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# Strictly positive definite multivariate covariance functions on spheres



Jean Carlo Guella a,\*, Valdir Antonio Menegatto a, Emilio Porcu b,c

- <sup>a</sup> Departamento de Matemática, ICMC-USP São Carlos, Caixa Postal 668, 13560-970 São Carlos SP, Brazil
- <sup>b</sup> School of Mathematics, Statistics and Physics, Newcastle University, NE1 7RU, United Kingdom
- <sup>c</sup> Departamento de Matemática, Universidad técnica Federico Santa María, 2360102 Valparaíso, Chile

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#### ABSTRACT

We study the strict positive definiteness of matrix-valued covariance functions associated to multivariate random fields defined over d-dimensional spheres of the (d+1)-dimensional Euclidean space. Characterization of strict positive definiteness is crucial to both estimation and cokriging prediction in classical geostatistical routines. We provide characterization theorems for high dimensional spheres as well as for the Hilbert sphere. We offer a necessary condition for positive definiteness on the circle. Finally, we discuss a parametric example which might turn to be useful for geostatistical applications.

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#### 1. Introduction

Positive definite functions are fundamental to many disciplines, such as mathematical analysis, probability theory, approximation theory, numerical analysis, machine learning techniques, and spatial statistics. They are crucial for the simulation of Gaussian random fields on subsets of Euclidean spaces as well as for the construction of certain classes of spatial point processes.

Spatial data observed over a subset of the *d*-dimensional Euclidean space are often modeled as a realization of a stationary and isotropic Gaussian field. This approach requires the fitting of a covariance model. As noted by Gneiting [17], a candidate function *C* is fitted to the observed correlations such that

$$\Sigma = \left[ C(\boldsymbol{x}_i, \boldsymbol{x}_j) \right]_{i,i=1}^N$$

is the covariance matrix for the random field restricted to arbitrary points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  in  $\mathbb{R}^d$ . The matrix  $\Sigma$  is positive semidefinite, and this is achieved for all N and all the points if and only if the kernel function C defined above is positive definite on  $\mathbb{R}^d$ . In the last years, the statistical analysis of vector-valued fields has become ubiquitous, and the reader is referred to the review in [16] as well to [6] and [12] for more details. Under such a framework, for a multivariate random field with p components, a candidate matrix-valued function C, is fitted to the observations so that the block matrix

 $\textit{E-mail addresses:} \ jeanguella@gmail.com\ (J.C.\ Guella),\ menegatt@icmc.usp.br\ (V.A.\ Menegatto),\ georgepolya01@gmail.com\ (E.\ Porcu).$ 

<sup>\*</sup> Corresponding author.

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \cdots & \Sigma_{1j} & \cdots & \Sigma_{1p} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \Sigma_{i1} & \cdots & \Sigma_{ij} & \cdots & \Sigma_{ip} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \Sigma_{p1} & \cdots & \cdots & \cdots & \Sigma_{pp} \end{bmatrix}$$

$$(1)$$

is the matrix-valued covariance block matrix for the p-valued random field restricted to any finite set  $\{x_1, \ldots, x_N\}$  of points in  $\mathbb{R}^d$ . Observe that each block  $\Sigma_{ij}$  reflects the cross covariance between the ith and jth components of the vector-valued random field. The blocks on the diagonal of  $\Sigma$  are called auto covariances.

The most popular estimation techniques, such as likelihood [24], typically rely on a Cholesky factorization of the matrices  $\Sigma$ . Calculation of the inverse is also the crux for getting the kriging predictor, which is basically the best linear unbiased predictor in the geostatistical context. If the function C is not strictly positive definite, then the associated matrices  $\Sigma$  might be singular. Such a problem has inspired constructive criticism in several branches of spatial statistics and numerical analysis, and the reader is referred to [3,4,11,13–15,19,28,33] for the geostatistical context, and to [9,25–27,36] for a mathematical treatise

Recently, there has been an intense activity around scalar and vector-valued fields defined globally over the whole of planet Earth, which is usually represented as a sphere. Motivating examples can be found in [1,2,8,22,29]. In this case, the matrix-valued function  $\mathbf{C}$  described above should depend on the geodesic distance, being the arc joining any pair of points located over the spherical shell. Positive definite real-valued functions over spheres have a long history and we refer the reader to the review by Gneiting [18] as well as the recent extensions in [5,20]. Their strict positive definiteness has been studied extensively in [10,25-27,34]. Positive definiteness for vector-valued random fields has been discussed in [3,30].

Characterization of strict positive definiteness for the matrix-valued case has been elusive so far. Our efforts in this paper are devoted to such a characterization. The plan of the paper is the following. Section 2 contains the necessary background material. Section 3 is devoted to the original results of this paper: we provide characterization theorems for high-dimensional spheres as well as for the Hilbert sphere. We offer a necessary condition for strict positive definiteness on the circle. In Section 4 we apply the main result in the paper to describe a large class of strictly positive definite multivariate covariance functions on all spheres.

# 2. Background and notation

We denote with  $\mathbb{S}^d$  the d-dimensional sphere embedded in  $\mathbb{R}^{d+1}$  and with  $\theta$  the geodesic distance on  $\mathbb{S}^d$  uniquely defined, for all  $\mathbf{x}, \mathbf{y} \in \mathbb{S}^d$ , through the relation

$$\theta(\mathbf{x}, \mathbf{y}) = \arccos(\mathbf{x} \cdot \mathbf{y}),$$

with  $\cdot$  being the canonical dot product in  $\mathbb{R}^{d+1}$ . We follow [29] when defining  $\Psi^p_d$  as the class of mappings  $\psi:[0,\pi]\to M^p$ , with  $M^p$  being the set of  $p\times p$  real matrices, such that the mapping  $\mathbf{C}:\mathbb{S}^d\times\mathbb{S}^d\to M^p$  defined, for all  $\mathbf{x},\mathbf{y}\in\mathbb{S}^d$ , through

$$C(x,y) = \psi\{\theta(x,y)\},\tag{2}$$

is symmetric and positive definite. The latter means that

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\boldsymbol{c}_{i}^{\mathsf{T}}\boldsymbol{C}(\boldsymbol{x}_{i},\boldsymbol{x}_{j})\boldsymbol{c}_{j}\geq0$$

for any integer  $N \ge 1$ , distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$  and vectors  $\mathbf{c}_1, \dots, \mathbf{c}_N$  in  $\mathbb{R}^p$ . If the last inequality is strict when  $\mathbf{c}_i \ne 0$  for at least one  $i \in \{1, \dots, N\}$ , then  $\mathbf{C}$  is called *strictly positive definite*. Rephrased,  $\mathbf{C}$  is the covariance function of some vector-valued Gaussian field  $\mathbf{Z}(\mathbf{x}) = (Z_1(\mathbf{x}), \dots, Z_p(\mathbf{x}))^{\mathsf{T}}$  on  $\mathbb{S}^d$ . Thus, a necessary requirement is that the diagonal members  $C_{ii}$  evaluated at zero, and being the variance of  $Z_i$ , are strictly positive.

