Cholesky decomposition, there is a complex $N \times N$ lower triangular matrix $A_m(N)$ such that $C_m(N) = A_m(N)A_m(N)^*$ the diagonal entries of $A_m(N)$ are real and positive and the matrix $A_0(N)$ is real. Denoting by $a_{nr}^{(m,N)}$ the $(n - m + 1, r - m + 1)$ entry of the matrix $A_m(N)$ if $N, m > 0$, the Cholesky decomposition of the matrix $C_m(N)$ can be written in the following form:

$$c_m(n, n') = \sum_{r=m}^{n \wedge n'} a_{nr}^{(m,N)} a_{n'r}^{(m,N)*},$$

for $n, n' = m, \ldots, N + m - 1$, where $x \wedge y$ denotes the minimum among x and y. If $M \geq N$, then by the Cholesky decomposition of the matrix $C_m(M)$ we have that:

$$\sum_{r=m}^{n \wedge n'} a_{nr}^{(m,M)} a_{n'r}^{(m,M)*} = \sum_{r=m}^{n \wedge n'} a_{nr}^{(m,N)} a_{n'r}^{(m,N)*},$$

for $n, n' = m, \ldots, N + m - 1$. Note the Cholesky decomposition of $C_m(N)$ is unique being $C_m(N)$ positive definite and therefore $a_{nr}^{(m,N)} = a_{nr}^{(m,M)}$ if $m \leq r \leq n \leq N+m-1 \leq M+m-1$. In particular, we have that $a_{nr}^{(m,n-m+1)} = a_{nr}^{(m,M)}$ for any quartet (m, r, n, M) where $m \leq r \leq n \leq M - m + 1$. Therefore, we can write $a_{nr}^{(m)}$ for $a_{nr}^{(m,n-m+1)}$ and

$$c_m(n, n') = \sum_{r=|m|}^{n \wedge n'} a_{nr}^{(m)} a_{n'r}^{(m)*}, \tag{42}$$

where for each r, $a_{rr}^{(m)} > 0$. Note that (42) holds also for $m < 0$ if we let $a_{nr}^{(-m)} = a_{nr}^{(m)*}$. Substituting (42) in (41) we obtain that, for every $m \in \mathbb{Z}$,

$$\sum_{n,n'=|m|}^{\infty} \sum_{r=|m|}^{n \wedge n'} a_{nr}^{(m)} a_{n'r}^{(m)*} b_{n,m} b_{n',m}^* = 0,$$

that is equivalent to:

$$\sum_{r=|m|}^{\infty} \sum_{n,n'=r}^{\infty} a_{nr}^{(m)} a_{n'r}^{(m)*} b_{n,m} b_{n',m}^* = 0,$$

which in turn is equivalent to:

$$\sum_{r=|m|}^{\infty} \left| \sum_{n=r}^{\infty} a_{nr}^{(m)} b_{n,m} \right|^2 = 0,$$

which implies that for every $r \geq |m|$

$$\sum_{n=r}^{\infty} a_{nr}^{(m)} b_{n,m} = 0. \tag{43}$$

Thus, for every fixed $m \in \mathbb{Z}$ and every fixed $r \geq |m|$ we can write:

$$\sum_{n=r+s}^{\infty} a_{n,r+s}^{(m)} b_{n,m} = 0, \tag{44}$$

for $s = 0, 1, 2, \ldots$ Recalling that $a_{r+s,r+s}^{(m)} > 0$ for each s, we can define a sequence $(d_s)_{s=0}^{\infty}$ according to the recursion:

$$d_0 = 1,\ d_1 = -\frac{a_{r+1,r}^{(m)}}{a_{r+1,r+1}^{(m)}}, \ldots, d_s = -\frac{1}{a_{r+s,r+s}^{(m)}} \sum_{l=0}^{s-1} d_l a_{r+s,r+l}^{(m)}, \ldots$$

This ensures that:

$$\sum_{s=0}^{t} d_s a_{r+t,r+s} = 0$$

for $t = 1, 2, \ldots$ and therefore by (44),

$$\begin{aligned}
0 &= \sum_{s=0}^{\infty} d_s \sum_{n=r+s}^{\infty} a_{n,r+s}^{(m)} b_{n,m} = \sum_{n=r}^{\infty} b_{n,m} \sum_{s=0}^{n-r} d_s a_{n,r+s}^{(m)} \\
&= b_{r,m} d_0 a_{r,r}^{(m)} + \sum_{n=r+1}^{\infty} b_{n,m} \sum_{s=0}^{n-r} d_s a_{n,r+s}^{(m)} \\
&= b_{r,m} a_{r,r}^{(m)} + \sum_{t=1}^{\infty} b_{r+t,m} \sum_{s=0}^{t} d_s a_{r+t,r+s}^{(m)} = b_{r,m} a_{r,r}^{(m)}.
\end{aligned}$$

