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Abstract

We consider spatial matrix-valued isotropic covariance functions in Euclidean spaces and provide a very short proof of a celebrated characterization result proposed by earlier literature. We then provide a characterization theorem to create a bridge between a class of matrix-valued functions and the class of matrix-valued positive semidefinite functions in finite-dimensional Euclidean spaces. We culminate with criteria of the Pólya type for matrix-valued isotropic covariance functions, and with a generalization of Schlather's class of multivariate spatial covariance functions.

We then challenge the problem of matrix-valued space-time covariance functions, and provide a general class that encompasses all the proposals on the Gneiting nonseparable class provided by earlier literature.

Key words: Completely monotone matrix-valued functions; Multiply monotone matrix-valued functions; Positive semidefinite matrix-valued functions; Multivariate Gneiting covariance.

1 Introduction

There is a huge literature for multivariate isotropic covariance functions in the field of spatial statistics, see Chilès and Delfiner (2012), Genton and Kleiber (2015) and the references therein for a comprehensive account. Applications cover as varied disciplines as geochemistry, natural resources assessment, geotechnics, geometallurgy, groundwater hydrology, climate, soil and environmental sciences. Multivariate covariance functions are positive semidefinite matrix-valued mappings, with the diagonal elements termed direct or auto-covariances, and the off-diagonal elements termed cross-covariances. The former quantify the spatial correlation structure of each variable under consideration, while the latter quantify the spatial correlation between each pair of variables.

While the statistical aspects regarding multivariate covariance functions have been repeatedly challenged in the past decade (see, for instance, Porcu and Zastavnyi, 2011, Bevilacqua et al., 2015 and De Iaco et al., 2019), the treatment of several mathematical questions has been elusive so far. The solution of such questions would be, in turn, important to solve other pressing statistical questions. This paper focuses on some of them. Specifically:

a. Continuous real-valued isotropic positive semidefinite functions have been characterized by Schoenberg (1938). The generalization to matrix-valued functions is informally suggested in Yaglom (1987) and subsequently formalized in Alonso-Malaver et al. (2015). In both works, however, proofs are lengthy and intricate. We provide this result with an elegant short proof.

b. Multiply monotone functions have been introduced by Williamson (1956), who proved a necessary and sufficient condition in terms of integral representation. We define matrix-valued multiply monotonicity, and show that the analogue of Williamson's result remains true in the matrix-valued case.

c. Gneiting (2001) provided criteria of the Pólya type for a real-valued function to be the isotropic part of a radial positive semidefinite function. We generalize those criteria to the matrix-valued case.

d. An elegant construction in Schlather (2010) provides a class of spatial multivariate covariance functions. Inspired by Aitken's identities (Menegatto and Oliveira, 2021, and references therein), we provide a generalization of Schlather's class.

e. We finally consider matrix-valued covariance functions defined in Euclidean spaces cross time, where these functions are stationary and isotropic in space, and stationary and symmetric in time. For real-valued functions defined in such product spaces, the Gneiting class (Gneiting, 2002) has been the cornerstone in space-time modeling, and we refer the reader to Porcu et al. (2021) for a thorough account. There have been several attempts of generalization of this class to the matrix-valued case, such as Bourotte et al. (2016) and very recently Menegatto and Oliveira (2021) and Dörr and Schlather (2021). The result proposed in this paper generalizes all the analogues of multivariate Gneiting classes proposed in earlier literature.

Most of our proofs rely on definitions of convexity and monotonicity with respect to matrix inequality, which in turn open for the definition of matrix-valued analogue classes of functions that have been celebrated, in the real-valued case, for over a century by the mathematical community.

The plan of the paper is the following. Section 2 provides the necessary mathematical background. Section 3 is split into two main subsections, where spatial (Section 3.1) and space-time (Section 3.2) problems are challenged. Concluding remarks in Section 4 close the paper.

2 Background

Throughout, bold letters refer to vectors and matrices, p, q and d denote positive integers, $\mathbf{0}$ and $\mathbf{1}$ denote the zero and all-ones matrices of size $p \times p$, ι denotes the imaginary unit, and $\top$ denotes the transposition operator. Also, continuity, differentiability, integrability, composition, exponentiation and pointwise limits involving matrix-valued functions are understood as elementwise.

2.1 Monotonicity and convexity of matrix-valued functions

The following definitions are the crux to generalize well-known classes of real-valued functions to the matrix-valued case.

Definition 1. *A matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is nonnegative with respect to matrix inequality if $\boldsymbol{\varphi}(x) \geq \mathbf{0}$ for any $x \in [0, +\infty)$, where $\geq$ refers to the partial ordering relation (Löewner order) between symmetric matrices: for two symmetric matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ of size $p \times p$, $\boldsymbol{A} \geq \boldsymbol{B}$ if $\boldsymbol{A} - \boldsymbol{B}$ is positive semidefinite.*

A necessary and sufficient condition for $\boldsymbol{\varphi}$ to be nonnegative with respect to matrix inequality is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the real-valued function

$$\varphi_{\boldsymbol{z}}(x) := \boldsymbol{z}^\top \boldsymbol{\varphi}(x)\boldsymbol{z}, \qquad x \geq 0, \tag{1}$$

is nonnegative.

Definition 2. *A matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is nonincreasing with respect to matrix inequality if $\boldsymbol{\varphi}(x) \geq \boldsymbol{\varphi}(x')$ when $0 \leq x \leq x'$. A nondecreasing function with respect to matrix inequality is defined analogously.*

A necessary and sufficient conditions for $\boldsymbol{\varphi}$ to be nonincreasing is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the real-valued function $\varphi_{\boldsymbol{z}}$ defined at (1) is nonincreasing (Boyd and Vandenberghe, 2004, Example 3.46).