Condition (2) in the definition above reflects the geodesic isotropy of C. In particular, the entries  $C_{ij}$  with  $i, j \in \{1, ..., p\}$  of an isotropic matrix function C satisfy, for all  $x, y \in \mathbb{S}^d$ ,  $A \in \mathcal{O}_d$  and  $i, j \in \{1, ..., p\}$ ,

$$C_{ij}(\boldsymbol{x},\boldsymbol{y}) = C_{ij}(A\boldsymbol{x},A\boldsymbol{y}), \tag{3}$$

where  $\mathcal{O}_d$  is the group of all orthogonal transformations on  $\mathbb{R}^{d+1}$ , a well-known fact from the analysis on spheres. We shall abuse notation when using equivalently  $\theta$  or  $\theta(\mathbf{x}, \mathbf{y})$  whenever no confusion can arise. The term geodesic isotropy is coined to distinguish from Euclidean isotropy or radial symmetry as in [12]. A relevant fact is that the mapping  $C_{ij}:[0,\pi]\to\mathbb{R}$ ,  $i\neq j$ , is not, in general, positive definite (for i=j, it obviously is). This in turn implies that the block  $\Sigma_{ij}$  in the matrix  $\Sigma$  in Eq. (1) is not necessarily positive semidefinite.

The case p=1 has been largely discussed since the seminal paper [31], where it is established that a continuous function  $\psi:[0,\pi]\to\mathbb{R}$  with  $\psi(0)=1$  such that  $C(\mathbf{x},\mathbf{y})=\psi(\theta)$  belongs to the class  $\Psi_d=\Psi_d^1$  if and only if

$$\forall_{\theta \in [0,\pi]} \quad \psi(\theta) = \sum_{k=0}^{\infty} b_{k,d} c_k(d,\cos\theta),\tag{4}$$

with  $\{b_{k,d}\}_{k=0}^{\infty}$  being a uniquely determined probability mass sequence. Following [5] and other references as well, we call  $\{b_{k,d}\}_{k=0}^{\infty}$  a d-Schoenberg sequence. Here,  $c_k(d,\cos\theta)$  is the normalized Gegenbauer polynomial, defined, for all  $x\in[-1,1]$ ,

$$c_k(d, x) = P_k^{(d-1)/2}(x)/P_k^{(d-1)/2}(1),$$

with  $P_k^{\lambda}$ ,  $\lambda > 0$ , generated by the intrinsic relation

$$(1+r^2-2r\cos\theta)^{-\lambda}=\sum_{k=0}^{\infty}r^kP_k^{\lambda}(\cos\theta)$$

valid for all  $r \in (-1, 1)$  and  $\theta \in [0, \pi]$ . The following well-known assertions [32] hold for d > 2:

- (i)  $|c_k(d, \cos \theta)| = 1$  if and only if either  $\theta = 0$  or  $\theta = \pi$ .
- (ii) For  $\theta \in (0, \pi)$ ,  $\lim_{k \to \infty} c_k(d, \cos \theta) = 0$ .

We shall make use of these properties through subsequent sections.

Taking advantage of the work of Schoenberg we can also define the limit class  $\Psi_{\infty}$  consisting instead of those continuous members  $\psi$  with  $\psi(0) = 1$  being identified through the series representation, valid for all  $\theta \in [0, \pi]$ ,

$$\psi(\theta) = \sum_{k=0}^{\infty} b_k \cos^k \theta, \tag{5}$$

which clearly shows that  $\psi \in \Psi_{\infty}$  if and only if  $\psi(\arccos X)$  is the probability generating function of some discrete random variable X with support on  $\mathbb{Z}_+$  and distributed according to the probability mass system  $\{b_k\}_{k=0}^{\infty}$ .

We call  $\widetilde{\Psi}_d^p$  the subclass of  $\Psi_d^p$  whose continuous members are the radial part of mappings C as in (2), being strictly positive definite. A characterization of the class  $\widetilde{\Psi}_d = \widetilde{\Psi}_d^1$  has emerged thanks to [10,25,27]. In particular, we have that  $\psi \in \widetilde{\Psi}_d$ , for  $d \ge 2$ , if and only if the d-Schoenberg coefficients  $b_{n,d}$  in the expansion (4) are strictly positive for infinitely many even and infinitely many odd ks. The class  $\widetilde{\Psi}_1$  consists of those members of  $\Psi_1$  such that for every integer  $n \geq 1$  and  $j \in \{0, \dots, n-1\}$ , there exists an integer k such that  $b_{|j+kn|,1}$  is strictly positive. The analogue of the result obtained for the class  $\widetilde{\Psi}_d$ , for  $d \geq 2$ , holds for the class  $\Psi_{\infty}$  in terms of infinitely many even and infinitely many odd positive coefficients  $b_k$  as defined through

A characterization for the class  $\Psi_q^p$  was essentially obtained in [21] and [35]. A recent alternative proof can be found in [7].

**Theorem 1.** The continuous mapping  $\psi : [0, \pi] \to M^p$  belongs to the class  $\Psi_d^p$  if and only if

$$\forall_{\theta \in [0,\pi]} \quad \psi(\theta) = \sum_{k=0}^{\infty} A_{k,d} c_k(d, \cos \theta), \tag{6}$$

where  $\{A_{k,d}\}\subset M^p$ , each  $A_k$  is positive semidefinite and  $\sum_{k=0}^{\infty}A_{k,d}<\infty$ .

A characterization for the analogous limit class  $\Psi^p_\infty$  has been described in [23]. However, characterizations for the classes  $\widetilde{\Psi}^p_d$  and  $\widetilde{\Psi}^p_\infty$  have been elusive and we are going to make them explicit in the next section. The matrix sequence  $\{A_{k,d}\}$  will be called a d-Schoenberg matrix sequence of  $\psi$  throughout. It is worth mentioning that the matrices  $A_k$  in the representation provided by the theorem above have real entries.

A neat exposition of the subsequent results relies on some notation. For a given  $d \in \mathbb{Z}_+$ , let  $\psi$  be a member of the class  $\Psi^p_d$  with d-Schoenberg matrix sequence  $\{A_{k,d}\}_{k=0}^{\infty}$  as in representation (6). We define

$$J(\psi, p) = \{k : A_{k,d} \neq 0\}.$$

Apparently, the function I depends on the dimension d, but this will not be emphasized in our notation because d is fixed throughout. We shall be sloppy when using J instead of  $J(\psi, p)$  whenever no confusion can arise. The set  $J(\psi, 1)$  with  $\psi \in \Psi_d$ has already been studied and the related result is reported below. It rephrases the findings of [10] and [27], respectively.

**Theorem 2.** Let d be a positive integer and let  $\psi \in \widetilde{\Psi}_d$ . Then, the following assertions hold:

- (i)  $\psi \in \widetilde{\Psi}_d$ ,  $d \ge 2$ , if and only if  $J(\psi, 1)$  contains infinitely many even and infinitely many odd integers. (ii)  $\psi \in \widetilde{\Psi}_1$  if and only if the set  $\{k : |k| \in J(\psi, 1)\}$  intersects every full arithmetic progression in  $\mathbb{Z}$ .

# 3. Results

We start by noting that, for every  $k \in \mathbb{Z}_+$  and a positive semidefinite  $A \in M^p$ , the mapping  $Ac_k(d, \cos \theta)$  belongs to the class  $\Psi^p_d \setminus \Psi^p_{d+1}$ . Thus, the proof of the following statement is obvious and omitted.

