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CHARACTERIZATION THEOREMS FOR PSEUDO CROSS-VARIOGRAMS

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Abstract

Pseudo cross-variograms appear naturally in the context of multivariate Brown–Resnick processes, and are a useful tool for analysis and prediction of multivariate random fields. We give a necessary and sufficient criterion for a matrix-valued function to be a pseudo cross-variogram, and further provide a Schoenberg-type result connecting pseudo cross-variograms and multivariate correlation functions. By means of these characterizations, we provide extensions of the popular univariate space–time covariance model of Gneiting to the multivariate case.

Keywords: Multivariate geostatistics; conditionally negative definite; positive definite; space–time covariance functions; Gneiting functions

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1. Introduction

With increasing availability of multivariate data and considerable improvements in computational feasibility, multivariate random fields have become a significant part of geostatistical modelling in recent years.

These random fields are usually assumed to be either second-order stationary or intrinsically stationary. An m-variate random field

$$\{\boldsymbol{Z}(\boldsymbol{x}) = (Z_1(\boldsymbol{x}), \ldots, Z_m(\boldsymbol{x}))^\top, \boldsymbol{x} \in \mathbb{R}^d\}$$

is called second-order stationary if it has a constant mean and if its auto- and cross-covariances

$$\mathrm{Cov}(Z_i(\boldsymbol{x}+\boldsymbol{h}), Z_j(\boldsymbol{x})), \quad \boldsymbol{x}, \boldsymbol{h} \in \mathbb{R}^d, \quad i, j = 1, \ldots, m,$$

exist and are functions of the lag $\boldsymbol{h}$ only. It is called intrinsically stationary if the increment process $\{\boldsymbol{Z}(\boldsymbol{x}+\boldsymbol{h}) - \boldsymbol{Z}(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d\}$ is second-order stationary for all $\boldsymbol{h} \in \mathbb{R}^d$. In this case, the function $\tilde{\boldsymbol{\gamma}} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$,

$$\tilde{\gamma}_{ij}(\boldsymbol{h}) = \frac{1}{2}\mathrm{Cov}(Z_i(\boldsymbol{x}+\boldsymbol{h}) - Z_i(\boldsymbol{x}), Z_j(\boldsymbol{x}+\boldsymbol{h}) - Z_j(\boldsymbol{x})), \quad \boldsymbol{x}, \boldsymbol{h} \in \mathbb{R}^d, \quad i, j = 1, \ldots, m,$$

is well-defined and is called a cross-variogram [19]. If we additionally assume that $Z_i(\boldsymbol{x}+\boldsymbol{h}) - Z_j(\boldsymbol{x})$ is square integrable and that $\mathrm{Var}(Z_i(\boldsymbol{x}+\boldsymbol{h}) - Z_j(\boldsymbol{x}))$ does not depend on $\boldsymbol{x}$ for all $\boldsymbol{x}, \boldsymbol{h} \in \mathbb{R}^d$,

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$i, j = 1, \ldots, m$, then we can also define the so-called pseudo cross-variogram $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ [20] via

$$\gamma_{ij}(\boldsymbol{h}) = \frac{1}{2}\mathrm{Var}(Z_i(\boldsymbol{x}+\boldsymbol{h}) - Z_j(\boldsymbol{x})), \quad \boldsymbol{x}, \boldsymbol{h} \in \mathbb{R}^d, \quad i, j = 1, \ldots, m.$$

Obviously, the diagonal entries of pseudo cross-variograms and cross-variograms coincide and contain univariate variograms $\gamma_{ii}(\boldsymbol{h}) = \frac{1}{2}\mathrm{Var}(Z_i(\boldsymbol{x}+\boldsymbol{h}) - Z_i(\boldsymbol{x}))$, $i = 1, \ldots, m$ [15, 16].

Both cross- and pseudo cross-variograms are commonly used in geostatistics to capture the degree of spatial dependence [5]. There is some controversy as to which one to use, since both have their benefits and drawbacks. The cross-variogram, on the one hand, is well-defined under weaker assumptions, but requires measurements of the quantities of interest at the same locations for estimation in practical applications [5]. Moreover, it only reproduces the symmetric part of a cross-covariance function of a stationary random field; see e.g. [30]. The pseudo cross-variogram, on the other hand, can capture asymmetry, and provides optimal co-kriging predictors without imposing any symmetry assumption on the cross-dependence structure [6, 29], but is difficult to interpret in practice due to considering differences of generally different physical quantities; cf. [6] and their account of it.