Definition 3. *A matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is convex with respect to matrix inequality if $\omega\boldsymbol{\varphi}(x) + (1-\omega)\boldsymbol{\varphi}(x') \geq \boldsymbol{\varphi}(\omega t + (1-\omega)t')$ for all $x, x' \in [0, +\infty)$ and all $\omega \in [0, 1]$.*

A necessary and sufficient condition for convexity with respect to matrix inequality is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the real-valued function $\varphi_{\boldsymbol{z}}$ defined at (1) is convex (Boyd and Vandenberghe, 2004, Example 3.48).

Definition 4. *A matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is 1-time monotone with respect to matrix inequality if it is nonnegative and nonincreasing. For $\mu \in \mathbb{N}$, a μ-times differentiable matrix-valued function $\boldsymbol{\varphi}$ is $(\mu+2)$-times monotone with respect to matrix inequality if $(-1)^k\boldsymbol{\varphi}^{(k)}$ is nonnegative, nonincreasing and convex for $k = 0, \ldots, \mu$, where $\boldsymbol{\varphi}^{(k)}$ denotes the k-th derivative of $\boldsymbol{\varphi}$.*

Using the above definitions, it is seen that a necessary and sufficient for $\boldsymbol{\varphi}$ to be $(\mu+1)$-times monotone is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the real-valued function $\varphi_{\boldsymbol{z}}$ defined at (1) is $(\mu+1)$-times monotone in the sense of Williamson (1956).

Definition 5. *An infinitely differentiable matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is completely monotone with respect to matrix inequality if it is multiply monotone with respect to matrix inequality for any positive integer μ.*

We observe that a necessary and sufficient for $\boldsymbol{\varphi}$ to be completely monotone is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the real-valued function $\varphi_{\boldsymbol{z}}$ defined at (1) is completely monotone, i.e., $\varphi_{\boldsymbol{z}}$ is infinitely often differentiable on the nonnegative real line and $(-1)^k\varphi_{\boldsymbol{z}}^{(k)}$ is nonnegative on $[0, +\infty)$ for any $k \in \mathbb{N}$. For a comprehensive account on completely monotone real-valued functions, the reader is referred to Schilling et al. (2010) and Porcu and Schilling (2011).

2.2 Isotropic covariance functions and pseudo-variograms in Euclidean spaces

Consider a second-order p-variate random field $\boldsymbol{Z}$ in $\mathbb{R}^d$ (i.e., a random field that possesses finite first- and second-order moments) with real-valued components. Without loss of generality, we hereunder assume the first-order moment (expectation) of $\boldsymbol{Z}$ to be the zero vector.

2.2.1 Covariance function

The spatial correlation structure of $\boldsymbol{Z}$ is characterized by its matrix-valued covariance function (a second-order moment), that is

$$\boldsymbol{K}(\boldsymbol{s}, \boldsymbol{s}') = \mathbb{E}(\boldsymbol{Z}(\boldsymbol{s})^\top \boldsymbol{Z}(\boldsymbol{s}')), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d,$$

with $\mathbb{E}$ denoting the expectation.

A necessary and sufficient condition for a function $\boldsymbol{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{p\times p}$ to be the covariance of a second-order p-variate random field in $\mathbb{R}^d$ is that $\boldsymbol{K}$ is positive semidefinite, i.e., the matrix of size $np \times np$ with generic entry $K_{ij}(\boldsymbol{s}_k, \boldsymbol{s}_\ell)$, where K_{ij} denotes the (i, j)-th entry of $\boldsymbol{K}$, is symmetric and positive semidefinite for any choice of the positive integer n and of the set of points $\{\boldsymbol{s}_1, \cdots, \boldsymbol{s}_n\}$ in $\mathbb{R}^d$. An alternative formulation is

$$\sum_{k,\ell=0}^{n} \boldsymbol{a}_k^\top \boldsymbol{K}(\boldsymbol{s}_k, \boldsymbol{s}_\ell)\boldsymbol{a}_\ell \geq 0,$$

for all $\boldsymbol{s}_1, \cdots, \boldsymbol{s}_n \in \mathbb{R}^d$ and $\boldsymbol{a}_1, \cdots, \boldsymbol{a}_n \in \mathbb{R}^p$.

The covariance function $\boldsymbol{K}$ is stationary and isotropic if it can be written as follows:

$$\boldsymbol{K}(\boldsymbol{s}, \boldsymbol{s}') = \boldsymbol{\varphi}(\|\boldsymbol{s} - \boldsymbol{s}'\|), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d, \tag{2}$$

where the matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is called the isotropic part of $\boldsymbol{K}$, and $\|\cdot\|$ is the Euclidean norm, defined through $\|\boldsymbol{s}-\boldsymbol{s}'\|^2 = \langle \boldsymbol{s}-\boldsymbol{s}', \boldsymbol{s}-\boldsymbol{s}'\rangle$, $\boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d$, with $\langle\cdot,\cdot\rangle$ the usual scalar product of the Cartesian coordinates.

We call Φ_d^p the class of continuous matrix-valued mappings $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ such that (2) is true for a covariance function $\boldsymbol{K}$ defined in $\mathbb{R}^d \times \mathbb{R}^d$.

2.2.2 Pseudo-variograms

Another second-order moment describing the spatial correlation structure of the random field $\boldsymbol{Z}$ (provided $\boldsymbol{Z}$ has square-integrable cross-increments) is its matrix-valued pseudo-variogram $\boldsymbol{\Gamma}$, with generic entry:

$$\Gamma_{ij}(\boldsymbol{s}, \boldsymbol{s}') = \frac{1}{2}\mathbb{E}\left([Z_i(\boldsymbol{s}) - Z_j(\boldsymbol{s}')]^2\right), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d,\, i, j = 1, \cdots, p,$$

with Z_i standing for the i-th component of $\boldsymbol{Z}$.