**Lemma 1.** Let d and p be positive integers and  $\psi \in \Psi_d^p$  with d-Schoenberg matrix sequence  $\{A_{k,d}\}_{k=0}^{\infty}$ . Then, for distinct points  $\mathbf{x}_1, \ldots, \mathbf{x}_N$  on  $\mathbb{S}^d$  and  $\{\mathbf{w}_1, \ldots, \mathbf{w}_N\} \subset \mathbb{R}^p$ , the following assertions are equivalent:

- (i)  $\sum_{i,j=1}^{N} \boldsymbol{w}_{i}^{\mathsf{T}} \psi \{\theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} \boldsymbol{w}_{j} = 0.$
- (ii)  $\sum_{i,j=1}^{N} \boldsymbol{w}_{i}^{\mathsf{T}} A_{k,d} \boldsymbol{w}_{j} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0$  for all  $k \in J$ .

Another formal statement along the same lines follows subsequently. A technical proof is needed in order to prove its validity.

**Lemma 2.** Let d and p be positive integers and  $\psi \in \Psi_d^p$  with d-Schoenberg matrix sequence  $\{A_{k,d}\}_{k=0}^{\infty}$ . Then, the following assertions are equivalent:

- (i)  $\psi \in \widetilde{\Psi}_d^p$ . (ii) For any integer  $N \geq 1$  and distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$ , no two of which are antipodal, the only solution  $(\mathbf{u}_1, \mathbf{v}_1), \dots, (\mathbf{u}_N, \mathbf{v}_N) \in \mathbb{R}^{2p}$  of the system

$$\forall_{k \in J} \quad \sum_{i,j=1}^{N} \{ \boldsymbol{u}_i + (-1)^k \boldsymbol{v}_i \}^{\mathsf{T}} A_{k,d} \{ \boldsymbol{u}_j + (-1)^k \boldsymbol{v}_j \} c_k \{ d, \cos \theta(\boldsymbol{x}_i, \boldsymbol{x}_j) \} = 0,$$

is the trivial one, i.e.,  $\boldsymbol{u}_1 = \boldsymbol{v}_1 = 0, \dots, \boldsymbol{u}_N = \boldsymbol{v}_N = 0.$ 

**Proof.** We give a constructive proof. Given distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$ , we define

$$\mathbf{y}_i = \begin{cases} \mathbf{x}_i & \text{if } i \in \{1, \dots, N\}, \\ -\mathbf{x}_{i-N} & \text{if } i \in \{N+1, \dots, 2N\}. \end{cases}$$

We note that  $\{y_1, \dots, y_{2N}\}$  is a set of 2N distinct points on  $\mathbb{S}^d$ . If (i) holds, Lemma 1 shows that the system

$$\forall_{k \in J} \quad \sum_{i=1}^{2N} \boldsymbol{w}_i^{\mathsf{T}} A_{k,d} \boldsymbol{w}_j c_k \{d, \cos \theta(\boldsymbol{x}_i, \boldsymbol{x}_j)\} = 0,$$

has a unique solution  $w_1, \ldots, w_{2N}$  in  $\mathbb{R}^p$ , being namely, the trivial one. Direct inspection shows that the system is precisely the one described in (ii), with  $\boldsymbol{u}_i = \boldsymbol{w}_i$  for all  $i \in \{1, ..., N\}$  and  $\boldsymbol{v}_i = \boldsymbol{w}_{i+N}$  for all  $i \in \{1, ..., N\}$ . Conversely, if (i) does not hold, we can pick distinct points  $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$  in  $\mathbb{S}^d$  for which the system

$$\forall_{k \in J} \quad \sum_{i,i=1}^{N} \boldsymbol{w}_{i}^{\mathsf{T}} A_{k,d} \boldsymbol{w}_{j} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0,$$

has more than one solution. But, if we consider m points  $y_1, \ldots, y_m$  in  $\mathbb{S}^d$  with  $m \leq N$ , no two of which are antipodal, so that  $\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N\}\subset\{\pm\boldsymbol{y}_1,\ldots,\pm\boldsymbol{y}_m\}$ , it is easily seen that the system

$$\forall_{k \in J} \quad \sum_{i,j=1}^{m} \{ \boldsymbol{u}_{i} + (-1)^{k} \boldsymbol{v}_{i} \}^{\mathsf{T}} A_{k,d} \{ \boldsymbol{u}_{j} + (-1)^{k} \boldsymbol{v}_{j} \} c_{k} \{ d, \cos \theta(\boldsymbol{y}_{i}, \boldsymbol{y}_{j}) \} = 0,$$

has, likewise, a nontrivial solution  $(\mathbf{u}_1, \mathbf{v}_1), \dots, (\mathbf{u}_m, \mathbf{v}_m)$ .

The following reformulation of Lemma 2 takes into account the evenness of the elements of J.

**Proposition 1.** Let d and p be positive integers and let  $\psi \in \Psi_d^p$  with d-Schoenberg matrix sequence  $\{A_{k,d}\}_{k=0}^{\infty}$ . Then, the following assertions are equivalent:

- (i)  $\psi \in \widetilde{\Psi}_d^p$ .
- (ii) For any integer  $N \geq 1$  and distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$ , no two of which are antipodal, the only solution  $(\mathbf{u}_1^o, \mathbf{u}_1^e), \dots, (\mathbf{u}_N^o, \mathbf{u}_N^e) \in \mathbb{R}^{2p}$  of the system

$$\begin{cases} \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{o})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{o} c_{k}(d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})) = 0 & \text{if } k \in J \cap (2\mathbb{Z}_{+} + 1), \\ \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e} c_{k}(d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})) = 0 & \text{if } k \in J \cap 2\mathbb{Z}_{+}, \end{cases}$$

is the trivial one.

**Proof.** If (ii) does not hold, we can find N distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$ , no two of which are antipodal, and N vectors  $(\mathbf{u}_i^o, \mathbf{u}_i^e) \in \mathbb{R}^{2p}$ , with at least one of them being nonzero, so that

$$\begin{cases} \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{o})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{o} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0 & \text{if } k \in J \cap (2\mathbb{Z}_{+} + 1), \\ \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0 & \text{if } k \in J \cap 2\mathbb{Z}_{+}, \end{cases}$$

holds. Now, consider

$$\begin{cases}
2\mathbf{u}_i = \mathbf{u}_i^o + \mathbf{u}_i^e & \text{if } i \in \{1, \dots, N\}, \\
2\mathbf{v}_i = \mathbf{u}_i^o - \mathbf{u}_i^e & \text{if } i \in \{1, \dots, N\}.
\end{cases}$$

Then, at least one pair  $(\boldsymbol{u}_i, \boldsymbol{v}_i)$  is nonzero and, in addition,

$$\forall_{k \in J} \quad \sum_{i,i=1}^{N} \{ \boldsymbol{u}_i + (-1)^k \boldsymbol{v}_i \}^{\mathsf{T}} A_{k,d} \{ \boldsymbol{u}_j + (-1)^k \boldsymbol{v}_j \} c_k \{ d, \cos \theta(\boldsymbol{x}_i, \boldsymbol{x}_j) \} = 0.$$

In particular, the arguments in Lemma 2 show that (i) does not hold. Conversely, if  $\psi \in \Psi_d^p \setminus \widetilde{\Psi}_d^p$ , we can make use of Lemma 2 and select N distinct points  $\mathbf{x}_1, \ldots, \mathbf{x}_N$  in  $\mathbb{S}^d$ , no two of which are antipodal, and vectors  $(\mathbf{u}_1, \mathbf{v}_1), \ldots, (\mathbf{u}_N, \mathbf{v}_N) \in \mathbb{R}^{2p}$ , with at least one of them being nonzero, so that

$$\forall_{k \in J} \quad \sum_{i,j=1}^{N} \{ \mathbf{u}_i + (-1)^k \mathbf{v}_i \}^{\mathsf{T}} A_{k,d} \{ \mathbf{u}_j + (-1)^k \mathbf{v}_j \} c_k \{ d, \cos \theta(\mathbf{x}_i, \mathbf{x}_j) \} = 0.$$

Let us now define

$$\begin{cases} \mathbf{u}_i^o = \mathbf{u}_i - \mathbf{v}_i & \text{if } i \in \{1, \dots, N\}, \\ \mathbf{u}_i^e = \mathbf{u}_i + \mathbf{v}_j & \text{if } i \in \{1, \dots, N\}. \end{cases}$$

Then, either  $\boldsymbol{u}_i^o \neq 0$  for some i, or  $\boldsymbol{u}_i^e \neq 0$  for some i. This in turn implies that  $(\boldsymbol{u}_1^o, \boldsymbol{u}_1^e), \dots, (\boldsymbol{u}_N^o, \boldsymbol{u}_N^e)$  is a nontrivial solution of the system in (ii). The proof is complete.  $\Box$ 

The following result offers a bridge from the class  $\Psi_d^p$ , with p>1 to the class  $\Psi_d$ .