We have just proved that $b_{r,m} a_{r,r}^{(m)} = 0$ for any $m \in \mathbb{Z}$ and any $r \geq |m|$. At this stage, recall once again that $a_{r,r}^{(m)} > 0$ for any (m, r). Therefore, for any $m \in \mathbb{Z}$ and any $r \geq |m|$, $b_{r,m} = 0$, namely by (40)

$$\sum_{j=1}^{k} a_j e^{\mathrm{i} m \ell_j} \bar{P}_n^m (\sin L_j) = 0 \tag{45}$$

for each $m \in \mathbb{Z}$ and each $n \in \{|m|, |m| + 1, \ldots\}$, proving *(ii)* . $\square$

Now we are ready to prove our main result.

A.3 Proof of Theorem 2

Proof. We aim at proving that if $(a_1, \dots, a_k) \in \mathbb{R}^k$, and $\boldsymbol{s}_1, \dots, \boldsymbol{s}_k$ are k distinct points in $\mathbb{S}^2$ such that the longitude and the latitude of $\boldsymbol{s}_j$ are $\ell_j \in (-\pi, \pi]$ and $L_j \in [-\pi/2, \pi/2]$, respectively ($j = 1, \dots, k$), and

$$\sum_{j,h=1}^{k} a_j K(L_j, L_h, \Delta\ell_{jh}) a_h = 0, \tag{46}$$

then $a_j = 0$ for $j = 1, \dots, k$.

By Lemma 5, letting $m = 0$, we obtain:

$$\sum_{j=1}^{k} a_j \bar{P}_n(\sin(L_j)) = 0 \tag{47}$$

for every $n \in \{0, 1, 2, \dots\}$, where $\bar{P}_n$ denotes the ordinary normalized Legendre polynomial of degree n.

By denoting $L_{(1)}, \dots, L_{(h)}$ the distinct elements among $L_1, \dots, L_k$ and letting $a_{(r)} = \sum_{j \in B_r} a_j$ where $B_r = \{j = 1, \dots, k : L_j = L_{(r)}\}$, as $r = 1, \dots, h$, the equation (47) becomes:

$$\sum_{j=1}^{h} a_{(j)} \bar{P}_n(\sin L_{(j)}) = 0 \tag{48}$$

for every $n \in \{0, 1, 2, \dots\}$.

At this stage, consider the following function:

$$p(L) = \sum_{n \in E} d_n \bar{P}_n(\sin L),$$

where E is a finite or infinite subset of $\{0, 1, 2, \dots\}$, so that by (48),

$$\sum_{j=1}^{h} a_{(j)} p(L_{(j)}) = 0. \tag{49}$$

There exist $\{d_n \in \mathbb{R} : n \in E\}$ for some set E such that $p(L_{(j)}) = a_{(j)}$ for $j = 1, \dots, h$. Indeed, we can just take $E = \{0, 1, \dots, h-1\}$ recalling that $\bar{P}_0, \dots, \bar{P}_{h-1}$ generate the h–dimensional polynomial space and that interpolation of arbitrary data at h nodes is possible. Hence, by (49), $\sum_{j=1}^{h} a_{(j)}^2 = 0$ and therefore $a_{(j)} = 0$, namely

$$\sum_{j \in B_r} a_j = 0, \quad j = 1, \dots, h. \tag{50}$$

Now note that if $L_j \in \{-\pi/2, \pi/2\}$ then $\boldsymbol{s}_j$ is a pole and therefore $L_i \neq L_j$ for any $i \neq j$ since $\boldsymbol{s}_1, \dots, \boldsymbol{s}_n$ are distinct points (*i.e.*, $B_r = \{j\}$ if $L_j \in \{-\pi/2, \pi/2\}$). Hence, by (50), we have just proved that if $L_j \in \{-\pi/2, \pi/2\}$ then $a_j = 0$.

