Admissible Nested Covariance Models over Spheres cross Time

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Abstract

Nested covariance models have been very popular in many branches of applied statistics, and in particular in geostatistics. A notorious limit of nested models is that the constants in the linear combination are bound to be nonnegative in order to preserve positive definiteness (admissibility). This paper studies nested models on d-dimensional spheres and spheres cross time. We show the exact interval of admissibility for the constants involved in the linear combinations. In particular, we show that at least one constant can be negative. One of the implications is that one can obtain a nested model attaining negative correlations. We provide characterization theorems for arbitrary linear combinations as well as for nonconvex combinations involving two covariance functions. We illustrate our findings through several examples involving nonconvex combinations of well-known parametric families of covariance functions.

Keywords: Covariance functions; Nested Models; Negative Covariance; Spheres.

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1 Introduction

Nested covariance models are linear combinations of covariance functions. They have an old history that can be traced back to geostatistics, and the reader is referred to Chilès and Delfiner (2012); Gregori et al. (2008); Journel and Huijbregts (1978); Wackernagel (2003); Porcu et al. (2006, 2013); Daley et al. (2015); De Iaco and Posa (2018) and Kleiber and Porcu (2015) for earlier as well as more recent examples.

The notorious limit in the construction of nested models is that the weights are bound to be nonnegative, in order to preserve positive definiteness. Such a drawback has been noted, for instance, by Gregori et al. (2008), who found conditions such that at least one negative weight in the linear combination of isotropic covariance functions in d-dimensional Euclidean spaces can be negative.

Admissible nested models with negative weights have important consequences to several branches of applied sciences. On the one hand, negative weights can allow for negative covariances or covariances oscillating between positive and negative values (see Yakhot et al., 1989). On the other hand, nested models with negative weights have recently become popular thanks to the notable approach by Bonat and Jørgensen (2016), who consider nontrivial extension for the Generalized Linear Model (GLM) to the case of multivariate covariates. The method is called multivariate covariance generalized linear model (MCGLM). In particular, the authors suggest to replace the identity matrix in the classical GLM setting with a matrix Ω that is implicitly specified through the relation

$$h(\Omega) = \sum_{k=0}^{N} \tau_k C_k,$$

where τ_k are real constants and C_k are known matrices reflecting the covariance structure. Since positive definite functions are closed under nonlinear combinations involving non negative constants, there is an apparent issue in specifying this model, in particular in knowing explicit restrictions for the parametric space of the constants τ_k. The idea of modelling a function of the covariance matrix by a linear structure goes back to Pourahmadi (1999, 2011) and Pan and Mackenzie (2003) among others (see Bonat and Jørgensen, 2016, for a thorough review). In particular, Bonat and Jørgensen (2016) emphasize the need to model the covariance structure explicitly, rather than treating it as a nuisance parameter. Taking verbatim from Bonat and Jørgensen (2016): *many researchers claim that a suitable covariance link function must provide an unrestricted and interpretable parameterization. Although laudable, such a goal is probably overoptimistic and does not seem to have been achieved yet, at least not for the general case.* The authors propose a numerical approach to this problem in order to get realistic values for $\tau_0, \dots, \tau_N$. This paper offers an analytic approach that allows to determine the exact range for the parameters involved in a arbitrary linear combination.
A third consequence of nested models with only nonnegative weights is that it has important implications in terms of statistical inference and testing, since, for instance, the value $\tau_k = 0$, for $k = 0, \dots, N$, lies on the boundary of the parameter space. Some criticism about this fact

is expressed in Bevilacqua et al. (2012).

The problem of linear combinations of covariance functions in Euclidean spaces has been considered in Gregori et al. (2008) who propose the special case of the product sum model (and similar extensions). Motivated by the increasing need of statistical techniques for global data, typically defined over the sphere representing planet Earth, this paper considers linear combinations of covariance functions defined over spheres or over spheres across time. The fact that such covariances are defined over spheres implies that the natural metric to be used is the geodesic distance, and this fact has a nontrivial implication in terms of mathematical framework needed to implement valid covariance functions.

There has been a fervent activity in the last five years around positive definite functions on spheres, as well as on positive definite functions on spheres cross time. The seminal paper by Gneiting (2013) provides a thorough overview of spherically isotropic positive definite kernels on sphere, with applications to probability theory, spatial statistics, numerical analysis and approximation theory, amongst others. Berg and Porcu (2017) provided the extension of the classical characterization theorem for positive definite functions on spheres to the case of the spheres cross time. Porcu et al. (2016) focussed on the geostatistical implications of using the geodesic distance for global data and the discrepancies in estimation and prediction when using the incorrect metric. The nonstationary case has been considered in Estrade et al. (2017). Regularity properties of Gaussian fields on spheres and spheres across time have been studied by Lang and Schwab (2015) and Clarke et al. (2018) respectively.

This paper determines the exact range for the weights involving arbitrary linear combinations of space or space-time covariance functions . The plan of the paper is the following: Section 2 contains the background material needed for understanding the problem. Section 3 provides results involving linear combinations of spatial covariance functions. Section 4 is devoted to the space-time case. We then offer, in Section 5, a list of examples that are useful for practitioners. The paper ends with a short discussion.

2 Mathematical Background

Let d be a positive integer. We define the d-dimensional unit sphere by $\mathbb{S}^d = \{\mathbf{x} \in \mathbb{R}^{d+1},\ \|\mathbf{x}\| = 1\}$, where $d \in \mathbb{N}$, and $\|\cdot\|$ is the Euclidean distance. The geodesic distance between any pair of points $\mathbf{x}, \mathbf{y}$ on $\mathbb{S}^d$ is defined as $\theta(\mathbf{x}, \mathbf{y}) = \arccos(\langle \mathbf{x}, \mathbf{y}\rangle)$, where $\langle \cdot, \cdot \rangle$ is the standard inner product on $\mathbb{R}^{d+1}$. Throughout the text, we use the abuse of notation θ for $\theta(\mathbf{x}, \mathbf{y})$ whenever no confusion can arise. Let $L^2(\mathbb{S}^d, \omega_d)$ be the space of squared-integrable real-valued functions on the sphere $\mathbb{S}^d$ with respect to the uniquely determined Haar measure on the sphere, denoted ω_d. The surface measure of the sphere has a total mass given by

$$\|\omega_d\| = \frac{2\pi^{(d+1)/2}}{\Gamma((d+1)/2)}.$$

Let X be a nonempty set. A function $\mathbb{K} : X \times X \to \mathbb{R}$ is called *positive definite on X* if for any system of constants $\{c_k\}_{k=1}^N \subset \mathbb{R}$ and any finite dimensional collection of points

$\{x_k\}_{k=1}^N \subset X$, one has

$$\sum_{k=1}^N \sum_{h=1}^N c_k \mathbb{K}(x_k, x_h) c_h \geq 0.$$

If the inequality above is strict when at least one c_k is nonzero, then $\mathbb{K}$ is called *strictly positive definite* (Menegatto, 1995).

2.1 The Class $\mathcal{P}(\mathbb{S}^d)$

We define $\mathcal{P}(\mathbb{S}^d)$ as the class of continuous functions $\psi : [0,\pi] \to \mathbb{R}$ with $\psi(0) = 1$ such that $\mathbb{K}(x,y) := \psi(\theta(x,y))$ is positive definite on $\mathbb{S}^d$. We also define $\mathcal{P}(\mathbb{S}^\infty) := \cap_{d\geq 1}\mathcal{P}(\mathbb{S}^d)$, with the inclusion relation $\mathcal{P}(\mathbb{S}^\infty) \subset \cdots \subset \mathcal{P}(\mathbb{S}^d) \subset \mathcal{P}(\mathbb{S}^{d-1}) \subset \cdots \subset \mathcal{P}(\mathbb{S}^1)$.