**Lemma 3.** Let d, p be positive integers. For  $\psi \in \Psi_d^p$  and  $\mathbf{v} \in \mathbb{R}^p$ , define, for all  $\theta \in [0, \pi]$ ,

$$g_{\mathbf{v}}(\theta) = \mathbf{v}^{\mathsf{T}} \boldsymbol{\psi}(\theta) \mathbf{v}. \tag{7}$$

Then, every function  $g_{\boldsymbol{v}}$  belongs to  $\Psi_d$ . Further, if  $\boldsymbol{v} \in \mathbb{R}^p \setminus \{\boldsymbol{0}\}$  and  $\boldsymbol{\psi} \in \widetilde{\Psi}_d^p$ , then  $g_{\boldsymbol{v}} \in \widetilde{\Psi}_d$ .

**Proof.** The first assertion follows from the fact that, for distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  on  $\mathbb{S}^d$  and real scalars  $c_1, \dots, c_N$ , we have

$$\sum_{i,j=1}^{N} c_i g_{\boldsymbol{v}} \{ \theta(\boldsymbol{x}_i, \boldsymbol{x}_j) \} c_j = \sum_{i,j=1}^{N} (c_i \boldsymbol{v})^{\mathsf{T}} \boldsymbol{\psi} \{ \theta(\boldsymbol{x}_i, \boldsymbol{x}_j) \} (c_j \boldsymbol{v}).$$

The second one follows from the fact that, if  $\psi \in \widetilde{\Psi}_d^p$ , then the quadratic form above is zero if and only if  $c_i \mathbf{v} = 0$  for all  $i \in \{1, ..., N\}$ . If  $\mathbf{v} \neq \mathbf{0}$ , the last condition reduces to  $c_i = 0$  for all  $i \in \{1, ..., N\}$ .  $\square$ 

We are now able to illustrate the main result of this section.

**Theorem 3.** Let  $d \geq 2$  and p be a positive integer. Let  $\psi \in \Psi_d^p$  with d-Schoenberg matrix sequence  $\{A_{k,d}\}_{k=0}^{\infty}$ . For  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , let  $g_{\mathbf{v}}$  be defined through Eq. (7). Then, the following assertions are equivalent:

- (i)  $\psi \in \widetilde{\Psi}_d^p$ .
- (ii) For every  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , the function  $g_{\mathbf{v}}$  belongs to the class  $\widetilde{\Psi}_d$ .
- (iii) For every  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , the set  $\{k : \mathbf{v}^{\mathsf{T}} A_{k,d} \mathbf{v} > 0\}$  contains infinitely many even and infinitely many odd integers.

**Proof.** The implication (i)  $\Rightarrow$  (ii) follows from Lemma 3.

We proceed by contradiction to prove (ii)  $\Rightarrow$  (iii). Let  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$  be such that  $\{k : \mathbf{v}^\intercal A_{k,d} \mathbf{v} > 0\}$  does not contain infinitely many even and infinitely many odd integers. Invoking again Lemma 3, we have that  $g_{\mathbf{v}}$  as defined through Eq. (7) is a member of the class  $\Psi_d$  for all  $\mathbf{v}$  fixed. Also, we have  $J(g_{\mathbf{v}}, 1) = \{k : \mathbf{v}^\intercal A_{k,d} \mathbf{v} > 0\}$ . In particular,  $J(g_{\mathbf{v}}, 1)$  fails to contain infinitely many even and infinitely many odd integers. By invoking Theorem 2, we conclude that  $g_{\mathbf{v}} \in \Psi_d \setminus \widetilde{\Psi}_d$ . Thus, (ii) implies (iii).

The implication (iii)  $\Rightarrow$  (i) is also shown by contradiction. In view of Proposition 1, there exist distinct points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  in  $\mathbb{S}^d$ , no two of which are antipodal, such that the system

$$\begin{cases} \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{o})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{o} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0 & \text{if } k \in J \cap (2\mathbb{Z}_{+} + 1), \\ \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0 & \text{if } k \in J \cap 2\mathbb{Z}_{+}, \end{cases}$$

has a nontrivial solution  $(\boldsymbol{u}_1^o, \boldsymbol{u}_1^e), \dots, (\boldsymbol{u}_N^o, \boldsymbol{u}_N^e)$  in  $\mathbb{R}^{2p}$ . We now proceed assuming that at least one  $\boldsymbol{u}_i^e$  is nonzero, and that the following holds:

$$\forall_{k \in J \cap 2\mathbb{Z}_{+}} \sum_{i,j=1}^{N} (\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 0.$$

$$(8)$$

The case in which at least one  $\mathbf{u}_i^o$  is nonzero and the other equality above holds can be handled in a similar fashion. Without loss of generality, we can now assume that  $\mathbf{u}_i^e \neq \mathbf{0}$  for all  $i \in \{1, ..., N\}$ . Indeed, otherwise we just work with less than N points. Due to assertion (iii), the set  $\{k : (\mathbf{u}_1^e)^\intercal A_{k,d} \mathbf{u}_1^e > 0\}$  contains infinitely many even integers. Since  $\{k \in J : (\mathbf{u}_1^e)^\intercal A_{k,d} \mathbf{u}_1^e > 0\}$  is infinite and  $\{1, ..., N\}$  is finite, we can select an infinite subset K of  $2\mathbb{Z}_+ \cap \{k : (\mathbf{u}_1^e)^\intercal A_{k,d} \mathbf{u}_1^e > 0\}$  and  $i_0 \in \{1, ..., N\}$  so that, for all  $i \in \{1, ..., N\}$  and  $k \in K$ ,

$$(\boldsymbol{u}_{i_0}^e)^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i_0}^e \geq (\boldsymbol{u}_i^e)^{\mathsf{T}}A_{k,d}\boldsymbol{u}_i^e.$$

Dividing both sides in Eq. (8) by  $(\boldsymbol{u}_{i_0}^e)^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i_0}^e$ , we can deduce that, for all  $k \in K$ ,

$$0 = \sum_{i,i=1}^{N} \frac{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i}^{e}}{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i_{0}}^{e}} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\} = 1 + \sum_{i,j\neq i=1}^{N} \frac{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i}^{e}}{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i_{0}}^{e}} + \sum_{i\neq j}^{N} \frac{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e}}{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i_{0}}^{e}} c_{k} \{d, \cos \theta(\boldsymbol{x}_{i}, \boldsymbol{x}_{j})\}.$$