From a theoretical perspective, pseudo cross-variograms are interesting objects, since they are not only found in multivariate geostatistics but also appear naturally in extreme value theory in the context of multivariate Brown–Resnick processes [8, 21]. However, pseudo cross-variograms, in contrast to cross-variograms, have not yet been sufficiently well understood. So far, elementary properties [7] are known, such as their relation to cross-variograms and cross-covariance functions [20, 22], their applicability to co-kriging [6, 20, 29], and limiting behaviour [21, 22], but a concise necessary and sufficient criterion for a matrix-valued function to be a pseudo cross-variogram is missing. This lack of an equivalent characterization makes it immensely difficult to show the validity of a function as a pseudo cross-variogram (cf. e.g. [13, p. 239]), unless it can be led back to an explicit construction of a random field as in [5] or [21].

Equivalent characterizations are well known for univariate variograms (see e.g. [11], [15]), and involve the notion of conditional negative definiteness. These characteristics are intimately connected to a result which can be mainly attributed to Schoenberg [2, 28], implying that a function $\gamma : \mathbb{R}^d \to \mathbb{R}$ is a univariate variogram if and only if $\exp(-t\gamma)$ is a correlation function for all $t > 0$ [11]. Such a characterization of γ in the multivariate case, however, seems to be untreated in the geostatistical literature. For cross-variograms, there is a result for the 'if' part [14, Theorem 10]. The 'only if' part is false in general; see e.g. [27, Remark 2]. See also [7].

The aim of this article is to fill these gaps. The key ingredient is to apply a stronger notion of conditional negative definiteness for matrix-valued functions than the predominant one in geostatistical literature. We discuss this notion in Section 2, and provide a first characterization of pseudo cross-variograms in these terms. This characterization leads to a Schoenberg-type result in terms of pseudo cross-variograms in Section 3, thus making a case for proponents of pseudo cross-variograms, at least from a theoretical standpoint. In Section 4 we apply this characterization and illustrate its power by extending versions of the very popular space–time covariance model of Gneiting [10] to the multivariate case.

Our presentation here is carried out in terms of pseudo cross-variograms in their original stationary form as introduced above. It is important to note that, with the exception of Corollary 2, all results presented here, which involve pseudo cross-variograms or conditionally negative definite matrix-valued functions as defined below, also hold for their respective non-stationary versions or kernel-based forms by straightforward adaptations. A non-stationary version of Corollary 2 is also available. The proofs follow the same lines.

2. Conditional negative definiteness for matrix-valued functions

Real-valued conditionally negative definite functions are essential to characterizing univariate variograms. A function $\gamma : \mathbb{R}^d \to \mathbb{R}$ is a univariate variogram if and only if $\gamma(0) = 0$ and γ is conditionally negative definite, that is, γ is symmetric and for all $n \geq 2$, $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n} \in \mathbb{R}^d$, $a_1, \ldots, a_n \in \mathbb{R}$ such that $\sum_{k=1}^n a_k = 0$, the inequality $\sum_{i=1}^n \sum_{j=1}^n a_i \gamma(\boldsymbol{x_i} - \boldsymbol{x_j}) a_j \leq 0$ holds [15]. An extended notion of conditional negative definiteness for matrix-valued functions is part of a characterization of cross-variograms. A function $\tilde{\boldsymbol{\gamma}} : \mathbb{R}^d \to \mathbb{R}^{m \times m}$ is a cross-variogram if and only if $\tilde{\boldsymbol{\gamma}}(\boldsymbol{0}) = \boldsymbol{0}$, $\tilde{\boldsymbol{\gamma}}(\boldsymbol{h}) = \tilde{\boldsymbol{\gamma}}(-\boldsymbol{h}) = \tilde{\boldsymbol{\gamma}}(\boldsymbol{h})^\top$ and

$$\sum_{i=1}^n \sum_{j=1}^n \boldsymbol{a_i}^\top \tilde{\boldsymbol{\gamma}}(\boldsymbol{x_i} - \boldsymbol{x_j}) \boldsymbol{a_j} \leq 0 \tag{1}$$

for $n \geq 2$, $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n} \in \mathbb{R}^d$, $\boldsymbol{a_1}, \ldots, \boldsymbol{a_n} \in \mathbb{R}^m$ such that $\sum_{k=1}^n \boldsymbol{a_k} = \boldsymbol{0}$ [14]. A function satisfying condition (1) is called an almost negative definite matrix-valued function in [31, p. 40].