Let us define the Gegenbauer polynomials $C_n^{(\lambda)}$ through the intrinsic relation (see Dai and Xu, 2013; Atkinson and Han, 2012)

$$(1 - 2xr + r^2)^{-\lambda} = \sum_{n=0}^\infty C_n^{(\lambda)}(x) r^n, \quad |r| < 1, \quad x \in [-1,1], \tag{2.1}$$

where $\lambda > 0$. For $\lambda = 0$, (2.1) has to be replaced by

$$\frac{1 - xr}{1 - 2xr + r^2} = \sum_{n=0}^\infty C_n^{(0)}(x) r^n, \quad |r| < 1, \quad x \in [-1,1],$$

where it is known that $C_n^{(0)}(x) = \cos(n \arccos x)$. For $\lambda > 0$, it is true that

$$\int_{-1}^1 (1-x^2)^{\lambda - 1/2} C_n^{(\lambda)}(x) C_m^{(\lambda)}(x) \, \mathrm{d}x = \frac{\pi \Gamma(n + 2\lambda) 2^{1-2\lambda}}{\Gamma^2(\lambda)(n+\lambda) n!} \delta_{m,n}, \tag{2.2}$$

with $\delta_{m,n}$ denoting the Kronecker delta. When $\lambda = 0$, Equation (2.2) simplifies to

$$\int_{-1}^1 (1-x^2)^{-1/2} C_n^{(0)}(x) C_m^{(0)}(x) \, \mathrm{d}x = \begin{cases} (\pi/2)\delta_{m,n} & \text{if } n > 0 \\ \pi \delta_{m,n} & \text{if } n = 0, \end{cases}$$

which is equivalent to the classical orthogonality relations of the family $\cos(nx), n = 0, 1, \ldots$ (Berg and Porcu, 2017). It is important to note that $C_n^{(\lambda)}(1) = (2\lambda)_n / n!$, with $(a)_n$ denoting the Pochammer symbol. Another important fact is that $|C_n^{(\lambda)}(x)| \leq C_n^{(\lambda)}(1)$, for $x \in [-1,1]$.

We now follow Berg and Porcu (2017) to illustrate the relation between Gegenbauer polynomials and spherical harmonics. A spherical harmonic of degree n for $\mathbb{S}^d$ is the restriction to $\mathbb{S}^d$ of a real-valued harmonic homogeneous polynomial in $\mathbb{R}^{d+1}$ of degree n. Together with the zero function, the spherical harmonics of degree n form a finite dimensional vector space denoted $\mathcal{H}_n(d)$. It is a subspace of the space $\mathcal{C}(\mathbb{S}^d)$ of continuous functions on $\mathbb{S}^d$. One has

$$N_n(d) := \dim \mathcal{H}_n(d) = \frac{(d)_{n-1}}{n!}(2n + d - 1), \; n \geq 1, \quad N_0(d) = 1,$$

(see Atkinson and Han, 2012).

Due to the fact that the spaces $\mathcal{H}_n(d)$ are mutually orthogonal subspaces of the Hilbert space $L^2(\mathbb{S}^d, \omega_d)$, which is in turn generated by them, we have that any $F \in L^2(\mathbb{S}^d, \omega_d)$ has an orthogonal expansion of the type

$$F = \sum_{n=0}^{\infty} S_n, \quad S_n \in \mathcal{H}_n(d), \quad \|F\|_2^2 = \sum_{n=0}^{\infty} \|S_n\|_2^2, \tag{2.3}$$

where the first series converges in $L^2(\mathbb{S}^d, \omega_d)$, and the second series is Parseval's equation. The orthogonal projection S_n of F onto $\mathcal{H}_n(d)$ is given by

$$S_n(\xi) = \frac{N_n(d)}{\|\omega_d\|} \int_{\mathbb{S}^d} \mathcal{G}_n(d, \xi \cdot \eta) F(\eta) \mathrm{d}\omega_d(\eta).$$

Here we are consistent with Berg and Porcu (2017) when using $\mathcal{G}_n(d,x)$ for the normalized Gegenbauer polynomial, being identically equal to 1 for $x = 1$ when $\lambda = (d-1)/2$, i.e., by

$$\mathcal{G}_n(d,x) = C_n^{((d-1)/2)}(x)/C_n^{((d-1)/2)}(1) = \frac{n!}{(d-1)_n} C_n^{((d-1)/2)}(x), \quad x \in [-1,1].$$

All these ingredients sum up to Schoenberg's theorem (Schoenberg, 1942).

Theorem 2.1. *(Schoenberg, 1942) A continuous function $\psi : [0,\pi] \to \mathbb{R}$ belongs to the class $\mathcal{P}(\mathbb{S}^d)$, $d = 1, 2, \ldots$, if and only if*

$$\psi(\theta) = \sum_{n=0}^{\infty} b_{n,d} \mathcal{G}_n(d, \cos\theta), \quad b_{n,d} \geq 0, \quad \theta \in [0,\pi], \tag{2.4}$$

for a uniquely determined probability mass sequence $(b_{n,d})_{n=0}^{\infty}$ given as

$$b_{n,d} = \frac{\|\omega_{d-1}\| N_n(d)}{\|\omega_d\|} \int_0^{\pi} \psi(x) \mathcal{G}_n(d, \cos x)(\sin x)^{d-1} \mathrm{d}x.$$

Some comments are in order. By analogy with what was done in Daley and Porcu (2014), the coefficients $b_{n,d}$ are called *d-Schoenberg coefficients* and the sequence $(b_{n,d})_{n=0}^{\infty}$ a *d-Schoenberg sequence* in Gneiting (2013). This stresses the fact that such a sequence is also related to the dimension of the sphere $\mathbb{S}^d$, where positive definiteness is attained.

When $d = 1$, the representation in Equation (2.4) reduces to

$$\psi(\theta) = \sum_{n=0}^{\infty} b_{n,1} \cos(n\theta), \quad b_{n,1} \geq 0, \quad \theta \in [0,\pi],$$

and for $d = 2$ the Gegenbauer polynomials simplify to Legendre polynomials.

The class $\mathcal{P}(\mathbb{S}^\infty)$ consists of those continuous mappings $\psi : [0,\pi] \to \mathbb{R}$ having expansion (see Schoenberg, 1942)

$$\psi(\theta) = \sum_{n=0}^{\infty} b_n (\cos\theta)^n, \quad b_n \geq 0, \quad \theta \in [0,\pi], \tag{2.5}$$

where $\sum_{n=1}^{\infty} b_n = 1$. By defining $\mathcal{G}_n(\infty, x) := x^n$, we can see how the representation (2.5) is of the same form as (2.4). A relation between the coefficients of Equations (2.4) and (2.5) can be found in a more general context in Berg et al. (2018).

A wealth of examples and interesting results are provided in Gneiting (2013). Observe that Gneiting makes explicit distinction between positive definite and strictly positive definite functions on spheres, the latter being attained when, in Equation (2.4), the d-Schoenberg coefficients are strictly positive for infinitely many even and odd n when $d \geq 2$ (Chen et al., 2003) and when $d = 1$, given integers $0 \leq j < n$, there exist $k \geq 0$ such that the d-Schoenberg coefficient $b_{nk+j,d}$ are strictly positive (Menegatto et al., 2006). Such a distinction is beyond the scope of this paper.

There is an explicit connection between Gaussian random fields and the class $\mathcal{P}(\mathbb{S}^d)$. Let $Z = \{Z(\mathbf{x}) \mid \mathbf{x} \in \mathbb{S}^d\}$ be a real-valued zero mean Gaussian random field. By Theorem 5.13 of Marinucci and Peccati (2011), Z admits a stochastic expansion being the analogue of (2.3). Such a representation is also called stochastic Peter-Weyl theorem on the sphere.

By well known facts, any positive definite function is the covariance function of a random process. For the reminder of the paper, we use equivalently both terminologies, whenever no confusion can arise.

2.2 The Class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$

We start by considering covariance functions on the real line. We call $\mathcal{P}(\mathbb{R})$ the class of continuous functions $\varphi : \mathbb{R} \to \mathbb{R}$ with $\varphi(0) = 1$ such that $\mathbb{K}(x, y) := \varphi(x - y)$ is positive definite on $\mathbb{R}$. By Bochner's theorem, such functions are represented as the Fourier transforms of probability measures μ:

$$\varphi(u) = \int_{-\infty}^{+\infty} \mathrm{e}^{iu\tau} \mu(\mathrm{d}\tau), \qquad u \in \mathbb{R}.$$

The hypothesis that $\varphi \in L^1(\mathbb{R})$ ensures that there exists a nonnegative mapping $\widehat{\varphi} \in L^1(\mathbb{R})$, such that

$$\varphi(u) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{iu\tau} \widehat{\varphi}(\tau) \mathrm{d}\tau, \qquad u \in \mathbb{R}. \tag{2.6}$$

We finally call $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ the class of continuous mappings $\psi : [0, \pi] \times \mathbb{R}$ with $\psi(0, 0) = 1$ such that the function $\mathbb{K} : \mathbb{S}^d \times \mathbb{S}^d \times \mathbb{R} \to \mathbb{R}$ defined through $\mathbb{K}(x, y, u) := \psi(\theta(x, y), u)$ is positive definite on $\mathbb{S}^d \times \mathbb{R}$.

We also define $\mathcal{P}(\mathbb{S}^\infty, \mathbb{R}) := \cap_{d \geq 1} \mathcal{P}(\mathbb{S}^d, \mathbb{R})$, with the inclusion relation $\mathcal{P}(\mathbb{S}^\infty, \mathbb{R}) \subset \cdots \subset \mathcal{P}(\mathbb{S}^d, \mathbb{R}) \subset \mathcal{P}(\mathbb{S}^{d-1}, \mathbb{R}) \subset \cdots \subset \mathcal{P}(\mathbb{S}^1, \mathbb{R})$.