Since each  $A_{k,d}$  is positive semidefinite, one has, for all  $k \in K$  and  $i \in \{1, ..., N\}$ ,

$$\frac{(\boldsymbol{u}_i^e)^{\scriptscriptstyle{\intercal}} A_{k,d} \boldsymbol{u}_i^e}{(\boldsymbol{u}_{i_0}^e)^{\scriptscriptstyle{\intercal}} A_{k,d} \boldsymbol{u}_{i_0}^e} \in [0,\,1].$$

From the Cauchy–Schwarz inequality, we also know that, for all  $k \in K$  and  $i \neq j$ ,

$$|(\boldsymbol{u}_{i}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{j}^{e}| \leq \sqrt{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i}^{e}} \sqrt{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i}^{e}} \leq \sqrt{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i_{0}}^{e}} \sqrt{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i_{0}}^{e}} = (\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}}A_{k,d}\boldsymbol{u}_{i_{0}}^{e}.$$

Hence, for all  $k \in K$  and  $i \neq j$ ,

$$\left| \frac{(\boldsymbol{u}_{i}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{j}^{e}}{(\boldsymbol{u}_{i_{0}}^{e})^{\mathsf{T}} A_{k,d} \boldsymbol{u}_{i_{0}}^{e}} \right| \leq 1.$$

Now, we can let  $k \to \infty$  in order to deduce that  $0 \ge 1$ , a contradiction.  $\square$ 

**Example 1.** Let  $\psi_1$ ,  $\psi_2$  be in the class  $\widetilde{\Psi}_d$  with  $J(\psi_1, 1) = 4\mathbb{Z}_+ \cup (4\mathbb{Z}_+ + 1)$  and  $J(\psi_2, 1) = (4\mathbb{Z}_+ + 2) \cup (4\mathbb{Z}_+ + 3)$ . We have immediately that  $\psi: [0, \pi] \to M^2$  defined, for all  $\theta \in [0, \pi]$ , through

$$\psi(\theta) = \begin{pmatrix} \psi_1(\theta) & 0 \\ 0 & \psi_2(\theta) \end{pmatrix},$$

belongs to the class  $\widetilde{\Psi}_d^2$ . However, none of the matrices  $A_{k,d}$  from the d-Schoenberg expansion of  $\psi$  are positive definite.

3.1. The class  $\widetilde{\Psi}_1^p$ : strict positive definiteness on the circle

We start with a technical lemma that opens for a new result.

**Lemma 4.** Let p be a positive integer and  $\psi \in \Psi_1^p$  with 1-Schoenberg matrix sequence  $\{A_{k,1}\}_{k=0}^{\infty}$ . Then, the following assertions are equivalent:

- (i)  $\psi \in \widetilde{\Psi}_1^p$ .
- (ii) For any integer  $N \geq 1$  and distinct points  $z_1, \ldots, z_N$  in  $\{z \in \mathbb{C} : |z| = 1\}$ , the only solution  $(\mathbf{w}_1, \ldots, \mathbf{w}_N) \in \mathbb{R}^{pN}$  of the system

$$\forall_{k \in J} \quad \left(\sum_{\alpha=1}^{N} z_{\alpha}^{k} \boldsymbol{w}_{\alpha}\right)^{\mathsf{T}} A_{k,1} \left(\sum_{\alpha=1}^{N} z_{\alpha}^{-k} \boldsymbol{w}_{\alpha}\right) = 0,$$

is the trivial one.

**Proof.** Due to Lemma 1, Assertion (i) is equivalent to the following condition: if N is a positive integer and  $\mathbf{x}_1, \dots, \mathbf{x}_N$  are distinct points on  $S^1$ , then the only solution  $(\mathbf{w}_1, \dots, \mathbf{w}_N) \in \mathbb{R}^p$  of the system

$$\forall_{k \in J} \quad \sum_{\alpha,\beta=1}^{N} \boldsymbol{w}_{\alpha}^{\mathsf{T}} A_{k,1} \boldsymbol{w}_{\beta} c_{k} \{1, \cos \theta(\boldsymbol{x}_{\alpha}, \boldsymbol{x}_{\beta})\} = 0$$

is the trivial one. If we write  $\mathbf{x}_{\alpha} = (\cos \theta_{\alpha}, \sin \theta_{\alpha})$  for all  $\theta_{\alpha} \in [0, 2\pi)$  and  $\alpha \in \{1, \dots, N\}$ , the proof will resume as long as we show that the system above corresponds to that in (ii). Since  $P_k^1(\cos \theta) = 2k^{-1}\cos k\theta$  for all  $\theta \in [0, \pi]$ , the previous equality becomes

$$\forall_{k \in J} \quad \sum_{\alpha,\beta=1}^{N} \boldsymbol{w}_{\alpha}^{\mathsf{T}} A_{k,1} \boldsymbol{w}_{\beta} (\cos k \theta_{\alpha} \cos k \theta_{\beta} + \sin \theta_{\alpha} \sin \theta_{\beta}) = 0.$$

Let  $a_{ii,k,1}$  be the (i,j)th element of  $A_{k,1}$ ,  $k \in \{0,\ldots\}$ . Then, we can write each  $a_{ii,k,1}$  in Gram format, i.e.,

$$\forall_{i,j\in\{1,\ldots,p\}} \quad a_{ij,k,1} = \boldsymbol{a}_{i,k} \cdot \boldsymbol{a}_{j,k},$$

where  $\mathbf{a}_{i,k} \in \mathbb{C}^p$  for all  $i \in \{1, ..., N\}$ , and  $\cdot$  is the inner product in  $\mathbb{C}^p$ , and the previous equality takes the form

$$\forall_{k \in J} \quad \left\| \sum_{i=1}^{p} \sum_{\alpha=1}^{N} w_{\alpha}^{i}(\cos k\theta_{\alpha}) \boldsymbol{a}_{i,k} \right\|^{2} + \left\| \sum_{i=1}^{p} \sum_{\alpha=1}^{N} w_{\alpha}^{i}(\sin k\theta_{\alpha}) \boldsymbol{a}_{i,k} \right\|^{2} = 0,$$

where  $\mathbf{w}_{\alpha} = (w_{\alpha}^{1}, \dots, w_{\alpha}^{p})$  for all  $\alpha \in \{1, \dots, N\}$  and  $\|\cdot\|$  is the usual norm in  $\mathbb{C}^{p}$ . However, this last equality is equivalent to

$$\forall_{k \in J} \quad \sum_{\mu=1}^{p} \sum_{\alpha=1}^{N} w_{\alpha}^{\mu} e^{ik\theta_{\alpha}} \boldsymbol{a}_{\mu,k} = 0.$$

After eliminating the Gram entries of the matrix, we are reduced to

$$\forall_{k\in J} \quad \sum_{\mu=1}^p \sum_{\alpha=1}^N \sum_{\nu=1}^p \sum_{\beta=1}^N w_{lpha}^{\mu} w_{eta}^{
u} e^{ik( heta_{lpha}- heta_{eta})} a_{\mu
u,k,1} = 0,$$

which is equivalent to

$$\forall_{k \in J} \left( \sum_{\alpha=1}^{N} e^{ik\theta_{\alpha}} \boldsymbol{w}_{\alpha} \right)^{\mathsf{T}} A_{k,1} \left( \sum_{\alpha=1}^{N} e^{-ik\theta_{\alpha}} \boldsymbol{w}_{\alpha} \right) = 0.$$

The proof is complete.  $\Box$ 

Theorem 3 has the following cousin in the case d = 1.