A necessary and sufficient condition for a function $\boldsymbol{\Gamma} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{p\times p}$ to be the pseudo-variogram of a second-order p-variate random field in $\mathbb{R}^d$ is that $\Gamma_{ii}(0) = 0$ for any $i = 1, \cdots, p$ and that $\boldsymbol{\Gamma}$ is conditionally negative semidefinite (Dörr and Schlather, 2021), i.e.,

$$\Gamma_{ij}(\boldsymbol{s}, \boldsymbol{s}') = \Gamma_{ji}(\boldsymbol{s}', \boldsymbol{s}), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d,\, i, j = 1, \cdots, p,$$

and

$$\sum_{i,j=0}^{n} \boldsymbol{a}_i^\top \boldsymbol{\Gamma}(\boldsymbol{s}_i, \boldsymbol{s}_j)\boldsymbol{a}_j \leq 0,$$

for any choice of the positive integer n, $\boldsymbol{s}_1, \cdots, \boldsymbol{s}_n \in \mathbb{R}^d$ and $\boldsymbol{a}_1, \cdots, \boldsymbol{a}_n \in \mathbb{R}^p$ such that $\sum_{i=1}^n \sum_{\ell=1}^p a_{i\ell} = 0$, with $a_{i\ell}$ standing for the ℓ-th component of $\boldsymbol{a}_i$. An alternative characterization (Dörr and Schlather, 2021) is that $\boldsymbol{\Gamma}$ is a pseudo-variogram if, and only if, $\exp(-a\boldsymbol{\Gamma})$ is a matrix-valued correlation function, i.e., a matrix-valued covariance function such that the diagonal entries are equal to 1 when $s = \boldsymbol{s}'$, for any $a > 0$.

The pseudo-variogram $\boldsymbol{\Gamma}$ is stationary and isotropic if it can be written as follows:

$$\boldsymbol{\Gamma}(\boldsymbol{s}, \boldsymbol{s}') = \boldsymbol{\gamma}(\|\boldsymbol{s} - \boldsymbol{s}'\|), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d, \tag{3}$$

where the matrix-valued function $\boldsymbol{\gamma} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is termed the isotropic part of $\boldsymbol{\Gamma}$. Hereafter, we call Υ_d^p the class of continuous matrix-valued mappings $\boldsymbol{\gamma} : [0, +\infty) \to \mathbb{R}^{p\times p}$ such that (3) is true for a pseudo-variogram $\boldsymbol{\Gamma}$ defined in $\mathbb{R}^d \times \mathbb{R}^d$.

2.3 Spatially isotropic and temporally symmetric covariance functions and pseudo-variograms in Euclidean spaces cross time

The isotropy assumption for a random field defined in the product space $\mathbb{R}^d \times \mathbb{R}$ is normally weakened by assuming the covariance function to depend on separate metrics in space ($\mathbb{R}^d$) and time ($\mathbb{R}$). Specifically, consider a zero-mean second-order stationary p-variate random field in $\mathbb{R}^d \times \mathbb{R}$. The random field is said to be spatially isotropic and temporally symmetric if its matrix-valued covariance function is of the form (Porcu et al., 2021)

$$\boldsymbol{K}\big((\boldsymbol{s}, t), (\boldsymbol{s}', t')\big) = \boldsymbol{\varphi}(\|\boldsymbol{s} - \boldsymbol{s}'\|, |\ t - t'\ |), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d, t, t' \in \mathbb{R}, \tag{4}$$

for some function $\boldsymbol{\varphi} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$.

We call $\Phi_{d,1}^p$ the class of continuous mappings $\boldsymbol{\varphi} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$ such that (4) is true for a covariance function $\boldsymbol{K}$ defined in $\mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$.

In the same way, spatial isotropy and temporal symmetry can be defined for the pseudo-variogram, when the latter is of the form

$$\boldsymbol{\Gamma}\big((\boldsymbol{s}, t), (\boldsymbol{s}', t')\big) = \boldsymbol{\gamma}(\|\boldsymbol{s} - \boldsymbol{s}'\|, |\ t - t'\ |), \quad \boldsymbol{s}, \boldsymbol{s}' \in \mathbb{R}^d, t, t' \in \mathbb{R}, \tag{5}$$

for some function $\boldsymbol{\gamma} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$. Hereinafter, we call $\Upsilon_{d,1}^p$ the class of continuous mappings $\boldsymbol{\gamma} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$ such that (5) is true for a pseudo-variogram $\boldsymbol{\Gamma}$ defined in $\mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$.

3 Results

3.1 Isotropic spatial models and the class Φ_d^p

The following result is crucial for most of the proofs provided in this section.

Lemma 1. *A necessary and sufficient condition for a continuous function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ to belong to Φ_d^p is that, for any $\boldsymbol{z} \in \mathbb{R}^p$, the function $\varphi_{\boldsymbol{z}}$ defined through (1) belongs to Φ_d^1.*

Proof. As the isotropic parts of continuous radial functions in $\mathbb{R}^d$, both $\boldsymbol{\varphi}$ and $\varphi_{\boldsymbol{z}}$ (for any fixed $\boldsymbol{z}$) have Fourier representations of the form

$$\boldsymbol{\varphi}(x) = \int_{\mathbb{R}^d} \cos(2\pi x\langle \boldsymbol{u}, \boldsymbol{e}_1\rangle)\boldsymbol{\chi}(\mathrm{d}\boldsymbol{u}), \quad x \in [0, +\infty),$$

and

$$\varphi_{\boldsymbol{z}}(x) = \int_{\mathbb{R}^d} \cos(2\pi x \langle \boldsymbol{u}, \boldsymbol{e}_1 \rangle) \chi_{\boldsymbol{z}}(\mathrm{d}\boldsymbol{u}), \quad x \in [0, +\infty),$$