A characterization of this class has become recently available (see Berg and Porcu, 2017): a continuous mapping $\phi : [0, \pi] \times \mathbb{R} \to \mathbb{R}$ belongs to the class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ if and only if

$$\phi(\theta, u) = \sum_{n=0}^{\infty} \lambda_{n,d}(u) \mathcal{G}_n(d, \cos\theta), \qquad (\theta, u) \in [0, \pi] \times \mathbb{R}, \tag{2.7}$$

with $\{\lambda_{n,d}(\cdot)\}_{n=0}^{\infty} \subset \mathcal{P}(\mathbb{R})$ such that $\sum_{n=1}^{\infty} \lambda_{n,d}(0) = 1$. Also, we have

$$\lambda_{n,d}(u) = \frac{N_n(d) \|\omega_{d-1}\|}{\|\omega_d\|} \int_0^{\pi} \phi(x, u) \mathcal{G}_n(d, \cos x) \sin(x)^{d-1} \, \mathrm{d}x.$$

Berg and Porcu (2017) use the term *Schoenberg function sequence* for $(\lambda_{n,d}(\cdot))_{n=0}^{\infty}$.

The class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ is having many applications to applied problems (see, for example Porcu et al., 2016, 2017).

3 Nested Models within the Class $\mathcal{P}(\mathbb{S}^d)$

We start by considering a simple strategy that allows to obtain covariances on spheres $\mathbb{S}^d$ as weighted sums of basic covariances with potentially negative weights. Specifically, let N be a positive integer and ψ_k, for $k = 1, 2, \dots, N$, a collection of elements of the class $\mathcal{P}(\mathbb{S}^d)$. Thus, for every k there exists an associated d-Schoenberg sequence $(b_{n,d}^{(k)})_{n=0}^{\infty}$, such that

$$\psi_k(\theta) = \sum_{n=0}^{\infty} b_{n,d}^{(k)} \mathcal{G}_n(d, \cos\theta), \quad \theta \in [0, \pi], \quad b_{n,d}^{(k)} \geq 0, \quad \sum_{n=0}^{\infty} b_{n,d}^{(k)} = 1. \tag{3.1}$$

For a given system $\{c_k : k = 1, 2, \dots, N\}$ of real constants, we now consider the function $C : [0, \pi] \to \mathbb{R}$ defined through

$$C(\theta) := \frac{1}{\kappa} \sum_{k=1}^{N} c_k \psi_k(\theta), \qquad \theta \in [0, \pi], \tag{3.2}$$

where $\kappa := \sum_{k=1}^{N} c_k \neq 0$ is a normalizing constant so that $C(0) = 1$. We now seek the conditions on the constants c_k such that C is still an element of $\mathcal{P}(\mathbb{S}^d)$. The answer is trivial if the constants c_k are restricted to be nonnegative. But the fact that at least one of them might be extended to a negative interval is what gives a motivation for a deep study of the problem.

A direct inspection shows that C has Schoenberg coefficients $b_{n,d}$ given by

$$b_{n,d} = \frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)},$$

and $\sum_{n=0}^{\infty} b_{n,d} = 1$. Thus, the application of Theorem 2.1 shows that C is an element of the class $\mathcal{P}(\mathbb{S}^d)$ if and only if the sequence $(b_{n,d})_{n=0}^{\infty}$ is nonnegative and summable.

Throughout the paper we assume $\kappa > 0$. We show below that at least one of the coefficients c_k can be negative while preserving the fact that $C \in \mathcal{P}(\mathbb{S}^d)$. A technical hypothesis is needed and we explicitly state it here for the convenience of the reader:

Hypothesis H1. *Let $b_{n,d}^{(k)}$ be the coefficients defined through Equation (3.1). We suppose throughout that $b_{n,d}^{(N)} > 0$ for all $n \in \mathbb{Z}_+$.*

Hypothesis H1 is indeed necessary to develop the rest of our findings. In fact, we can now write

$$b_{n,d} = \frac{1}{\kappa} b_{n,d}^{(N)} \left[\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} + c_N \right], \quad n \in \mathbb{Z}_+.$$

By assuming $\kappa > 0$ (for $\kappa < 0$, see Remark 3.4) we obtain that $b_{n,d} \geq 0$, $n \in \mathbb{Z}_+$, if, and only if,

$$\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} + c_N \geq 0, \quad n \in \mathbb{Z}_+. \tag{3.3}$$

Next, inspired by Gregori et al. (2008), we define

$$M_k := \sup\left\{\frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} : n \in \mathbb{Z}_+\right\}, \qquad m_k := \inf\left\{\frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} : n \in \mathbb{Z}_+\right\}, \quad k = 1, 2, \dots, N-1. \tag{3.4}$$

Note that $m_k \geq 0$ and $M_k > 0$, for $k = 1, 2, \dots, N-1$. The following lemma will simplify the exposition of the results following subsequently.

Lemma 3.1. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d)$, $k = 1, \dots, N$, with associated d-Schoenberg coefficients $b_{n,d}^{(k)}$ and assume the Hypothesis* H1. *Let $C : [0, \pi] \to \mathbb{R}$ be the function defined through Equation (3.2) such that $\kappa > 0$. Then, the following assertions hold true.*

(i) If $C \in \mathcal{P}(\mathbb{S}^d)$, then

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[M_k \mathbf{1}_{\{c_k \geq 0\}} + m_k \mathbf{1}_{\{c_k < 0\}}\right]. \tag{3.5}$$

(ii) If

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[M_k \mathbf{1}_{\{c_k < 0\}} + m_k \mathbf{1}_{\{c_k \geq 0\}}\right], \tag{3.6}$$

then $C \in \mathcal{P}(\mathbb{S}^d)$.

Proof. We give a constructive proof. Suppose $C \in \mathcal{P}(\mathbb{S}^d)$, then $b_{n,d} \geq 0$ for all n. From Equation (3.3) we get

$$0 \leq \sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} + c_N \leq \sum_{\substack{k=1 \\ c_k \geq 0}}^{N-1} c_k M_k + \sum_{\substack{k=1 \\ c_k < 0}}^{N-1} c_k m_k + c_N.$$

This is exactly (3.5).

Now we assume that (3.6) is true. We need to prove that $b_{n,d} \geq 0$ for all n. By Equation (3.6),

$$\begin{aligned}\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} + c_N &\geq \sum_{\substack{k=1 \\ c_k \geq 0}}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} + \sum_{\substack{k=1 \\ c_k < 0}}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} - \sum_{\substack{k=1 \\ c_k < 0}}^{N-1} c_k M_k - \sum_{\substack{k=1 \\ c_k \geq 0}}^{N-1} c_k m_k \\ &= \sum_{\substack{k=1 \\ c_k \geq 0}}^{N-1} c_k \left(\frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} - m_k\right) + \sum_{\substack{k=1 \\ c_k < 0}}^{N-1} c_k \left(\frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} - M_k\right) \geq 0, \quad n \in \mathbb{Z}_+.\end{aligned}$$

Therefore, by (3.3), $b_{n,d} \geq 0$ for all n. ■

The special case $N = 2$ allows for a complete characterization of the problem.

Proposition 3.2. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d)$ with associated d-Schoenberg coefficients $b_{n,d}^{(k)}$, $k = 1, 2$. Suppose that Hypothesis* H1 *holds. Let $c_1, c_2 \in \mathbb{R}$ such that $c_1 + c_2 > 0$. Then,*

$$C(\theta) = \frac{1}{c_1 + c_2}\left[c_1 \psi_1(\theta) + c_2 \psi_2(\theta)\right], \qquad \theta \in [0, \pi],$$

belongs to $\mathcal{P}(\mathbb{S}^d)$ if, and only if,

$$c_2 \geq -c_1 \left[M_1 \mathbf{1}_{\{c_1 < 0\}} + m_1 \mathbf{1}_{\{c_1 \geq 0\}}\right]. \tag{3.7}$$

Proof. Suppose that $\psi \in \mathcal{P}(\mathbb{S}^d)$. By Equation (3.3),

$$c_2 \geq -c_1 \frac{b_{n,d}^{(1)}}{b_{n,d}^{(2)}}, \quad n \in \mathbb{Z}_+.$$

We now note that all numbers $b_{n,d}^{(1)}/b_{n,d}^{(2)}$, $n \in \mathbb{Z}_+$ are nonnegative, which in turn implies that M_1 and m_1 are nonnegative. Previous inequality implies that

$$\begin{cases} c_2 \geq -c_1 M_1, & c_1 < 0 \\ c_2 \geq -c_1 m_1, & c_1 \geq 0 \end{cases}$$

This is exactly Equation (3.7). The converse is shown through straight application of Lemma 3.1. ∎

An important case follows.