**Theorem 4.** Let p be a positive integer and let  $\psi \in \widetilde{\Psi}_1^p$  with 1-Schoenberg matrix sequence  $\{A_{k,1}\}_{k=0}^{\infty}$ . Then, for each  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , the set  $\{k: \mathbf{v}^\intercal A_{|k|,1} \mathbf{v} > 0\}$  intersects every full arithmetic progression in  $\mathbb{Z}$ .

**Proof.** Assume  $\psi \in \widetilde{\Psi}_1^p$ . Let  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$  and define  $g_{\mathbf{v}}(\theta) = \mathbf{v}^{\mathsf{T}} \psi(\theta) \mathbf{v}$  for all  $\theta \in [0, \pi]$ . It is manifest that  $g_{\mathbf{v}}$  is a member of the class  $\widetilde{\Psi}_1$ . Thanks to Theorem 2, we have that  $\{k : |k| \in J(\psi, 1)\}$  intersects every arithmetic progression in  $\mathbb{Z}$ . However, since  $J(\psi, 1) = \{k : \mathbf{v}^{\mathsf{T}} A_{k,1} \mathbf{v} > 0\}$ , the set  $\{k : \mathbf{v}^{\mathsf{T}} A_{|k|,1} \mathbf{v} > 0\}$  must intersect each arithmetic progression in  $\mathbb{Z}$ . The proof is complete.  $\square$ 

A proof for the sufficiency of the condition in the previous theorem is still elusive.

3.2. The class  $\widetilde{\Psi}_{\infty}^{p}$ 

Our findings are now completed by considering the class  $\widetilde{\Psi}_{\infty}^{p}$ 

**Theorem 5.** Let p be a positive integer and let  $\psi$  be a member of the class  $\Psi_{\infty}^p$  having a uniquely determined expansion

$$\psi(\theta) = \sum_{k=0}^{\infty} A_k \cos^k \theta,$$

valid for all  $\theta \in [0, \pi]$ , with Schoenberg matrix sequence  $\{A_k\} \subset M^p$  of positive semidefinite matrices such that  $\sum_k A_k < \infty$ . Then, the following assertions are equivalent:

- (i)  $\psi \in \widetilde{\Psi}^p_{\infty}$ .
- (ii) For every  $\mathbf{v} \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , both sets  $\{k : \mathbf{v}^{\mathsf{T}} A_k \mathbf{v} > 0\} \cap 2\mathbb{Z}_+$  and  $\{k : \mathbf{v}^{\mathsf{T}} A_k \mathbf{v} > 0\} \cap (2\mathbb{Z}_+ + 1)$  are infinite.

**Proof.** Assume (i) holds and let  $\mathbf{v} \in \mathbb{R}^{\ell}$ . For  $\mathbf{v} \in \mathbb{R}^{p} \setminus \{\mathbf{0}\}$ , let us consider the function  $g_{\mathbf{v}} : [0, \pi] \to \mathbb{R}$  defined through Eq. (7). It is easy to see that  $g_{\mathbf{v}} \in \widetilde{\Psi}_{\infty}$  for all  $\mathbf{v}$ . By (i) and from Theorem 2.8 in [25] we can write, for all  $\theta \in [0, \pi]$ ,

$$g_{\mathbf{v}}(\theta) = \sum_{k=0}^{\infty} b_k \cos^k \theta,$$

with  $b_k \geq 0$  for all  $k \in \mathbb{N}$ ,  $\sum_{k=0}^{\infty} b_k < \infty$ , and both sets  $\{k: b_k > 0\} \cap 2\mathbb{Z}_+$  and  $\{k: b_k > 0\} \cap (2\mathbb{Z}_+ + 1)$  being infinite. Since

$$g_{\mathbf{v}}(\theta) = \mathbf{v}^{\mathsf{T}} \left( \sum_{k=0}^{\infty} A_k \cos^k \theta \right) \mathbf{v} = \sum_{k=0}^{\infty} (\mathbf{v}^{\mathsf{T}} A_k \mathbf{v}) \cos^k \theta,$$

for all  $\theta \in [0, \pi]$ , we then have that (ii) follows by uniqueness of MacLaurin series representations. Conversely, assume (ii) holds. It suffices to show that  $\psi \in \widetilde{\Psi}_d^p$  for all d. Fix  $d \ge 1$  and write

$$(\cos \theta)^{k} = \sum_{0 \le 2j \le k} b(d, k, j) P_{k-2j}^{(d-1)/2}(\cos \theta),$$

for all  $\theta \in [0, \pi]$ , with all the b(d, k, j) being positive. It follows that, for all  $\theta \in [0, \pi]$ ,

$$\psi(\theta) = \sum_{k=0}^{\infty} A_k (\cos \theta)^k = \sum_{k=0}^{\infty} A_k \left\{ \sum_{0 \le 2j \le k} b(d, k, j) P_{k-2j}^{(d-1)/2} (\cos \theta) \right\} = \sum_{k=0}^{\infty} A'_k C_k^{(d-1)/2} (\cos \theta),$$

where

$$A'_{k} = \begin{cases} \sum_{\substack{j=k \ j \in 2\mathbb{Z}_{+}}}^{\infty} b(d, k, j) A_{j} & \text{if } k \text{ is even,} \\ \sum_{\substack{j=k \ i \in 2\mathbb{Z}_{+}+1}}^{\infty} b(d, k, j) A_{j} & \text{if } k \text{ is odd.} \end{cases}$$

Each  $A'_k$  is positive semidefinite. If  $\mathbf{v}^{\mathsf{T}}A_k\mathbf{v}>0$  for some k, then

$$\boldsymbol{v}^{\mathsf{T}}A_k'\boldsymbol{v} = \boldsymbol{v}^{\mathsf{T}}\left\{\sum_{\substack{j=k\\j\in2\mathbb{Z}_+}}^{\infty}b(d,k,j)A_j\right\}\boldsymbol{v} = \sum_{\substack{j=k\\j\in2\mathbb{Z}_+}}^{\infty}b(d,k,j)\boldsymbol{v}^{\mathsf{T}}A_j\boldsymbol{v} = b(d,k,j)\boldsymbol{v}^{\mathsf{T}}A_k\boldsymbol{v} + \sum_{\substack{j=k+2\\j\in2\mathbb{Z}_+}}^{\infty}b(d,k,j)A_j > 0,$$

i.e.,  $\{k: \mathbf{v}^{\mathsf{T}} A_k \mathbf{v} > 0\} \cap 2\mathbb{Z}_+ \subset \{k: \mathbf{v}^{\mathsf{T}} A_k' \mathbf{v} > 0\} \cap 2\mathbb{Z}_+$ . By assumption (ii), the set above is infinite. Proceeding analogously, we conclude that  $\{k: \mathbf{v}^{\mathsf{T}} A_k' \mathbf{v} > 0\} \cap (2\mathbb{Z}_+ + 1)$  is likewise infinite. Invoking the main theorem in [10], we conclude that  $\mathbf{\psi} \in \widetilde{\Psi}_{\infty}^p$ .  $\square$ 

An alternative proof of the previous theorem can be achieved fulfilling the details in these arguments:  $\psi \in \widetilde{\Psi}^p_{\infty}$  if and only if  $\psi \in \widetilde{\Psi}^p_d$ , for every d. However, Theorem 3 shows that the previous assertion is equivalent to  $g_{\boldsymbol{v}} \in \widetilde{\Psi}_d$ , for  $\boldsymbol{v} \in \mathbb{R}^p \setminus \{\boldsymbol{0}\}$  and every d. By the definition of  $\widetilde{\Psi}_d$ , this is also equivalent to  $g_{\boldsymbol{v}} \in \widetilde{\Psi}_{\infty}$ , for  $\boldsymbol{v} \in \mathbb{R}^p \setminus \{\boldsymbol{0}\}$ .