where $\boldsymbol{e}_1 = (1, 0, \ldots, 0)$ is a unit vector in $\mathbb{R}^d$, $\boldsymbol{\chi}$ is a bounded matrix-valued measure defined in $\mathbb{R}^d$, with each entry being real-valued and $\boldsymbol{\chi}(-B) = \boldsymbol{\chi}(B)$ for any Borel set of $\mathbb{R}^d$, and $\chi_{\boldsymbol{z}} = \boldsymbol{z}^\top \boldsymbol{\chi} \boldsymbol{z}$ is a bounded real-valued measure defined in $\mathbb{R}^d$. Owing to Cramér's criterion on positive semidefinite radial functions in $\mathbb{R}^d$ (Cramér, 1940; Yaglom, 1987), the following assertions are clearly equivalent: (i) $\boldsymbol{\varphi}$ belongs to Φ_d^p, (ii) for any Borel set $B \subset \mathbb{R}^d$, $\boldsymbol{\chi}(B)$ is a positive semidefinite matrix, (iii) for any $\boldsymbol{z} \in \mathbb{R}^p$ and any Borel set $B \subset \mathbb{R}^d$, $\chi_{\boldsymbol{z}}(B)$ is nonnegative, and (iv) for any $\boldsymbol{z} \in \mathbb{R}^p$, $\varphi_{\boldsymbol{z}}$ belongs to Φ_d^1. □

To illustrate our subsequent findings, we define the function $\Omega_d : [0, +\infty) \to \mathbb{R}$ through the identity

$$\Omega_d(x) = \Gamma\left(\frac{d}{2}\right)\left(\frac{2}{x}\right)^{\frac{d}{2}-1} J_{\frac{d}{2}-1}(x), \qquad x \geq 0,$$

where J_ν is the Bessel function of the first kind of order ν (Olver et al., 2010, formula 10.2.2). We start with a result for which two lengthy proofs are available in Yaglom (1987) and Alonso-Malaver et al. (2015). We provide here a straightforward proof.

Theorem 1 (Yaglom, 1987)**.** *Let $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p \times p}$. Then $\boldsymbol{\varphi}$ belongs to Φ_d^p if and only if*

$$\boldsymbol{\varphi}(x) = \int_0^{+\infty} \Omega_d(rx) \mathrm{d}\boldsymbol{F}(r), \qquad x \geq 0, \tag{6}$$

where $\boldsymbol{F}$ is a bounded matrix-valued measure that is nondecreasing with respect to matrix inequality.

Proof. We invoke Lemma 1 to claim that the function $\boldsymbol{\varphi}$ belongs to Φ_d^p if and only if $\varphi_{\boldsymbol{z}}$, defined at (1), belongs to Φ_d^1 for every $\boldsymbol{z} \in \mathbb{R}^p$. Hence, we invoke Schoenberg's theorem (Schoenberg, 1938) to claim that this is equivalent to the existence of a nondecreasing and bounded measure $F_{\boldsymbol{z}}$, defined on the nonnegative real line, such that

$$\varphi_{\boldsymbol{z}}(x) = \int_0^{+\infty} \Omega_d(rx) \mathrm{d}F_{\boldsymbol{z}}(r), \qquad x \geq 0.$$

Since $\boldsymbol{z} \mapsto \varphi_{\boldsymbol{z}} = \boldsymbol{z}^\top \boldsymbol{\varphi} \boldsymbol{z}$ is a quadratic form in $\boldsymbol{z}$, so is $\boldsymbol{z} \mapsto F_{\boldsymbol{z}}$. This implies that $F_{\boldsymbol{z}}(\cdot) = \boldsymbol{z}^\top \boldsymbol{F}(\cdot) \boldsymbol{z}$ for some matrix-valued measure $\boldsymbol{F}$, which proves (6). To complete the proof, we note that the real-valued measure $F_{\boldsymbol{z}}$ is bounded and nondecreasing for any $\boldsymbol{z} \in \mathbb{R}^p$ if and only if the matrix-valued measure $\boldsymbol{F}$ is bounded and nondecreasing with respect to matrix inequality. □

Our next results are the matrix-valued counterpart of what has been provided by Williamson (1956) to characterize the class of real-valued multiply monotone functions. In what follows, $(\cdot)_+$ denotes the positive part function.

Theorem 2. *Let μ be a positive integer and $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$. Then, $\boldsymbol{\varphi}$ is μ-times monotone with respect to matrix inequality if and only if*

$$\boldsymbol{\varphi}(x) = \int_0^{+\infty} (1 - rx)_+^{\mu-1}\, \mathrm{d}\boldsymbol{F}(r), \qquad x \geq 0,$$

with $\boldsymbol{F}$ is a matrix-valued measure that is nondecreasing with respect to matrix inequality and nonnegative with respect to matrix inequality.

Proof. The proof comes by noting that $\boldsymbol{\varphi}$ is μ-times monotone with respect to matrix inequality if and only if $\varphi_{\boldsymbol{z}}$ in (1) is μ-times monotone on the nonnegative real line for any $\boldsymbol{z} \in \mathbb{R}^p$. We invoke Williamson (1956) to claim that the latter is equivalent to $\varphi_{\boldsymbol{z}}$ being identically equal to

$$\varphi_{\boldsymbol{z}}(x) = \int_0^{+\infty} (1 - rx)_+^{\mu-1}\, \mathrm{d}F_{\boldsymbol{z}}(r), \qquad x \geq 0,$$

where $F_{\boldsymbol{z}}$ is a nondecreasing and nonnegative real-valued measure. Arguments as in the proof of Theorem 1 allow writing $F_{\boldsymbol{z}} = \boldsymbol{z}^\top \boldsymbol{F} \boldsymbol{z}$ for some matrix-valued measure $\boldsymbol{F}$. As $F_{\boldsymbol{z}}$ is nondecreasing and nonnegative for any $\boldsymbol{z} \in \mathbb{R}^p$, $\boldsymbol{F}$ turns out to be nondecreasing and nonnegative with respect to matrix inequality. $\square$

Theorem 2 allows generalizing the definition of multiply monotone matrix-valued functions to fractional orders, as stated next, which appears as a multivariate extension of the definition proposed by Williamson (1956) for real-valued functions.