Corollary 3.3. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d)$ with associated d-Schoenberg coefficients $b_{n,d}^{(k)}$, $k = 1,2$. Suppose that Hypothesis* H1 *holds. Let $\rho \in \mathbb{R}$. Then,*

$$C = \rho\psi_1 + (1-\rho)\psi_2 \tag{3.8}$$

belongs to $\mathcal{P}(\mathbb{S}^d)$ if, and only if,

$$\frac{1}{1-\max\{1, M_1\}} \leq \rho \leq \frac{1}{1-\min\{1, m_1\}}, \tag{3.9}$$

where the left side is $-\infty$ if the maximum is 1 and 0 if the maximum is $+\infty$. The right side is $+\infty$ if the minimum is 1.

Proof. We consider Proposition 3.2 with $c_1 = \rho$ and $c_2 = 1-\rho$. Then

$$\begin{cases} \rho(1-M_1) \leq 1, & \rho < 0 \\ \rho(1-m_1) \leq 1, & \rho \geq 0. \end{cases}$$

This is equivalent to (3.9). ∎

Remark 3.4. If $\kappa < 0$, we can proceeding in the same way as before and then Equations (3.5), (3.6) and (3.7) become, respectively,

$$c_N \leq -\sum_{k=1}^{N-1} c_k \left[M_k \mathbf{1}_{\{c_k \leq 0\}} + m_k \mathbf{1}_{\{c_k > 0\}}\right], \quad c_N \leq -\sum_{k=1}^{N-1} c_k \left[M_k \mathbf{1}_{\{c_k > 0\}} + m_k \mathbf{1}_{\{c_k \leq 0\}}\right],$$
$$c_2 \leq -c_1 \left[M_1 \mathbf{1}_{\{c_1 > 0\}} + m_1 \mathbf{1}_{\{c_1 \leq 0\}}\right].$$

Note that under the hypotheses of Corollary 3.3, $c_1 + c_2 = 1 > 0$, for all $\rho \in \mathbb{R}$.

4 Product-Sum Models with Potentially Negative Weights within the Class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$

4.1 A Product-Sum Model

Product-sum models have been first proposed by De Iaco and coauthors (see De Iaco et al., 2001). We start this section by recalling that the class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ is a convex cone, being closed under the topology of pointwise convergence. This implies that, for given $\psi \in \mathcal{P}(\mathbb{S}^d)$ and $\varphi \in \mathcal{P}(\mathbb{R})$, the function $(\theta, u) \mapsto \phi(\theta, u) = \psi(\theta)\varphi(u)$, $(\theta, u) \in [0, \pi] \times \mathbb{R}$, belongs to the class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$. In virtue of Theorem 3.3 in Berg and Porcu (2017), this in turn implies that the model

$$\phi(\theta, u) = \sum_{n=1}^{\infty} \lambda_{n,d}(u)\mathcal{G}_n(d, \cos\theta), \quad \sum_{n=1}^{\infty} \lambda_{n,d}(0) < \infty, \quad \lambda_{n,d} \in \mathcal{P}(\mathbb{R}),$$

has d-Schoenberg functions $\lambda_{n,d}$ given by

$$\lambda_{n,d}(u) = b_{n,d}\varphi(u), \quad u \in \mathbb{R},$$

with $b_{n,d}$ being the d-Schoenberg coefficients of ψ as in (2.4).

This remark opens for a simple modeling strategy that we will illustrate now. Consider a finite dimensional collection of functions $\varphi_k \in \mathcal{P}(\mathbb{R})$, $k = 1, 2, \ldots, N$ such that, for all k, $\varphi_k \in L_1(\mathbb{R})$. This implies that each φ_k can be uniquely written as in (2.6) , with $\widehat{\varphi}_k$ being the Fourier pair of φ_k. In particular, we have $\widehat{\varphi}_k(w) \geq 0$, for $w \in \mathbb{R}$ and $\widehat{\varphi}_k \in L_1(\mathbb{R})$ because of Parseval's identity.

Now, let $c_k \in \mathbb{R}$ and $\psi_k \in \mathcal{P}(\mathbb{S}^d)$, $k = 1, 2 \ldots, N$. Consider the function $C : [0, \pi] \times \mathbb{R} \to \mathbb{C}$ defined by

$$C(\theta, u) := \frac{1}{\kappa} \sum_{k=1}^{N} c_k \psi_k(\theta)\varphi_k(u), \qquad (\theta, u) \in [0, \pi] \times \mathbb{R}. \tag{4.1}$$

Apparently, C has d-Schoenberg functions given by

$$\lambda_{n,d}(u) = \frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)} \varphi_k(u), \quad n \in \mathbb{Z}_+, \quad u \in \mathbb{R},$$

and of course we have that $\sum_{n=1}^{\infty} \lambda_{n,d}(0) < \infty$ and $\lambda_{n,d} \in L_1(\mathbb{R})$. Now, note that

$$\begin{aligned} \lambda_{n,d}(u) &= \frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)} \varphi_k(u) = \frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)} \int_{-\infty}^{\infty} e^{iwu} \widehat{\varphi}_k(w) \mathrm{d}w \\ &= \int_{-\infty}^{\infty} e^{iwu} \left(\frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)} \widehat{\varphi}_k(w) \right) \mathrm{d}w, \quad n \in \mathbb{Z}_+, \quad u \in \mathbb{R}, \end{aligned}$$

that is,

$$\widehat{\lambda}_{n,d}(w) = \frac{1}{\kappa} \sum_{k=1}^{N} c_k b_{n,d}^{(k)} \widehat{\varphi}_k(w), \quad w \in \mathbb{R}.$$

Since $b_{n,d}^{(k)}, \widehat{\varphi}_k(w) \geq 0$, for all n, k, w, we have to find conditions on the scalars c_k so that

$$\widehat{\lambda}_{n,d}(w) \geq 0, \quad w \in \mathbb{R},$$

in order to guarantee that C belongs to the class $\mathcal{P}(\mathbb{S}^d,\mathbb{R})$. A technical hypothesis is again needed to ensure that we can go further with our findings.

Hypothesis H2. *Let $\widehat{\varphi}_k$ be the Fourier pair of φ_k as in the Equation (2.6). We suppose throughout that $\widehat{\varphi}_N(w) > 0$, for all $w \in \mathbb{R}$.*

If Hypotheses H1 and H2 hold, then we can write

$$\widehat{\lambda}_{n,d}(w) = \frac{1}{\kappa} b_{n,d}^{(N)} \widehat{\varphi}_N(w) \left[\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)} \widehat{\varphi}_k(w)}{b_{n,d}^{(N)} \widehat{\varphi}_N(w)} + c_N \right], \quad n \in \mathbb{Z}_+, \quad w \in \mathbb{R}.$$

Since $\kappa > 0$ (see Remark 4.4 for $\kappa < 0$), then $\widehat{\lambda}_{n,d}(w) \geq 0$, $n \in \mathbb{Z}_+$, $w \in \mathbb{R}$, if, and only if,

$$\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)} \widehat{\varphi}_k(w)}{b_{n,d}^{(N)} \widehat{\varphi}_N(w)} + c_N \geq 0, \quad n \in \mathbb{Z}_+, \quad w \in \mathbb{R}. \tag{4.2}$$

Now, defining

$$\widetilde{M}_k := \sup\left\{ \frac{\widehat{\varphi}_k(w)}{\widehat{\varphi}_N(w)} : w \in \mathbb{R} \right\}, \qquad \widetilde{m}_k := \inf\left\{ \frac{\widehat{\varphi}_k(w)}{\widehat{\varphi}_N(w)} : w \in \mathbb{R} \right\}, \quad k = 1, 2, \ldots, N-1,$$

we obtain the following.

Lemma 4.1. *Let C as defined at (4.1) with $\kappa > 0$ and assume the Hypotheses* H1 *and* H2*. Then the following assertions hold true.*

(i) If $C \in \mathcal{P}(\mathbb{S}^d,\mathbb{R})$, then

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[M_k \widetilde{M}_k \mathbf{1}_{\{c_k \geq 0\}} + m_k \widetilde{m}_k \mathbf{1}_{\{c_k < 0\}} \right]. \tag{4.3}$$

(ii) If

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[M_k \widetilde{M}_k \mathbf{1}_{\{c_k < 0\}} + m_k \widetilde{m}_k \mathbf{1}_{\{c_k \geq 0\}} \right], \tag{4.4}$$

then $C \in \mathcal{P}(\mathbb{S}^d,\mathbb{R})$.