A pseudo cross-variogram $\boldsymbol{\gamma}$ has similar, but only necessary properties; see [7]. It holds that $\gamma_{ii}(\boldsymbol{0}) = 0$, and $\gamma_{ij}(\boldsymbol{h}) = \gamma_{ji}(-\boldsymbol{h})$, $i, j = 1, \ldots, m$. Additionally, a pseudo cross-variogram is an almost negative definite matrix-valued function as well, but inequality (1), loosely speaking, cannot enforce non-negativity on the secondary diagonals. Therefore we consider the following stronger notion of conditional negative definiteness; see [9].

Definition 1. A function $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m \times m}$ is called conditionally negative definite if

$$\gamma_{ij}(\boldsymbol{h}) = \gamma_{ji}(-\boldsymbol{h}), \quad i, j = 1, \ldots, m, \tag{2a}$$

$$\sum_{i=1}^n \sum_{j=1}^n \boldsymbol{a_i}^\top \boldsymbol{\gamma}(\boldsymbol{x_i} - \boldsymbol{x_j}) \boldsymbol{a_j} \leq 0, \tag{2b}$$

for all $n \in \mathbb{N}$, $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n} \in \mathbb{R}^d$, $\boldsymbol{a_1}, \ldots, \boldsymbol{a_n} \in \mathbb{R}^m$ such that

$$\boldsymbol{1_m}^\top \sum_{k=1}^n \boldsymbol{a_k} = 0$$

with $\boldsymbol{1_m} := (1, \ldots, 1)^\top \in \mathbb{R}^m$.

Obviously, the set of conditionally negative definite matrix-valued functions is a convex cone which is closed under integration and pointwise limits, if existing. In the univariate case, the concepts of conditionally and almost negative definite functions coincide, reproducing the traditional notion of real-valued conditionally negative definite functions. The main difference between them is the broader spectrum of vectors for which inequality (2b) has to hold, in that the sum of all components has to be zero instead of each component of the sum itself. This modification in particular includes sets of linearly independent vectors in the pool of admissible test vector families, resulting in more restrictive conditions on the secondary diagonals. Indeed, choosing $n = 2$, $\boldsymbol{x_1} = \boldsymbol{h} \in \mathbb{R}^d$, $\boldsymbol{x_2} = \boldsymbol{0}$, and $\boldsymbol{a_1} = \boldsymbol{e_i}$, $\boldsymbol{a_2} = -\boldsymbol{e_j}$ in Definition 1 with $\{\boldsymbol{e_1}, \ldots, \boldsymbol{e_m}\}$ denoting the canonical basis in $\mathbb{R}^m$, we have $\gamma_{ij}(\boldsymbol{h}) \geq 0$ for a conditionally negative definite

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function $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ with $\gamma_{ii}(\mathbf{0}) = 0$, $i, j = 1, \ldots, m$, fitting the non-negativity of a pseudo cross-variogram. In fact, the latter condition on the main diagonal and the conditional negative definiteness property are sufficient to characterize pseudo cross-variograms.

Theorem 1. *Let $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$. Then there exists a centred Gaussian random field $\mathbf{Z}$ on $\mathbb{R}^d$ with pseudo cross-variogram $\boldsymbol{\gamma}$ if and only if $\gamma_{ii}(\mathbf{0}) = 0$, $i = 1, \ldots, m$, and $\boldsymbol{\gamma}$ is conditionally negative definite.*