Definition 6. *For $\mu \in \mathbb{R}$, $\mu \geq 1$, the matrix-valued function $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ is μ-times monotone with respect to matrix inequality if and only if*

$$\boldsymbol{\varphi}(x) = \int_0^{+\infty} (1 - rx)_+^{\mu-1}\, \mathrm{d}\boldsymbol{F}(r), \qquad x \geq 0, \tag{7}$$

with $\boldsymbol{F}$ is a matrix-valued measure that is nondecreasing with respect to matrix inequality and nonnegative with respect to matrix inequality.

In particular, for $2\mu \in \mathbb{N}$, the truncated power function $0 \leq x \mapsto (1 - x)_+^{\mu+1}$ belongs to the class $\Phi^1_{2\mu+1}$ (Zastavnyi, 2000). Hence, the integral representation in (7) in concert with Lemma 1 and with the fact that $\Phi^1_{2\mu+1}$ is closed under scale mixtures, provides the following direct implication.

Corollary 1. *Let $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ be $(\mu + 2)$-times monotone with respect to matrix inequality, with $2\mu \in \mathbb{N}$. Then, $\boldsymbol{\varphi}$ belongs to the class $\Phi^p_{2\mu+1}$.*

The convexity of given order derivatives of a real-valued function defined on the nonnegative real line has been used by Gneiting (2001) to provide criteria for a candidate function to belong to the class Φ^1_d. We now generalize such a criterion to the matrix-valued case.

Theorem 3 (Multivariate Gneiting criterion)**.** *Let $\boldsymbol{\varphi} : [0, +\infty) \to \mathbb{R}^{p\times p}$ be continuous, with $\boldsymbol{\varphi}(x) = [\varphi_{ij}(x)]_{i,j=1}^{p}$ such that $\varphi_{ii}(0) = 1$, $i = 1, \dots, p$ and $\lim_{t\to\infty} \boldsymbol{\varphi}(x) = \mathbf{0}$. Let k, ℓ be nonnegative integers, with at least one of them being strictly positive. Let*

$$\boldsymbol{\eta}_1(x) = \left(-\frac{\mathrm{d}}{\mathrm{d}u}\right)^k \boldsymbol{\varphi}\left(\sqrt{u}\right)\Big|_{u=x^2}.$$

If there exists $\alpha \geq \frac{1}{2}$ such that

$$\boldsymbol{\eta}_2(x) = \left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)^{k+\ell-1} \left[-\frac{\mathrm{d}}{\mathrm{d}x}\boldsymbol{\eta}_1(x^\alpha)\right]$$

is convex with respect to matrix inequality on $[0, +\infty)$, then $\boldsymbol{\varphi} \in \Phi_d^p$, for $d = 1, \dots, 2\ell + 1$.

Proof. If $\boldsymbol{\varphi}$ satisfies the conditions of Theorem 3 for $\alpha > \frac{1}{2}$, then so it does for $\alpha = \frac{1}{2}$ as well (Gneiting, 2001). Hence, it suffices to prove the result for $\alpha = \frac{1}{2}$. By assumption, $\boldsymbol{\eta}_2$ is convex with respect to matrix inequality. Therefore, the real-valued function $\eta_{2,\boldsymbol{z}}(\cdot) := \boldsymbol{z}^\top \boldsymbol{\eta}_2(\cdot)\boldsymbol{z}$ is convex for every $\boldsymbol{z} \in \mathbb{R}^p$. Proposition 2.1 in Gneiting (2001) shows that

$$\eta_{2,\boldsymbol{z}}(x) = \int_0^{+\infty} \psi_{k+\ell}(rx)\,\mathrm{d}F_{\boldsymbol{z}}(r), \qquad x \geq 0,$$

where $F_{\boldsymbol{z}}$ is a probability measure depending on $\boldsymbol{z} \in \mathbb{R}^p$, and $\psi_{k+\ell}$ is the k-fold application of the montée operator (Matheron, 1965, formula I.4.18) applied to the Euclid's hat (Schaback, 1995), which belongs to the class $\Phi^1_{2\ell+1}$. Since this class is closed under scale mixtures, this ensures that $\eta_{2,\boldsymbol{z}} \in \Phi^1_{2\ell+1}$ for any $\boldsymbol{z} \in \mathbb{R}^p$, and that $\boldsymbol{\eta}_2$ belongs to $\Phi^p_{2\ell+1}$, based on Lemma 1 and on the identity $F_{\boldsymbol{z}} = \boldsymbol{z}^\top \boldsymbol{F}\boldsymbol{z}$ as established in the proof of Theorem 1. The fact that $\Phi^p_{2\ell+1}$ is contained in Φ^p_d for any $d = 1, \cdots, 2\ell$ (Alonso-Malaver et al., 2015) completes the proof. □

The Schlather class (Schlather, 2010) of multivariate covariance functions has been recently generalized by Menegatto and Oliveira (2021). We provide here a generalization of both contributions through matrix-valued mappings that are completely monotone with respect to matrix inequality.