Proof. If $C \in \mathcal{P}(\mathbb{S}^d,\mathbb{R})$, then $\widehat{\lambda}_{n,d}(w) \geq 0$ for all n and w. By (4.2),

$$0 \leq \sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}}{b_{n,d}^{(N)}} \frac{\widehat{\varphi}_k(w)}{\widehat{\varphi}_N(w)} + c_N \leq \sum_{\substack{k=1 \\ c_k \geq 0}}^{N-1} c_k M_k \widetilde{M}_k + \sum_{\substack{k=1 \\ c_k < 0}}^{N-1} c_k m_k \widetilde{m}_k + c_N.$$

This is exactly (4.3).

If (4.4) holds, we need prove that $\widehat{\lambda}_{n,d}(w) \geq 0$ for all n and $w \in \mathbb{R}$. By (4.4),

$$\begin{aligned}\sum_{k=1}^{N-1} c_k \frac{b_{n,d}^{(k)}\widehat{\varphi}_k(w)}{b_{n,d}^{(N)}\widehat{\varphi}_N(w)} + c_N &\geq \sum_{\substack{k=1\\c_k\geq 0}}^{N-1} c_k \frac{b_{n,d}^{(k)}\widehat{\varphi}_k(w)}{b_{n,d}^{(N)}\widehat{\varphi}_N(w)} + \sum_{\substack{k=1\\c_k<0}}^{N-1} c_k \frac{b_{n,d}^{(k)}\widehat{\varphi}_k(w)}{b_{n,d}^{(N)}\widehat{\varphi}_N(w)} \\ &\qquad - \sum_{\substack{k=1\\c_k<0}}^{N-1} c_k M_k \widetilde{M_k} - \sum_{\substack{k=1\\c_k\geq 0}}^{N-1} c_k m_k \widetilde{m_k} \\ &= \sum_{\substack{k=1\\c_k\geq 0}}^{N-1} c_k \left(\frac{b_{n,d}^{(k)}\widehat{\varphi}_k(w)}{b_{n,d}^{(N)}\widehat{\varphi}_N(w)} - m_k\widetilde{m_k}\right) + \sum_{\substack{k=1\\c_k<0}}^{N-1} c_k \left(\frac{b_{n,d}^{(k)}\widehat{\varphi}_k(w)}{b_{n,d}^{(N)}\widehat{\varphi}_N(w)} - M_k\widetilde{M_k}\right) \geq 0,\end{aligned}$$

for all $n \in \mathbb{Z}_+$ and $w \in \mathbb{R}$. By Equation (4.2), $\widehat{\lambda}_{n,d}(w) \geq 0$, $n \in \mathbb{Z}_+$, $w \in \mathbb{R}$. ∎

For the special case $N = 2$ we attain the following characterization.

Proposition 4.2. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d)$ with associated d-Schoenberg coefficients $b_{n,d}^{(k)}$ and $\varphi_k \in \mathcal{P}(\mathbb{R})$, $k = 1, 2$. Let $c_1, c_2 \in \mathbb{R}$ such that $c_1 + c_2 > 0$. Suppose that Hypothesis* H1 *and* H2 *hold. Then,*

$$C = \frac{1}{c_1 + c_2}\left[c_1\psi_1\varphi_1 + c_2\psi_2\varphi_2\right]$$

belongs to $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ if and only if

$$c_2 \geq -c_1\left[M_1\widetilde{M}_1\mathbf{1}_{\{c_1<0\}} + m_1\widetilde{m}_1\mathbf{1}_{\{c_1\geq 0\}}\right]. \tag{4.5}$$

Proof. Suppose that $C \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$. By Equation (4.2),

$$c_2 \geq -c_1 \frac{b_{n,d}^{(1)}\widehat{\varphi}_1(w)}{b_{n,d}^{(2)}\widehat{\varphi}_2(w)}, \quad n \in \mathbb{Z}_+, \quad w \in \mathbb{R}.$$

Since all numbers $b_{n,d}^{(1)}/b_{n,d}^{(2)}$, $n \in \mathbb{Z}_+$, $\widehat{\varphi}_1(w)/\widehat{\varphi}_2(w)$, $w \in \mathbb{R}$, and $M_1, \widetilde{M}_1, m_1, \widetilde{m}_1$ are nonnegative, in particular, the previous inequality implies

$$\begin{cases} c_2 \geq -c_1 M_1\widetilde{M}_1, & c_1 < 0 \\ c_2 \geq -c_1 m_1\widetilde{m}_1, & c_1 \geq 0. \end{cases}$$

This is Equation (4.5). The converse is obtained from Lemma 4.1. ∎

An immediate consequence is:

Corollary 4.3. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d)$ with associated d-Schoenberg coefficients $b_{n,d}^{(k)}$ and $\varphi_k \in \mathcal{P}(\mathbb{R})$, $k = 1, 2$. Suppose that Hypothesis* H1 *and* H2 *hold. Let $\rho \in \mathbb{R}$. Then,*

$$C = \rho\psi_1\varphi_1 + (1-\rho)\psi_2\varphi_2 \tag{4.6}$$

belongs to $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ if and only if

$$\frac{1}{1 - \max\{1, M_1\widetilde{M}_1\}} \leq \rho \leq \frac{1}{1 - \min\{1, m_1\widetilde{m}_1\}}, \tag{4.7}$$

where the left side is $-\infty$ if the maximum is 1 and 0 if the maximum is $+\infty$. The right side is $+\infty$ if the minimum is 1.

Remark 4.4. If $\kappa < 0$, we can proceeding in the same way as before and then Equations (4.3), (4.4) and (4.5) become, respectively,

$$c_N \le -\sum_{k=1}^{N-1} c_k \left[M_k \widetilde{M_k} \mathbf{1}_{\{c_k \le 0\}} + m_k \widetilde{m_k} \mathbf{1}_{\{c_k > 0\}} \right], \quad c_N \le -\sum_{k=1}^{N-1} c_k \left[M_k \widetilde{M_k} \mathbf{1}_{\{c_k > 0\}} + m_k \widetilde{m_k} \mathbf{1}_{\{c_k \le 0\}} \right],$$
$$c_2 \le -c_1 \left[M_1 \widetilde{M}_1 \mathbf{1}_{\{c_1 > 0\}} + m_1 \widetilde{m}_1 \mathbf{1}_{\{c_1 \le 0\}} \right].$$

4.2 A General Formulation within the Class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$

This section faces the most general and tricky case within the class $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$. Examples of functions in this class can be found in Porcu et al. (2017). We consider a collection $\{\psi_k : k = 1, \dots, N\} \subset \mathcal{P}(\mathbb{S}^d, \mathbb{R})$, and constants $c_k \in \mathbb{R}$, for $k = 1, 2, \dots, N$. Consider the function $C : [0, \pi] \times \mathbb{R} \to \mathbb{C}$ defined by

$$C(\theta, u) := \frac{1}{\kappa} \sum_{k=1}^{N} c_k \psi_k(\theta, u), \qquad (\theta, u) \in [0, \pi] \times \mathbb{R}. \tag{4.8}$$

Using (2.7) we get that C has d-Schoenberg functions given by

$$\lambda_{n,d}(u) = \frac{1}{\kappa} \sum_{k=1}^{N} c_k \lambda_{n,d}^{(k)}(u), \quad n \in \mathbb{Z}_+, \quad u \in \mathbb{R},$$

where $\sum_{n=1}^{\infty} \lambda_{n,d}(0) < \infty$ and $\lambda_{n,d} \in L_1(\mathbb{R})$. For this, note that, since

$$\begin{aligned} \lambda_{n,d}(u) &= \frac{1}{\kappa} \sum_{k=1}^{N} c_k \int_{-\infty}^{\infty} e^{iuw} \widehat{\lambda}_{n,d}^{(k)}(w) \mathrm{d}w \\ &= \int_{-\infty}^{\infty} e^{iuw} \left(\frac{1}{\kappa} \sum_{k=1}^{N} c_k \widehat{\lambda}_{n,d}^{(k)}(w) \right) \mathrm{d}w, \quad n \in \mathbb{Z}_+, \quad u \in \mathbb{R}, \end{aligned}$$

we have

$$\widehat{\lambda}_{n,d}(w) = \frac{1}{\kappa} \sum_{k=1}^{N} c_k \widehat{\lambda}_{n,d}^{(k)}(w), \quad n \in \mathbb{Z}_+, \quad w \in \mathbb{R}.$$

Thus, we have to find conditions on the scalars c_k so that

$$\widehat{\lambda}_{n,d}(w) \ge 0, \quad w \in \mathbb{R}, \quad n \in \mathbb{Z}_+.$$

The following additional hypothesis is needed subsequently.