Proof. The proof is analogous to the univariate one in [15]. Let $\mathbf{Z}$ be an m-variate random field with pseudo cross-variogram $\boldsymbol{\gamma}$. Obviously, $\gamma_{ii}(\mathbf{0}) = 0$ and $\gamma_{ij}(\boldsymbol{h}) = \gamma_{ji}(-\boldsymbol{h})$ for all $\boldsymbol{h} \in \mathbb{R}^d$, $i, j = 1, \ldots, m$. Define an m-variate random field $\tilde{\mathbf{Z}}$ via $\tilde{Z}_i(\boldsymbol{x}) = Z_i(\boldsymbol{x}) - Z_1(\mathbf{0})$, $\boldsymbol{x} \in \mathbb{R}^d$, $i = 1, \ldots, m$. Then $\mathbf{Z}$ and $\tilde{\mathbf{Z}}$ have the same pseudo cross-variogram, and

$$\mathrm{Cov}(\tilde{Z}_i(\boldsymbol{x}), \tilde{Z}_j(\boldsymbol{y})) = \gamma_{i1}(\boldsymbol{x}) + \gamma_{j1}(\boldsymbol{y}) - \gamma_{ij}(\boldsymbol{x} - \boldsymbol{y})$$

(see also [22, equation (6)]), that is,

$$\mathrm{Cov}(\tilde{\mathbf{Z}}(\boldsymbol{x}), \tilde{\mathbf{Z}}(\boldsymbol{y})) = \boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + \mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y}) - \boldsymbol{\gamma}(\boldsymbol{x} - \boldsymbol{y}), \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d,$$

with $\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x}) := (\gamma_{11}(\boldsymbol{x}), \ldots, \gamma_{m1}(\boldsymbol{x}))^\top$. For $\mathbf{1}_{\boldsymbol{m}}^\top \sum_{k=1}^m \boldsymbol{a}_{\boldsymbol{k}} = 0$, we thus have

$$\begin{aligned} 0 &\le \mathrm{Var}\left(\sum_{i=1}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \tilde{\mathbf{Z}}(\boldsymbol{x}_{\boldsymbol{i}})\right) \\ &= \sum_{i=1}^n \sum_{j=1}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \big(\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x}_i)\mathbf{1}_{\boldsymbol{m}}^\top + \mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{x}_j) - \boldsymbol{\gamma}(\boldsymbol{x}_{\boldsymbol{i}} - \boldsymbol{x}_{\boldsymbol{j}})\big)\boldsymbol{a}_{\boldsymbol{j}} \\ &= -\sum_{i=1}^n \sum_{j=1}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\boldsymbol{i}} - \boldsymbol{x}_{\boldsymbol{j}})\boldsymbol{a}_{\boldsymbol{j}}. \end{aligned}$$

Now let $\boldsymbol{\gamma}$ be conditionally negative definite and $\gamma_{ii}(\mathbf{0}) = 0$, $i = 1, \ldots, m$. Let $\boldsymbol{a}_{\mathbf{1}}, \ldots, \boldsymbol{a}_{\boldsymbol{n}} \in \mathbb{R}^m$, $\boldsymbol{x}_{\mathbf{1}}, \ldots, \boldsymbol{x}_{\boldsymbol{n}} \in \mathbb{R}^d$ be arbitrary, $\boldsymbol{x}_{\mathbf{0}} = \mathbf{0} \in \mathbb{R}^d$ and

$$\boldsymbol{a}_{\mathbf{0}} = \left(-\mathbf{1}_{\boldsymbol{m}}^\top \sum_{k=1}^n \boldsymbol{a}_{\boldsymbol{k}}, 0, \ldots, 0\right) \in \mathbb{R}^m.$$

Then

$$\begin{aligned} 0 &\le -\sum_{i=0}^n \sum_{j=0}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\boldsymbol{i}} - \boldsymbol{x}_{\boldsymbol{j}})\boldsymbol{a}_{\boldsymbol{j}} \\ &= -\sum_{i=1}^n \sum_{j=1}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\boldsymbol{i}} - \boldsymbol{x}_{\boldsymbol{j}})\boldsymbol{a}_{\boldsymbol{j}} - \sum_{i=1}^n \boldsymbol{a}_{\boldsymbol{i}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\boldsymbol{i}} - \boldsymbol{x}_{\mathbf{0}})\boldsymbol{a}_{\mathbf{0}} - \sum_{j=1}^n \boldsymbol{a}_{\mathbf{0}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\mathbf{0}} - \boldsymbol{x}_{\boldsymbol{j}})\boldsymbol{a}_{\boldsymbol{j}} \\ &\quad - \boldsymbol{a}_{\mathbf{0}}^\top \boldsymbol{\gamma}(\boldsymbol{x}_{\mathbf{0}} - \boldsymbol{x}_{\mathbf{0}})\boldsymbol{a}_{\mathbf{0}}. \end{aligned}$$