Theorem 4. *Let $\boldsymbol{f} : [0, +\infty) \to \mathbb{R}^{p\times p}$ be bounded and completely monotone with respect to matrix inequality. For $i, j = 1, \dots, p$, let $\boldsymbol{G}_{ij} : [0, +\infty) \to \mathbb{R}^{q\times q}$ and $\boldsymbol{H}_{ij} : [0, +\infty) \to \mathbb{R}^q$ be such that*

(1) $\boldsymbol{G}_{ij} \in \Phi_d^q$;

(2) $\left[\boldsymbol{v}^\top \boldsymbol{G}_{ij}(\cdot)\boldsymbol{v}\right]_{i,j=1}^p \in \Upsilon_d^p$ for any $\boldsymbol{v} \in \mathbb{R}^q$;

(3) $\left[\mathrm{e}^{\iota \boldsymbol{H}_{ij}(\|\cdot\|)^\top \boldsymbol{v}}\right]_{i,j=1}^p$ is positive semidefinite in $\mathbb{R}^d$, for any $\boldsymbol{v} \in \mathbb{R}^q$.

Then, the mapping $\boldsymbol{K}:[0,+\infty)\to\mathbb{R}^{p\times p}$ *defined through*

$$\boldsymbol{K}(x) := \boldsymbol{f}\circ\left[\frac{\boldsymbol{H}_{ij}(x)^\top\boldsymbol{G}_{ij}^{-1}(x)\boldsymbol{H}_{ij}(x)}{\sqrt{\det\left(\boldsymbol{G}_{ij}(x)\right)}}\right]_{i,j=1}^{p}, \qquad x\geq 0, \tag{8}$$

with $\circ$ *denoting the elementwise composition, belongs to* Φ_d^p*.*

Proof. A constructive proof is provided. We note that $\boldsymbol{f}$ is completely monotone with respect to matrix inequality if and only if the mapping $f_{\boldsymbol{z}} = \boldsymbol{z}^\top\boldsymbol{f}\boldsymbol{z}$ is completely monotone for any $\boldsymbol{z}\in\mathbb{R}^p$, which is equivalent to (Schilling et al., 2010)

$$f_{\boldsymbol{z}}(u) = \int_0^{+\infty} \mathrm{e}^{-ru}\mathrm{d}F_{\boldsymbol{z}}(r), \qquad u\geq 0,$$

for a bounded, nonnegative and nondecreasing measure $F_{\boldsymbol{z}}$. This in turn proves that

$$\boldsymbol{f}(u) = \int_0^{+\infty} \mathrm{e}^{-ru}\mathrm{d}\boldsymbol{F}(r), \qquad u\geq 0, \tag{9}$$

where the matrix-valued measure $\boldsymbol{F}$, defined such that $F_{\boldsymbol{z}} = \boldsymbol{z}^\top\boldsymbol{F}\boldsymbol{z}$, is bounded, nonnegative with respect to matrix inequality and nondecreasing with respect to matrix inequality. We now invoke the generalized Aitken's formula (Menegatto and Oliveira, 2021) in concert with Fubini's theorem to rewrite (8) as

$$\boldsymbol{K}(x) = \frac{1}{\pi^{q/2}}\int_0^{+\infty}\left[\int_{\mathbb{R}^q}\mathrm{e}^{-\boldsymbol{v}^\top\boldsymbol{G}_{ij}(x)\boldsymbol{v}}\,\mathrm{e}^{2\iota\sqrt{r}\boldsymbol{H}_{ij}(x)^\top\boldsymbol{v}}\mathrm{d}\boldsymbol{v}\right]_{i,j=1}^{p}\mathrm{d}\boldsymbol{F}(r), \quad x\geq 0.$$

Both mappings $x\mapsto\left[\mathrm{e}^{-\boldsymbol{v}^\top\boldsymbol{G}_{ij}(x)\boldsymbol{v}}\right]_{i,j=1}^{p}$ and $x\mapsto\left[\mathrm{e}^{2\iota\sqrt{r}\boldsymbol{H}_{ij}(x)^\top\boldsymbol{v}}\right]_{i,j=1}^{p}$ belong to Φ_d^p for any $\boldsymbol{v}\in\mathbb{R}^q$ and $r\geq 0$, owing to a characterization of pseudo-variograms (see Section 2.2.2) and to the second and third theorem's assumptions. The proof is completed, insofar as the function $\boldsymbol{K}$ appears as the scale mixture, with respect to the matrix $\boldsymbol{F}$, of an inner integral that belongs to the class Φ_d^p for any nonnegative r. □

Some comments are in order. The formulations proposed by Schlather (2010) and Menegatto and Oliveira (2021) escape from the isotropy assumption. Our proof can easily be extended to cover the anisotropic case, but this case is out of the scope of the paper. A second relevant comment is that Schlather (2010) and Menegatto and Oliveira (2021) adopt the choice $\boldsymbol{\varphi} = \boldsymbol{1}\varphi$, for φ a completely monotone. The latter authors also consider the mapping $\left[\boldsymbol{v}^\top\boldsymbol{G}_{ij}(\cdot)\boldsymbol{v}\right]_{i,j=1}^{p}$ to belong to a broader class than Υ_d^p, based on a less restrictive definition of conditional negative semidefiniteness, which is seemingly incorrect in view of Theorem 3.2 of Dörr and Schlather (2021).

3.2 Spatially isotropic and temporally symmetric models and the class $\Phi_{d,1}^p$

We start with a straightforward extension of Lemma 1, the proof of which is omitted.

Lemma 2. *A necessary and sufficient condition for a continuous function* $\boldsymbol{\varphi} : [0,+\infty)\times[0,+\infty) \to \mathbb{R}^{p\times p}$ *to belong to* $\Phi_{d,1}^p$ *is that, for any* $\boldsymbol{z} \in \mathbb{R}^p$*, the function* $\varphi_{\boldsymbol{z}}$ *defined through*

$$\varphi_{\boldsymbol{z}}(x,t) := \boldsymbol{z}^\top \boldsymbol{\varphi}(x,t)\boldsymbol{z}, \qquad x,t \geq 0, \tag{10}$$

belongs to $\Phi_{d,1}^1$.