Hypothesis H3. *Let C as in (4.8), where $\psi_k \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$, for all $k = 1, 2, \dots, N$. Let $\widehat{\lambda}_{n,d}^{(k)}$ be the Fourier pair of the coefficients $\lambda_{n,d}^{(k)}$ associated to C. We suppose throughout that $\widehat{\lambda}_{n,d}^{(N)}(w) > 0$, for all $w \in \mathbb{R}$ and $n \in \mathbb{Z}_+$.*

If Hypothesis H3 holds, then we have

$$\widehat{\lambda}_{n,d}(w) = \widehat{\lambda}_{n,d}^{(N)}(w) \left[\sum_{k=1}^{N-1} c_k \frac{\widehat{\lambda}_{n,d}^{(k)}(w)}{\widehat{\lambda}_{n,d}^{(N)}(w)} + c_N \right], \quad w \in \mathbb{R}, \quad n \in \mathbb{Z}_+.$$

Since $\kappa > 0$ (see Remark 4.8 for $\kappa < 0$), we have that $\widehat{\lambda}_{n,d}(\cdot)$ is nonnegative if, and only if,

$$\sum_{k=1}^{N-1} c_k \frac{\widehat{\lambda}_{n,d}^{(k)}(w)}{\widehat{\lambda}_{n,d}^{(N)}(w)} + c_N \geq 0, \quad w \in \mathbb{R}, \quad n \in \mathbb{Z}_+.$$

Let $n \in \mathbb{Z}_+$ fixed and define

$$M_{n,k} := \sup\left\{\frac{\widehat{\lambda}_{n,d}^{(k)}(w)}{\widehat{\lambda}_{n,d}^{(N)}(w)} : w \in \mathbb{R}\right\}, \qquad m_{n,k} := \inf\left\{\frac{\widehat{\lambda}_{n,d}^{(k)}(w)}{\widehat{\lambda}_{n,d}^{(N)}(w)} : w \in \mathbb{R}\right\}, \quad k = 1, 2, \ldots, N-1.$$

Note that $m_{n,k} \geq 0$ and $M_{n,k} > 0$, for $k = 1, 2, \ldots, N-1$.

Defining

$$\breve{M}_k := \sup\left\{M_{n,k} : n \in \mathbb{Z}_+\right\}, \qquad \breve{m}_k := \inf\left\{m_{n,k} : n \in \mathbb{Z}_+\right\}, \quad k = 1, 2, \ldots, N-1,$$

similarly to the previous cases we have the following lemma.

Lemma 4.5. *Let C as defined at (4.8) with $\kappa > 0$ and assume the Hypotheses* H3*. Then the following assertions hold true.*

(i) If $C \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$, then

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[\breve{M}_k \mathbf{1}_{\{c_k \geq 0\}} + \breve{m}_k \mathbf{1}_{\{c_k < 0\}}\right].$$

(ii) If

$$c_N \geq -\sum_{k=1}^{N-1} c_k \left[\breve{M}_k \mathbf{1}_{\{c_k < 0\}} + \breve{m}_k \mathbf{1}_{\{c_k \geq 0\}}\right],$$

then $C \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$.

For the particular case $N = 2$ we have the following characterizations.

Proposition 4.6. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$ such that Hypothesis* H3 *is satisfied, for $k = 1, 2$. Let $c_1, c_2 \in \mathbb{R}$ with $c_1 + c_2 > 0$. Then,*

$$C = \frac{1}{c_1 + c_2}\left[c_1\psi_1 + c_2\psi_2\right]$$

belongs to $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ if, and only if,

$$c_2 \geq -c_1\left[\breve{M}_1 \mathbf{1}_{\{c_1 < 0\}} + \breve{m}_1 \mathbf{1}_{\{c_1 \geq 0\}}\right].$$

Corollary 4.7. *Let $\psi_k \in \mathcal{P}(\mathbb{S}^d, \mathbb{R})$ such that Hypothesis* H3 *is satisfied, for $k = 1, 2$. Let $\rho \in \mathbb{R}$. Then,*

$$C = \rho\psi_1 + (1-\rho)\psi_2$$

belongs to $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ if, and only if,

$$\frac{1}{1-\max\{1,\breve{M}_1\}} \le \rho \le \frac{1}{1-\min\{1,\breve{m}_1\}},$$

where the left side is $-\infty$ if the maximum is 1 and 0 if the maximum is $+\infty$. The right side is $+\infty$ if the minimum is 1.

Remark 4.8. If $\kappa < 0$, then the equations in Lemma 4.5 and Proposition 4.6 become, respectively,

$$c_N \le -\sum_{k=1}^{N-1} c_k \left[\breve{M}_k \mathbf{1}_{\{c_k \le 0\}} + \breve{m}_k \mathbf{1}_{\{c_k > 0\}}\right], \quad c_N \le -\sum_{k=1}^{N-1} c_k \left[\breve{M}_k \mathbf{1}_{\{c_k > 0\}} + \breve{m}_k \mathbf{1}_{\{c_k \le 0\}}\right],$$

$$c_2 \le -c_1 \left[\breve{M}_1 \mathbf{1}_{\{c_1 > 0\}} + \breve{m}_1 \mathbf{1}_{\{c_1 \le 0\}}\right].$$

5 Examples

In this section we give classes of the functions that belong to $\mathcal{P}(\mathbb{S}^d)$, $\mathcal{P}(\mathbb{S}^\infty)$ or $\mathcal{P}(\mathbb{R})$ so that the functions in (3.8) and (4.6) are respectively spatial and space-time covariance functions. We consider some of the most celebrated models on spheres for which an explicit expression of the Schoenberg coefficient is available. We also provide the supremum and infimum necessary so that the range of the parameter ρ in (3.9) and (4.7) becomes well determined.

5.1 Examples from $\mathcal{P}(\mathbb{S}^d)$ and $\mathcal{P}(\mathbb{S}^\infty)$

This section illustrates some examples from Corollary 3.3, that is, $C(\theta) = \rho\psi_1(\theta) + (1-\rho)\psi_2(\theta)$. Thus, necessary ingredients are:

1. Parametric classes within the classes $\mathcal{P}(\mathbb{S}^d)$ and $\mathcal{P}(\mathbb{S}^\infty)$ for ψ_1 and ψ_2.
2. Computation of M_1 and m_1 as in Corollary 3.3.

In particular, we consider the following parametric classes:

- Multiquadric functions:

  Let $p_1, p_2 \in (0,1)$, τ_1, τ_2 be positive integers and σ_1, σ_2 positive real numbers. The functions

  $$\psi_k(\theta) = \sigma_k^2 \left(\frac{1-p_k}{1-p_k\cos\theta}\right)^{\tau_k}, \quad 0 \le \theta \le \pi, \quad k = 1,2, \tag{5.1}$$

  belong to the class $\mathcal{P}(\mathbb{S}^\infty)$ and their coefficients in the expansion are given by (Arafat et al., 2018)

  $$b_n^{(k)} = b_n^{(k)}(p_k,\tau_k) = \sigma_k^2 \binom{\tau_k + n - 1}{n} p_k^n (1-p_k)^{\tau_k}, \quad n = 0,1,\ldots, \quad k = 1,2.$$

- Multiquadric functions and $\mathcal{P}(\mathbb{S}^d)$:

  Let $d \geq 2$. A reparameterization of (5.1) with $p_k = 2\delta_k/(1+\delta_k^2)$, with $\delta_k \in (0,1)$, for $k = 1, 2$, provide us the functions

$$\psi_k(\theta) = \sigma_k^2 \frac{(1-\delta_k)^{2\tau_k}}{(1+\delta_k^2 - 2\delta_k \cos\theta)^{\tau_k}}, \quad 0 \leq \theta \leq \pi, \quad k = 1, 2. \tag{5.2}$$

  If $\tau_k = (d-1)/2$, then ψ_k belongs to the class $\mathcal{P}(\mathbb{S}^d)$, and their d-Schoenberg coefficients are given by (see Equation (4.31) of Møller et al., 2018)

$$b_{n,d}^{(k)} = \sigma_k^2 (1-\delta_k)^{d-1} \binom{d+n-2}{n} \delta_k^n.$$

- Sine Power functions:

  Let $\alpha_1, \alpha_2 \in (0,2)$ and σ_1, σ_2 be positive real numbers. Then the functions

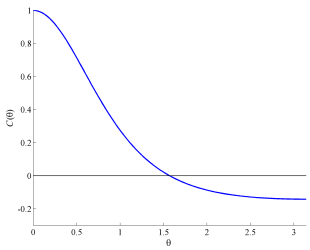
$$\psi_k(\theta) = \sigma_k^2 \left[1 - \left(\sin\frac{\theta}{2}\right)^{\alpha_k}\right], \quad 0 \leq \theta \leq 2\pi, \quad k = 1, 2, \tag{5.3}$$

  belong to the class $\mathcal{P}(\mathbb{S}^\infty)$, and their Schoenberg coefficients are given by (Soubeyrand et al., 2008; Gneiting, 2013)

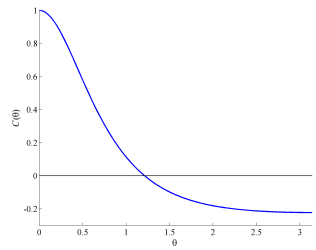
$$b_n^{(k)} = -\frac{\sigma_k^2}{\sqrt{2}} \frac{1}{(n+1)!} \prod_{m=0}^{n} \left(m - \frac{\alpha_k}{2}\right), \quad n = 0, 1, \ldots, \quad k = 1, 2.$$

In the above cases, the supremum M_1 and the infimum m_1 required in Corollary 3.3 can be found by simple techniques.