Hence , the equation (45) becomes:

$$\sum_{r=1}^{h} \sum_{j \in B_r} a_j e^{\mathrm{i}m\ell_j} \bar{P}_n^m(\sin L_{(r)}) = 0, \tag{51}$$

for each $m \in \mathbb{Z}$ and each $n \in \{|m|, |m|+1, \dots\}$. Since $\overline{P}_n^m(\pm 1) = 0$, (51) becomes:

$$\sum_{r \in A} \sum_{j \in B_r} a_j e^{\mathrm{i}m\ell_j} \bar{P}_n^m(\sin L_{(r)}) = 0 \tag{52}$$

where $A = \{r = 1, \dots, h : L_r \notin \{-\pi/2, \pi/2\}\}$, for each $m \in \mathbb{Z}$ and each $n \in \{|m|, |m|+1, \dots\}$. Moreover, since we have just proved that $a_j = 0$ if $L_j = \pm\pi/2$, then we need to show that $a_j = 0$ for all $j \in B_r$ and for all $r \in A$.

By Lemma 4, (52) implies that:

$$\sum_{j \in B_r} a_j e^{\mathrm{i}m\ell_j} = 0 \tag{53}$$

for every $m \in \mathbb{Z}$ and $r \in A$. At this stage, observe that $\ell_i \neq \ell_j$ when $i, j \in B_r$ because in this case $L_i = L_j$ and $\boldsymbol{s}_i \neq \boldsymbol{s}_j$. Moreover, the matrix of the system (53) is Vandermonde–like associated to the distinct points $e^{\mathrm{i}\ell_j}$, $j \in B_r$ for each $r \in A$. Therefore, (53) implies that $a_j = 0$ for each $j = 1, \dots, k$ such that $L_j \notin \{-\pi/2, \pi/2\}$ and the proof is complete. □

A.4 Proof of Theorem 3

Proof. In order to evaluate the integral in the right hand side of (19), we can plug in (17) and swap the double series and the triple integral if the following is verified:

$$\int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} \sum_{n,n'=0}^{\infty} \sum_{m=-(n \wedge n')}^{n \wedge n'} g_{m_0,n_0,n'_0}^{(m,n,n')}(\Delta\ell, L, L') \mathrm{d}\Delta\ell \mathrm{d}L \mathrm{d}L' < \infty, \tag{54}$$

where:

$$g_{m_0,n_0,n'_0}^{(m,n,n')}(\Delta\ell, L, L') = \left| e^{im\Delta\ell} \bar{P}_n^m(\sin L) \bar{P}_{n'}^m(\sin L') c_m(n,n') e^{-\mathrm{i}m_0\Delta\ell} \bar{P}_{n_0}^{m_0}(\sin L) \bar{P}_{n'_0}^{m_0}(\sin L') \cos L \cos L' \right|$$

for every $m_0 \in \mathbb{Z}$ and $n_0, n'_0 \geq |m_0|$. Trivially,

$$g_{m_0,n_0,n'_0}^{(m,n,n')}(\Delta\ell, L, L') \leq \left| \bar{P}_n^m(\sin L) \bar{P}_{n'}^m(\sin L') c_m(n,n') \bar{P}_{n_0}^{m_0}(\sin L) \bar{P}_{n'_0}^{m_0}(\sin L') \right|. \tag{55}$$

At this stage, note that by (12),

$$\left|\bar{P}_n^m(\sin L)\right| \leq \sqrt{n+\frac{1}{2}},$$

for every $m, n \in \mathbb{Z}$ with $n \geq |m|$, and therefore (55) yields:

$$g_{m_0,n_0,n_0'}^{(m,n,n')}(\Delta\ell, L, L') \leq \left|\bar{P}_n^m(\sin L)\bar{P}_{n'}^m(\sin L')c_m(n,n')\sqrt{(n_0+1/2)(n_0'+1/2)}\right|,$$

which, by the Cauchy–Schwartz inequality and (12), in turn yields:

$$\begin{aligned}\sum_{m=-(n\wedge n')}^{n\wedge n'} g_{m_0,n_0,n_0'}^{(m,n,n')}(\Delta\ell, L, L') \quad &\leq \quad \sqrt{\left(n_0+\frac{1}{2}\right)\left(n_0'+\frac{1}{2}\right)\left(n+\frac{1}{2}\right)\left(n'+\frac{1}{2}\right)} \\ &\times \sup_{m\in\{-(n\wedge n'),\ldots,n\wedge n'\}} \left|c_m(n,n')\right|,\end{aligned}$$

which by (18) implies that (54) is verified. It is therefore possible to plug (17) into the integral in (19) and swap the double sum with the triple integral. In this way, due to the orthogonality of the associated Legendre polynomials $\{\bar{P}_n^m(\sin L) : n \in \mathbb{N}\}$ given by (6) and of $\{e^{im\ell} : m \in \mathbb{Z}\}$, and due to (7), (19) is obtained. □

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