#### 3.3. Complex matrix functions

The setting in Section 2 can be slightly changed by letting  $M^p$  be the set of all complex  $p \times p$  matrices instead. In that case, we need to use complex vectors  $\mathbf{c}_i$  in the definition of positive definiteness and we may suppress the symmetry assumption on the matrix functions  $\mathbf{C}$ . Indeed, in this new setting, a positive definite matrix function is automatically hermitian. Theorem 1 still holds, but the matrices  $A_{k,d}$  may have off diagonal complex entries. All the results in Section 3 remain, with some pertinent adaptations in the proofs: the replacement of real vectors with complex ones and the replacement of the transposition operation with conjugate-transposition. The details will not be included here.

### 4. An application

We consider an example based on the class  $\Psi_{\infty}$ . Let  $\psi:[0,\pi]\to\mathbb{R}$  belong to the class  $\Psi_{\infty}$ , with probability mass system  $\{a_n\}_{n=0}^{\infty}$ . Let  $B=[B_{ii}]\in M^p$  be a nonzero positive semidefinite matrix with diagonal entries  $B_{kk}\in[0,1]$ . We denote by  $B^{(k)}$ the kth Hadamard power of B. We consider the matrix-valued function  $\psi$  with Schoenberg matrix sequence  $\{a_k B^{(k)}\}$ . Clearly, we have that  $\psi \in \Psi_p^{\infty}$ . Since B is nonzero, we also have that  $J(\psi, p) = J(\psi, 1)$ . As an application of Theorem 3, we can prove the following.

**Theorem 6.** Let  $\psi$ ,  $\psi$  and B be as in the previous paragraph. Write B in Gram format, i.e.,  $B = [\mathbf{x}_{\mu} \cdot \mathbf{x}_{\nu}]_{\mu,\nu=1}^{p}$ , where  $\mathbf{x}_{\mu} \in \mathbb{R}^{p}$  for all  $\mu \in \{1, \ldots, p\}$ . Then, the following assertions are equivalent:

- $\begin{array}{ll} \text{(i)} \;\; \pmb{\psi} \in \widetilde{\varPsi}_{\infty}^{\,p}. \\ \text{(ii)} \;\; \psi \in \widetilde{\varPsi}_{\infty}, \, \text{the } \pmb{x}_i \, \text{are nonzero and } \pmb{x}_{\mu} \neq \pm \pmb{x}_{\nu}, \, \mu \neq \nu. \end{array}$

**Proof.** If  $\psi \in \widetilde{\Psi}^p_{\infty}$ , the equality  $J(\psi, p) = J(\psi, 1)$  reveals that each function  $g_{\nu}, \nu \in \mathbb{R}^p \setminus \{\mathbf{0}\}$ , belongs to  $\widetilde{\Psi}_{\infty}$ . That being said, write  $\{e_1, \dots, e_p\}$  to denote the canonical basis of  $\mathbb{R}^p$ . If  $\mathbf{x}_i = \mathbf{0}$  for some i, direct computation reveals that  $g_{e_i}$  is a constant function and that is a contradiction. If  $\mathbf{x}_i = \mathbf{x}_j$  for some pair (i,j) with  $i \neq j$ , then another calculation reveals that  $g_{\mathbf{e}_i - \mathbf{e}_i} = 0$ , another contradiction. Finally, if  $\mathbf{x}_i = -\mathbf{x}_i$  for some pair (i,j) with  $i \neq j$ , then yet another calculation reveals that  $g_{e_i+e_i}$  is an odd function, a contradiction as well. These arguments resolve the implication (i)  $\Rightarrow$  (ii). In order to prove the converse implication, we will assume (ii) holds and that  $\psi \notin \widetilde{\Psi}_{\infty}^p$  and will reach a contradiction. The second assumption above reveals that the function  $g_{\boldsymbol{v}}$  does not belong to  $\widetilde{\Psi}_{\infty}^p$ , for some nonzero vector  $\boldsymbol{v} = (v_1, \dots, v_p) \in \mathbb{R}^p$ . In particular, the set

$$\{k: a_k \mathbf{v}^{\mathsf{T}} B^{(k)} \mathbf{v} > 0\} = \{k \in I(\psi, 1): \mathbf{v}^{\mathsf{T}} B^{(k)} \mathbf{v} > 0\}$$

must fail to contain infinitely many even and infinitely many odd integers. We will proceed assuming that it contains finitely many odd integers, the other case being similar. Pick  $k_0 \in \mathbb{Z}_+$  so that, for all  $k \geq k_0$  and  $k \in 2\mathbb{Z}_+ \cap J(\psi, 1)$ ,

$$0 = \mathbf{v}^{\mathsf{T}} B^{(k)} \mathbf{v} = \sum_{\mu, \nu=1}^p v_{\mu} v_{\nu} (\mathbf{x}_{\mu} \cdot \mathbf{x}_{\nu})^k.$$

Without loss of generality, we can assume that  $\mathbf{x}_1 \cdot \mathbf{x}_1 \geq \mathbf{x}_\mu \cdot \mathbf{x}_\mu$  for all  $\mu \in \{1, \dots, p\}$ . For  $\mu \neq \nu$ , we have that  $\mathbf{x}_\mu \neq \pm \mathbf{x}_\nu$ and, consequently,

$$(\mathbf{x}_{\mu} + \mathbf{x}_{\nu}) \cdot (\mathbf{x}_{\mu} + \mathbf{x}_{\nu}) > 0 > -(\mathbf{x}_{\mu} - \mathbf{x}_{\nu}) \cdot (\mathbf{x}_{\mu} - \mathbf{x}_{\nu}).$$

Hence.

$$2|\boldsymbol{x}_{\mu}\cdot\boldsymbol{x}_{\nu}|<\boldsymbol{x}_{\mu}\cdot\boldsymbol{x}_{\mu}+\boldsymbol{x}_{\nu}\cdot\boldsymbol{x}_{\nu}\leq 2\boldsymbol{x}_{1}\cdot\boldsymbol{x}_{1}$$

and we can conclude that, for all  $\mu \neq \nu$ ,

$$\lim_{k\to\infty}\frac{|\boldsymbol{x}_{\mu}\cdot\boldsymbol{x}_{\nu}|^k}{(\boldsymbol{x}_1\cdot\boldsymbol{x}_1)^k}=0.$$

Next, define  $E_1 = \{\mu : \mathbf{x}_{\mu} \cdot \mathbf{x}_{\mu} = \mathbf{x}_1 \cdot \mathbf{x}_1\}$ . If  $\mu \notin E_1$ , it is promptly seen that

$$\lim_{k\to\infty}\frac{|\boldsymbol{x}_{\mu}\cdot\boldsymbol{x}_{\mu}|^k}{(\boldsymbol{x}_1\cdot\boldsymbol{x}_1)^k}=0.$$