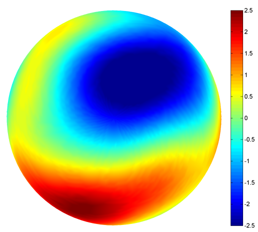
As an illustration, Figure 1 displays two nested Multiquadratic covariance functions corresponding to Table 1 and realizations of Gaussian random fields with such covariance functions. The covariance reaches a minimum less than -0.141 in the first case and -0.222 in the second case.



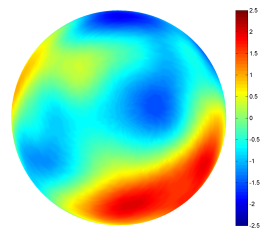
(a) $p_1 = 0.5$; $p_2 = 0.2$; $\tau_1 = 2$; $\tau_2 = 1$; $\sigma_1 = 1$; $\sigma_2 = 1$



(b) $\delta_1 = 0.5$; $\delta_2 = 0.2$; $\sigma_1 = 1$; $\sigma_2 = 1$



(c)



(d)

Figure 1: Nested Multiquadric covariance functions with the above specified parameters (a,b) and ρ calculated with the minimum allowed value in Equation (3.9), and realizations of Gaussian random fields with such covariance functions (c,d).

Table 1: Bounds m_1 and M_1 associated to ρ in Equations (3.8) and (3.9). Here $\tau_k \in \mathbb{Z}_+$, $p_k \in (0,1)$, $\delta_k \in (0,1)$ and $\sigma_k > 0$, $k = 1,2$. Here, both ψ_1 and ψ_2 belong to the Multiquadric family as in (5.1).

Parameters	m_1	M_1
$\tau_1 \geq \tau_2$, $p_1 > p_2$	$\left(\frac{\sigma_1}{\sigma_2}\right)^2 \frac{(1-p_1)^{\tau_1}\Gamma(\tau_2)}{(1-p_2)^{\tau_2}\Gamma(\tau_1)}$	$+\infty$
$\tau_1 \leq \tau_2$, $p_1 < p_2$	0	$\left(\frac{\sigma_1}{\sigma_2}\right)^2 \frac{(1-p_1)^{\tau_1}\Gamma(\tau_2)}{(1-p_2)^{\tau_2}\Gamma(\tau_1)}$
Some setting but considering Equation (5.2) for both ψ_1 and ψ_2.		
Parameters	m_1	M_1
$\delta_1 > \delta_2$	$\left(\frac{\sigma_1}{\sigma_2}\right)^2 \left(\frac{1-\delta_1}{1-\delta_2}\right)^{d-1}$	$+\infty$
$\delta_1 < \delta_2$	0	$\left(\frac{\sigma_1}{\sigma_2}\right)^2 \left(\frac{1-\delta_1}{1-\delta_2}\right)^{d-1}$

Table 2: Upper bounds m_1 and M_1 for ρ as in Equation (3.9). Here $\alpha_k \in (0,2)$, $\sigma_k > 0$, $k = 1,2$. Both ψ_1 and ψ_2 in (3.8) belong to the Sine Power family as in (5.3)

Parameters	m_1	M_1
$\alpha_1 > \alpha_2$	0	$\frac{\alpha_1}{\alpha_2}\left(\frac{\sigma_1}{\sigma_2}\right)^2$
$\alpha_1 < \alpha_2$	$\frac{\alpha_1}{\alpha_2}\left(\frac{\sigma_1}{\sigma_2}\right)^2$	$+\infty$

Table 3: Upper bounds m_1 and M_1 for ρ as in Equation (3.9). Here $\sigma_k > 0$, $k = 1, 2$. Here, ψ_1 is the Multiquadric as in (5.1) and ψ_2 is the Sine Power as in (5.3).

Parameters	m_1	M_1
$p_1 \in \left(0, \frac{1}{2}\right)$, $\alpha_2 \in (0, 2)$ $\tau_1 \in \mathbb{Z}_+ \setminus \{0\}$ $n_0 \geq \max\left\{\tau_1, \frac{4p_1-2}{1-2p_1}\right\}^*$	0	$\max\left\{-\sqrt{2}\left(\frac{\sigma_1}{\sigma_2}\right)^2 \frac{(1-p_1)^{\tau_1}}{\Gamma(\tau_1)} \times \frac{\Gamma(\tau_1+n)}{\prod_{m=0}^{n}(2m-\alpha_2)}(n+1) \times (2p_1)^n : n = 0, 1, \ldots, n_0\right\}$
$\alpha_2 = p_1 \in \left(0, \frac{2}{5}\right)$ $\tau_1 = 1$	0	$2\sqrt{2}\left(\frac{\sigma_1}{\sigma_2}\right)^2 \frac{1-p_1}{p_1}$
$\alpha_2 = p_1 \in \left(\frac{2}{5}, \frac{1}{2}\right)$ $\tau_1 = 1$	0	$8\sqrt{2}\left(\frac{\sigma_1}{\sigma_2}\right)^2 \frac{1-p_1}{2-p_1}$

*If $p_1 \in \left(0, \frac{1}{4}\right)$, then $\max\left\{\tau_1, \frac{4p_1-2}{1-2p_1}\right\} = \tau_1$.

5.2 Examples from the Classes $\mathcal{P}(\mathbb{S}^d, \mathbb{R})$ and $\mathcal{P}(\mathbb{S}^\infty, \mathbb{R})$

Let $\alpha_{G_k} \in \mathbb{R}_+$ and $\sigma_{G_k} > 0$, $k = 1, 2$. It is known that Gauss functions given by

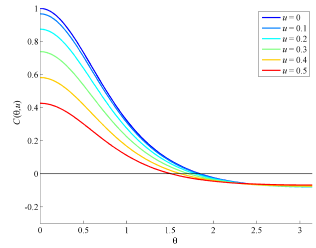
$$\varphi_{G_k}(u) = \sigma_{G_k}^2 \exp(-\alpha_{G_k}|u|^2), \quad k = 1, 2, \tag{5.4}$$

belong to the class $\mathcal{P}(\mathbb{R})$. The supremum and infimum, $\widetilde{M}_1, \widetilde{m}_1$, needed in Proposition 4.2 and Corollary 4.3 are available in Table 1 in Gregori et al. (2008).

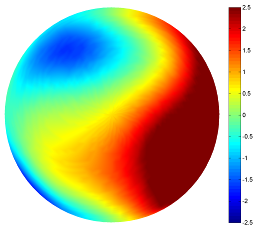
Using Table 1 in Gregori et al. (2008) and the tables of the previous subsection, we obtain Tables 4 – 6 below.

Here all parameters are subscripted in each case with the initial of the used function.

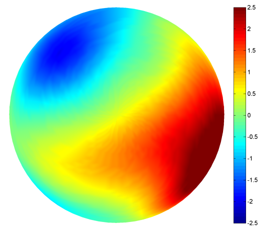
As an illustration, Figure 2 displays a nested Multiquadric coupled with Gauss covariance function corresponding to Table 4 and a realization of a Gaussian random field with such a covariance function. The covariance reaches a minimum less than −0.079.



(a) $p_{Mq_1} = 0.5$; $p_{Mq_2} = 0.2$; $\tau_{Mq_1} = 2$; $\tau_{Mq_2} = 1$; $\alpha_{G_1} = 3$; $\alpha_{G_2} = 2$; $\sigma_{M_1} = \sigma_{M_2} = \sigma_{G_1} = \sigma_{G_2} = 1$



(b)



(c)

Figure 2: Nested Multiquadric coupled with Gauss covariance function with the above specified parameters (a) and ρ calculated with the minimum allowed value in Equation (4.7), and realization of a Gaussian random field with such a covariance function at two time instants: (b) $t = 0$ and (c) $t = 0.3$.