Proposition 1. *Let* $\boldsymbol{\varphi} : [0,+\infty)\times[0,+\infty) \to \mathbb{R}^{p\times p}$ *be continuous and absolutely integrable. Then,* $\boldsymbol{\varphi} \in \Phi_{d,1}^p$ *if and only if the mapping* $\boldsymbol{\phi}_\xi : [0,+\infty) \to \mathbb{R}^{p\times p}$ *defined through*

$$\boldsymbol{\phi}_\xi(t) = 2\pi t^{1-\frac{d}{2}} \int_0^{+\infty} x^{\frac{d}{2}} J_{\frac{d}{2}-1}(2\pi\xi x)\, \boldsymbol{\varphi}(x,t)\mathrm{d}x, \quad t \geq 0,$$

belongs to the class Φ_1^p *for almost all* $\xi \geq 0$.

Proof. We provide a constructive proof. In view of Lemma 2, $\boldsymbol{\varphi}$ belongs to the class $\Phi_{d,1}^p$ if and only if the mapping $\varphi_{\boldsymbol{z}}$ defined through (10) belongs to the class $\Phi_{d,1}^1$ for any $\boldsymbol{z} \in \mathbb{R}^p$. We invoke Theorem 1 in Gneiting (2002) to claim that this is equivalent to the mapping

$$\phi_{\boldsymbol{z},\xi}(t) = 2\pi t^{1-\frac{d}{2}} \int_0^{+\infty} x^{\frac{d}{2}} J_{\frac{d}{2}-1}(2\pi\xi x)\, \varphi_{\boldsymbol{z}}(x,t)\mathrm{d}x = \boldsymbol{z}^\top \boldsymbol{\phi}_\xi(t)\boldsymbol{z}, \quad t \geq 0,$$

to belong to Φ_1^1 for all $\boldsymbol{z} \in \mathbb{R}^p$ and almost all $\xi \in [0,+\infty)$. In turn, this is true if and only if $\boldsymbol{\phi}_\xi$ belongs to Φ_1^p for almost all $\xi \in [0,+\infty)$ (Lemma 1). The proof is completed. □

Gneiting (2002) proved that the mapping

$$\varphi(x,t) = \frac{1}{\psi(t^2)^{\frac{d}{2}}} f\left(\frac{x^2}{\psi(t^2)}\right), \qquad x,t \geq 0, \tag{11}$$

belongs to the class $\Phi_{d,1}^1$ provided f is completely monotone and bounded on the nonnegative real line, and ψ is a strictly positive Bernstein function (a primitive of a completely monotone function). The converse of this assertion, for f being completely monotone, was provided by Zastavnyi and Porcu (2011), who showed that the following more general form belongs to $\Phi_{d,1}^1$:

$$\varphi(x,t) = \frac{1}{(1+\gamma(t))^{\frac{d}{2}}} f\left(\frac{x^2}{1+\gamma(t)}\right), \qquad x,t \geq 0,$$

where f is completely monotone and bounded on the nonnegative real line, and γ is a continuous variogram, i.e., a conditionally negative semidefinite real-valued function; the assumption of continuity of γ was subsequently lifted by Allard et al. (2020). The constant 1 added to this variogram is needed to avoid a division by zero when $t = 0$.

Theorem 5. *Let $\boldsymbol{f} : [0, +\infty) \to \mathbb{R}^{p\times p}$ be bounded and completely monotone with respect to matrix inequality. Let $\boldsymbol{\gamma} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$ belong to $\Upsilon^p_{d,1}$. Then, the mapping $\boldsymbol{\varphi} : [0, +\infty) \times [0, +\infty) \to \mathbb{R}^{p\times p}$ determined through*

$$\boldsymbol{\varphi}(x, t) = \frac{1}{(1 + \boldsymbol{\gamma}(x, t))^{\frac{d}{2}}} \boldsymbol{f}\left(\frac{x^2}{1 + \boldsymbol{\gamma}(x, t)}\right), \qquad x, t \geq 0,$$

where all operations are taken elementwise, belongs to the class $\Phi^p_{d,1}$.

Proof. A constructive proof is provided. We invoke representation (9) to write $\boldsymbol{\varphi}$ as

$$\boldsymbol{\varphi}(x, t) = \frac{1}{(1 + \boldsymbol{\gamma}(x, t))^{\frac{d}{2}}} \int_0^{+\infty} \mathrm{e}^{-r\frac{x^2}{1+\boldsymbol{\gamma}(x,t)}} \,\mathrm{d}\boldsymbol{F}(r), \quad x, t \geq 0.$$

Using the fact that a Gaussian (squared exponential) function is the d-dimensional Fourier transform of another Gaussian function (Lantuéjoul, 2002), one obtains the equivalent expression:

$$\boldsymbol{\varphi}(x, t) = \frac{1}{(2\pi)^{\frac{d}{2}}} \int_0^{+\infty} \int_{\mathbb{R}^d} \cos(\sqrt{2r}x\langle \boldsymbol{u}, \boldsymbol{e}_1\rangle)\, \mathrm{e}^{-\frac{\|u\|^2(1+\boldsymbol{\gamma}(x,t))}{2}} \mathrm{d}\boldsymbol{u}\, \mathrm{d}\boldsymbol{F}(r), \quad x, t \geq 0. \tag{12}$$

As the matrix-valued measure $\boldsymbol{F}$ is nondecreasing with respect to matrix inequality, $\mathrm{d}\boldsymbol{F}(r) = \boldsymbol{F}(r + \mathrm{d}r) - \boldsymbol{F}(r)$ is positive semidefinite for any $r \geq 0$. This implies that the mapping $(x, t) \mapsto \mathrm{d}\boldsymbol{F}(r) \cos(\sqrt{2r}x\langle \boldsymbol{u}, \boldsymbol{e}_1\rangle)$ belongs to $\Phi^p_{d,1}$ for any $r \geq 0$ and $\boldsymbol{u} \in \mathbb{R}^d$. So does the mapping $(x, t) \mapsto \exp(-\frac{\|u\|^2(1+\boldsymbol{\gamma}(x,t))}{2})$ (Dörr and Schlather, 2021, corollary 3.4). Accordingly, the integrand in (12) belongs to $\Phi^p_{d,1}$, and so does $\boldsymbol{\varphi}$ because $\Phi^p_{d,1}$ is closed under scale mixtures. The proof is completed. □