It is now clear that letting  $k \to \infty$  with  $k \in 2\mathbb{Z}_+ \cap J(\psi, 1)$  in the equality

$$\sum_{\mu,\nu=1}^p v_\mu v_\nu \frac{(\boldsymbol{x}_\mu \cdot \boldsymbol{x}_\nu)^k}{(\boldsymbol{x}_1 \cdot \boldsymbol{x}_1)^k} = 0,$$

valid for all  $k \in 2\mathbb{Z}_+ \cap J(\psi, 1)$  and  $k \geq k_0$ , results in

$$\sum_{\mu\in E_1} v_\mu v_\mu = 0,$$

i.e.,  $v_{\mu}=0$ ,  $\mu\in E_1$ . In particular,  $v_1=0$ . The procedure can be repeated to the set  $E_2=\{\mu\not\in E_1: \mathbf{x}_{\mu}\cdot\mathbf{x}_{\mu}=\mathbf{x}_{\mu_1}\cdot\mathbf{x}_{\mu_1}\}$  after we pick  $\mu_1 \notin E_1$  and assume that  $\mathbf{x}_{\mu} \cdot \mathbf{x}_{\mu} \leq \mathbf{x}_{\mu_1} \cdot \mathbf{x}_{\mu_1}$ ,  $\mu \notin E_1$ . The conclusion is

$$\sum_{\mu \in E_2} v_\mu v_\mu = 0$$

so that  $v_{\mu_1}=0$ . After finitely many steps, we reach  $v_1=\cdots=v_p=0$ , i.e.,  ${\bf v}=0$ , an obvious contradiction.  $\Box$ 

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#### References

- [1] A. Alegria, M. Bevilacqua, E. Porcu, Likelihood-based inference for multivariate space-time wrapped-Gaussian fields, J. Stat. Comput. Simul. 86 (2016) 2583–2597.
- A. Alegria, E. Porcu, R. Furrer, J. Mateu, Covariance functions for multivariate Gaussian fields evolving temporally over planet Earth, Technical Report, 2017. arXiv: 1701.06010v1.
- [3] C.E. Alonso-Malaver, E. Porcu, R. Giraldo, Multivariate and multiradial Schoenberg measures with their dimension walks, J. Multivariate Anal. 133 (2015) 251–265.
- [4] S. Banerjee, On geodetic distance computations in spatial modeling, Biometrics 61 (2005) 617-625.
- 151 C. Berg, E. Porcu, From Schoenberg coefficients to Schoenberg functions, Constr. Approx. 45 (2017) 217-241.
- [6] M. Bevilacqua, A.S. Hering, E. Porcu, On the flexibility of multivariate covariance models: Comment on the paper by Genton and Kleiber, Statist. Sci. 30 (2015) 167–169.
- [7] R.N. Bonfim, V.A. Menegatto, Strict positive definiteness of multivariate covariance functions on compact two-point homogeneous spaces, J. Multivariate Anal. 152 (2016) 237–248.
- [8] S. Castruccio, J. Guinness, An evolutionary spectrum approach to incorporate large-scale geographical descriptors on global processes, J. R. Stat. Soc. Ser. C 66 (2017) 329–344.
- [9] K.-F. Chang, Strictly positive definite functions, J. Approx. Theory 87 (1996) 148–158.
- [10] D. Chen, V.A. Menegatto, X. Sun, A necessary and sufficient condition for strictly positive definite functions on spheres, Proc. Amer. Math. Soc. 131 (2003) 2733–2740.
- [11] N. Cressie, Fitting variogram models by weighted least squares, J. Int. Assoc. Math. Geol. 17 (1985) 563-586.
- [12] D.J. Daley, E. Porcu, M. Bevilacqua, Classes of compactly supported covariance functions for multivariate random fields, Stoch. Environ. Res. Risk Assess. 29 (2015) 1249–1263.
- [13] S. De Iaco, D.E. Myers, D. Posa, On strict positive definiteness of product and product-sum covariance models, J. Statist. Plann. Inference 141 (2011) 1132–1140.
- [14] S. De Iaco, D.E. Myers, D. Posa, Strict positive definiteness of a product of covariance functions, Comm. Statist, Theory Methods 40 (2011) 4400–4408.
- [15] S. De Iaco, P. Posa, Strict positive definiteness in geostatistics, Stoch. Environ. Res. Risk. Assess. 32 (2018) 577-590.
- [16] M.G. Genton, W. Kleiber, Cross-covariance functions for multivariate geostatistics, Statist. Sci. 30 (2015) 147–163.
- [17] T. Gneiting, Compactly supported correlation functions, J. Multivariate Anal. 83 (2002) 493–508.
- [18] T. Gneiting, Strictly and non-strictly positive definite functions on spheres, Bernoulli 19 (2013) 1327-1349.
- [19] P. Gregori, E. Porcu, J. Mateu, Z. Sasvári, On potentially negative space time covariances obtained as sum of products of marginal ones, Ann. Inst. Statist. Math. 60 (2008) 865–882.
- [20] J.C. Guella, V.A. Menegatto, From Schoenberg coefficients to Schoenberg functions: A unifying framework, Preprint, 2016.
- [21] E.J. Hannan, Multiple Time Series, Wiley, New York, 1970.
- [22] M. Jun, M.L. Stein, Nonstationary covariance models for global data, Ann. Appl. Stat. 2 (2008) 1271-1289.
- [23] C. Ma, Stationary and isotropic vector random fields on spheres, Math. Geosci. 44 (2012) 765–778.
- [24] K.V. Mardia, R.J. Marshall, Maximum likelihood estimation of models for residual covariance in spatial regression, Biometrika 71 (1984) 135–146.
- [25] V.A. Menegatto, Strictly positive definite kernels on the Hilbert sphere, Appl. Anal. 55 (1994) 91-101.
- [26] V.A. Menegatto, Strictly positive definite kernels on the circle, Rocky Mountain J. Math. 25 (1995) 1149-1163.
- [27] V.A. Menegatto, C.P. Oliveira, A.P. Peron, Strictly positive definite kernels on subsets of the complex plane, Comput. Math. Appl. 51 (2006) 1233–1250.
- [28] D.E. Myers, A. Journel, Variograms with zonal anisotropies and noninvertible kriging systems, Math. Geol. 22 (1990) 779–785.
- [29] E. Porcu, M. Bevilacqua, M.G. Genton, Spatio-temporal covariance and cross-covariance functions of the great circle distance on a sphere, J. Amer. Statist. Assoc. 111 (2016) 888–898.
- [30] E. Porcu, V. Zastavnyi, Characterization theorems for some classes of covariance functions associated to vector-valued random fields, J. Multivariate Anal. 102 (2011) 1293–1301.
- [31] I.J. Schoenberg, Positive definite functions on spheres, Duke Math. J. 9 (1942) 96-108.
- [32] G. Szegö, Orthogonal Polynomials, fourth ed., in: American Mathematical Society, Colloquium Publications, vol. XXIII, American Mathematical Society, Providence. RI. 1975.
- [33] T. Xie, D.E. Myers, Fitting matrix-valued variogram models by simultaneous diagonalization I, Theory Math. Geol. 27 (1995) 867-875.
- [34] Y. Xu, E.W. Cheney, Strictly positive definite functions on spheres, Proc. Amer. Math. Soc. 116 (1992) 977–981.
- [35] A.M. Yaglom, Correlation Theory of Stationary and Related Random Functions, Vol. I, Basic Results, Springer, New York, 1987.
- [36] W. Zu Castell, F. Filbir, R. Szwarc, Strictly positive definite functions in  $\mathbb{R}^d$ , J. Approx. Theory 137 (2005) 277–280.