Table 4: Upper bounds $m_1\widetilde{m}_1$ and $M_1\widetilde{M_1}$ for ρ as in Equation (4.7). Here $\tau_{Mq_k} \in \mathbb{Z}_+$, $p_{Mq_k} \in (0,1)$, $\delta_{Mq_k} \in (0,1)$ and $\sigma_{Mq_k}, \sigma_{G_k} > 0$, $\alpha_{G_k} \in \mathbb{R}_+$, $k = 1, 2$. Both ψ_1 and ψ_2 are Multiquadric functions as in (5.1) and both φ_1, φ_2 are Gauss functions as in (5.4).

Parameters	$m_{Mq_1,Mq_2} m_{G_1,G_2}$	$M_{Mq_1,Mq_2} M_{G_1,G_1}$
$\tau_{Mq_1} \geq \tau_{Mq_2}$ $p_{Mq_1} > p_{Mq_2}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$+\infty$
$\tau_{Mq_1} \geq \tau_{Mq_2}$ $p_{Mq_1} > p_{Mq_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	$\left(\frac{\sigma_{M_1}}{\sigma_{M_2}}\right)^2 \frac{(1-p_{Mq_1})^{\tau_{Mq_1}}\Gamma(\tau_{Mq_2})}{(1-p_{Mq_2})^{\tau_{Mq_2}}\Gamma(\tau_{Mq_1})} \times \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$	$+\infty$
$\tau_{Mq_1} \leq \tau_{Mq_2}$ $p_{Mq_1} < p_{Mq_2}$	0	$\left(\frac{\sigma_{M_1}}{\sigma_{M_2}}\right)^2 \frac{(1-p_{Mq_1})^{\tau_{Mq_1}}\Gamma(\tau_{Mq_2})}{(1-p_{Mq_2})^{\tau_{Mq_2}}\Gamma(\tau_{Mq_1})} \times \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$

Continuation of Table 4		
Parameters	$m_{Mq_1,Mq_2}m_{G_1,G_2}$	$M_{Mq_1,Mq_2}M_{G_1,G_1}$
$\alpha_{G_1} < \alpha_{G_2}$		
$\tau_{Mq_1} \leq \tau_{Mq_2}$ $p_{Mq_1} < p_{Mq_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$
Both ψ_1 and ψ_2 are Multiquadric functions as in (5.2) and both φ_1, φ_2 are Gauss functions as in (5.4)		
$\delta_{Mq_1} > \delta_{Mq_2}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$+\infty$
$\delta_{Mq_1} > \delta_{Mq_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	$\left(\frac{\sigma_{Mq_1}}{\sigma_{Mq_2}}\right)^2 \left(\frac{1-\delta_{Mq_1}}{1-\delta_{Mq_2}}\right)^{d-1} \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$	$+\infty$
$\delta_{Mq_1} < \delta_{Mq_2}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$\left(\frac{\sigma_{Mq_1}}{\sigma_{Mq_2}}\right)^2 \left(\frac{1-\delta_{Mq_1}}{1-\delta_{Mq_2}}\right)^{d-1} \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$
$\delta_{Mq_1} < \delta_{Mq_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$

Table 5: Upper bounds $m_1\widetilde{m}_1$ and $M_1\widetilde{M}_1$ for ρ as in Equation (4.7). Here $\alpha_{SP_k} \in (0,2)$, $\alpha_{G_k} \in \mathbb{R}_+$ and $\sigma_{SP_k}, \sigma_{G_k} > 0$, $k = 1,2$. Both ψ_1 and ψ_2 are Sine Power functions as in (5.3) and both φ_1, φ_2 are Gauss functions as in (5.4).

Parameters	$m_{SP_1,SP_2} m_{G_1,G_2}$	$M_{SP_1,SP_2} M_{G_1,G_2}$
$\alpha_{SP_1} > \alpha_{SP_2}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$\frac{\alpha_{SP_1}}{\alpha_{SP_2}}\left(\frac{\sigma_{SP_1}}{\sigma_{SP_2}}\right)^2 \times \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$
$\alpha_{SP_1} > \alpha_{SP_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$
$\alpha_{SP_1} < \alpha_{SP_2}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$+\infty$
$\alpha_{SP_1} < \alpha_{SP_2}$ $\alpha_{G_1} \geq \alpha_{G_2}$	$\frac{\alpha_{SP_1}}{\alpha_{SP_2}}\left(\frac{\sigma_{SP_1}}{\sigma_{SP_2}}\right)^2 \times \times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$	$+\infty$

Table 6: Upper bounds $m_1\widetilde{m}_1$ and $M_1\widetilde{M}_1$ for ρ as in Equation (4.7). Here $\sigma_{Mq}, \sigma_{SP}, \sigma_{G_k} > 0$ and $\alpha_{G_k} \in \mathbb{R}_+$, $k = 1, 2$. Here ψ_1 is Multiquadric function as in (5.1), ψ_2 is a Sine Power function as (5.3) and φ_1, φ_2 are Gauss functions as in (5.4)

Parameters	$m_{Mq,SP} m_{G_1,G_2}$	$M_{Mq,SP} M_{G_1,G_2}$
$p_{Mq} \in \left(0, \frac{1}{2}\right)$, $\alpha_{SP} \in (0, 2)$ $\tau_{Mq} \in \mathbb{Z}_+ \setminus \{0\}$ $n_0 \geq \max\left\{\tau_{Mq}, \frac{4p_{Mq}-2}{1-2p_{Mq}}\right\}$ $\alpha_{G_1} < \alpha_{G_2}$	0	$C^{\dagger}_{Mq,SP} \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$
$p_{Mq} \in \left(0, \frac{1}{2}\right)$, $\alpha_{SP} \in (0, 2)$ $\tau_{Mq} \in \mathbb{Z}_+ \setminus \{0\}$ $n_0 \geq \max\left\{\tau_{Mq}, \frac{4p_{Mq}-2}{1-2p_{Mq}}\right\}$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$
$\alpha_{SP} = p_{Mq} \in \left(0, \frac{2}{5}\right)$ $\tau_{Mq} = 1$ $\alpha_{G_1} < \alpha_{G_2}$	0	$2\sqrt{2}\left(\frac{\sigma_{Mq}}{\sigma_{SP}}\right)^2 \frac{1-p_{Mq}}{p_{Mq}}$ $\times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$
$\alpha_{SP} = p_{Mq} \in \left(0, \frac{2}{5}\right)$ $\tau_{Mq} = 1$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$
$\alpha_{SP} = p_{Mq} \in \left(\frac{2}{5}, \frac{1}{2}\right)$ $\tau_{Mq} = 1$ $\alpha_{G_1} < \alpha_{G_2}$	0	$8\sqrt{2}\left(\frac{\sigma_{Mq}}{\sigma_{SP}}\right)^2 \frac{1-p_{Mq}}{2-p_{Mq}}$ $\times \left(\frac{\sigma_{G_1}}{\sigma_{G_2}}\right)^2 \left(\frac{\alpha_{G_2}}{\alpha_{G_1}}\right)^{1/2}$
$\alpha_{SP} = p_{Mq} \in \left(\frac{2}{5}, \frac{1}{2}\right)$ $\tau_{Mq} = 1$ $\alpha_{G_1} \geq \alpha_{G_2}$	0	$+\infty$

$$^{\dagger}C_{Mq,SP} := \max_{n \in \{0,1,\ldots,n_0\}} \left\{ -\sqrt{2}\left(\frac{\sigma_{Mq}}{\sigma_{SP}}\right)^2 \frac{(1-p_{Mq})^{\tau_{Mq}}}{\Gamma(\tau_{Mq})} \frac{\Gamma(\tau_{Mq}+n1)}{\prod_{m=0}^{n}(2m-\alpha_{SP})} (n+1)\,(2p_{Mq})^n \right\}$$

6 Discussion

We have provided simple strategies that allow to obtain admissible nested covariance models with (some) negative coefficients. Our findings allow to enrich the classes of covariance functions on spheres as well as spheres cross time. In particular, our model allow for potential negative correlations at large distances over the sphere representing planet Earth.

A subsequent step in our research will be to consider a more general class of processes over spheres, called axially symmetric in Jones (1963). Such a class is more suitable for modeling climate processes, that are notoriously stationary with respect to longitude, but nonstationary with respect to latitude.

Another important research for the future will be to consider the regularity properties of Gaussian fields with admissible nested covariance functions. This would imply to emulate the tours de force in Lang and Schwab (2015) and in Clarke et al. (2018).

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