Some comments are in order. Theorem 5 generalizes Theorem 1 in Bourotte et al. (2016), where the authors use a specific choice of the function $\boldsymbol{\gamma}$ and take $\boldsymbol{f} = \mathbf{1}f$, with f a completely monotone function. Theorem 5 also generalizes Theorem 4.3 in Dörr and Schlather (2021), where it is assumed that the entries f_{ij} of $\boldsymbol{f}$ are Stieltjes functions. The generalization is threefold: first, Stieltjies functions are a subset of completely monotone functions. Second, assuming f_{ij} to be a Stieltjes function implies the corresponding measure in its integral representation (9) to be nonnegative on $[0, +\infty)$, which is not required by our definition of multivariate complete monotonicity, where the off-diagonal elements of $\boldsymbol{F}$ might be negative-valued. Third, the matrix-valued function $\boldsymbol{\gamma}$ controlling the temporal structure depends on both the spatial and temporal lags, which provides a highly-versatile and nonseparable covariance model allowing complex interactions between space and time.

Let us mention a few examples of parametric forms for $\boldsymbol{\gamma}$:

- $\boldsymbol{\gamma}(x,t) = \widetilde{\boldsymbol{\gamma}}(t)$, with $\widetilde{\boldsymbol{\gamma}} \in \Upsilon_1^p$;
- $\boldsymbol{\gamma}(x,t) = \alpha_1\widetilde{\boldsymbol{\gamma}}_1(x) + \alpha_2\widetilde{\boldsymbol{\gamma}}_2(t)$, with $\alpha_1 > 0$, $\alpha_2 > 0$, $\widetilde{\boldsymbol{\gamma}}_1 \in \Upsilon_d^p$ and $\widetilde{\boldsymbol{\gamma}}_2 \in \Upsilon_1^p$;
- $\boldsymbol{\gamma}(x,t) = \widetilde{\boldsymbol{\gamma}}(\sqrt{\alpha x^2 + t^2})$, with $\alpha > 0$ and $\widetilde{\boldsymbol{\gamma}} \in \Upsilon_{d+1}^p$.

As for $\boldsymbol{f}$, versatile examples can be constructed based on the Matérn function defined through

$$\mathcal{M}(u;\alpha,\nu) = \frac{2^{1-\nu}}{\Gamma(\nu)}\,(\alpha u)^{\nu/2}\,\mathcal{K}_\nu(\sqrt{\alpha u}), \qquad u \geq 0, \alpha > 0, \nu > 0, \tag{13}$$

where $\mathcal{K}_\nu$ is the modified Bessel function of the second kind of order ν (Olver et al., 2010, formula 10.27.4). We note that $\mathcal{M}(\cdot;\alpha,\nu)$ is completely monotone for all $\alpha > 0$ and $\nu > 0$. Yet, it is not a Stieltjes function. Hence, the Matérn function cannot be used for the purpose of Theorem 4.3 in Dörr and Schlather (2021), but can be used for the purpose of Theorem 5. Indeed, the function $\boldsymbol{f} : [0, +\infty) \to \mathbb{R}^{p\times p}$ having elements

$$f_{ij}(u) = \rho_{ij}\mathcal{M}(u;\alpha_{ij},\nu_{ij}), \qquad u \geq 0,$$

is bounded and completely monotone with respect to matrix inequality if the matrix-valued parameters $\boldsymbol{\alpha} = [\alpha_{ij}]_{i,j=1}^p$, $\boldsymbol{\nu} = [\nu_{ij}]_{i,j=1}^p$ and $\boldsymbol{\rho} = [\rho_{ij}]_{i,j=1}^p$ fulfill any of the sufficient validity conditions established by Gneiting et al. (2010), Apanasovich et al. (2012) or Emery et al. (2020), insofar as, under such conditions, $\boldsymbol{f}$ can be written as a mixture of completely monotone real-valued functions of the form (13) weighted by positive semidefinite matrices.

4 Concluding remarks

We provided a collection of mathematical results that were currently lacking in the literature. Let us elaborate more on the impact of these results.

Theorems 2 and 3 allow building members of the class Φ_d^p for a given positive integer d. This is relevant, for instance, to the construction of multivariate covariance functions that are compactly supported over balls with given radii embedded in $\mathbb{R}^d$. The literature on this subject is scarce, with Daley et al. (2015) being a notable exception. On another note, the mathematical techniques proposed in this paper would allow generalizing other minor criteria for positive semidefiniteness, such as the one proposed in Gneiting (2000).

Theorem 4 provides a flexible formulation for members of the class Φ_d^p that does not allow for compact supports. Such a construction, though, allows for straightforward reparameterizations of the mappings $\boldsymbol{G}_{ij}$ and $\boldsymbol{H}_{ij}$ to achieve anisotropies and nonstationarities in space.

Our multivariate analogue of the Gneiting class as provided in Theorem 5 allows for a substantial improvement of previous proposals, with special emphasis on the improvement of the formulation proposed by Dörr and Schlather (2021).

An open problem that would be certainly relevant is to replace the function $\boldsymbol{f}$ in Theorem 5 with a member of Φ_d^p, for a given d, so as to achieve multivariate covariance functions of the Gneiting type that are compactly supported in space. In the real-valued case, the recent contribution by Porcu et al. (2020) might be a good starting point.

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