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Since $\gamma_{11}(\mathbf{0})=0$, and $\boldsymbol{a}_{\mathbf{0}}^{\top}\boldsymbol{\gamma}(\boldsymbol{x}_{\mathbf{0}}-\boldsymbol{x}_j)\boldsymbol{a}_j=\boldsymbol{a}_j^{\top}\boldsymbol{\gamma}(\boldsymbol{x}_j)\boldsymbol{a}_{\mathbf{0}}$ due to property (2a), we get that

$$\begin{aligned}0&\le-\sum_{i=0}^{n}\sum_{j=0}^{n}\boldsymbol{a}_i^{\top}\boldsymbol{\gamma}(\boldsymbol{x}_i-\boldsymbol{x}_j)\boldsymbol{a}_j\\&=\sum_{i=1}^{n}\sum_{j=1}^{n}\boldsymbol{a}_i^{\top}\big(\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x}_i)\mathbf{1}_m^{\top}+\mathbf{1}_m\boldsymbol{\gamma}_{\mathbf{1}}^{\top}(\boldsymbol{x}_j)-\boldsymbol{\gamma}(\boldsymbol{x}_i-\boldsymbol{x}_j)\big)\boldsymbol{a}_j,\end{aligned}$$

that is,

$$(\boldsymbol{x},\boldsymbol{y})\mapsto\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x})\mathbf{1}_m^{\top}+\mathbf{1}_m\boldsymbol{\gamma}_{\mathbf{1}}^{\top}(\boldsymbol{y})-\boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y})$$

is a matrix-valued positive definite kernel. Let

$$\{\boldsymbol{Z}(\boldsymbol{x})=(Z_1(\boldsymbol{x}),\dots,Z_m(\boldsymbol{x}))^{\top},\ \boldsymbol{x}\in\mathbb{R}^d\}$$

be a corresponding centred Gaussian random field. We have to show that $\operatorname{Var}(Z_i(\boldsymbol{x}+\boldsymbol{h})-Z_j(\boldsymbol{x}))$ is independent of $\boldsymbol{x}$ for all $\boldsymbol{x},\boldsymbol{h}\in\mathbb{R}^d$, $i,j=1,\dots,m$. We even show that $\boldsymbol{x}\mapsto Z_i(\boldsymbol{x}+\boldsymbol{h})-Z_j(\boldsymbol{x})$ is weakly stationary for $i,j=1,\dots,m$:

$$\begin{aligned}&\operatorname{Cov}(Z_i(\boldsymbol{x}+\boldsymbol{h})-Z_j(\boldsymbol{x}),Z_i(\boldsymbol{y}+\boldsymbol{h})-Z_j(\boldsymbol{y}))\\&\quad=\gamma_{i1}(\boldsymbol{x}+\boldsymbol{h})+\gamma_{i1}(\boldsymbol{y}+\boldsymbol{h})-\gamma_{ii}(\boldsymbol{x}-\boldsymbol{y})+\gamma_{j1}(\boldsymbol{x})+\gamma_{j1}(\boldsymbol{y})-\gamma_{jj}(\boldsymbol{x}-\boldsymbol{y})\\&\qquad-\gamma_{j1}(\boldsymbol{x})-\gamma_{i1}(\boldsymbol{y}+\boldsymbol{h})+\gamma_{ji}(\boldsymbol{x}-\boldsymbol{y}-\boldsymbol{h})-\gamma_{i1}(\boldsymbol{x}+\boldsymbol{h})-\gamma_{j1}(\boldsymbol{y})+\gamma_{ij}(\boldsymbol{x}+\boldsymbol{h}-\boldsymbol{y})\\&\quad=-\gamma_{ii}(\boldsymbol{x}-\boldsymbol{y})-\gamma_{jj}(\boldsymbol{x}-\boldsymbol{y})+\gamma_{ji}(\boldsymbol{x}-\boldsymbol{y}-\boldsymbol{h})+\gamma_{ij}(\boldsymbol{x}-\boldsymbol{y}+\boldsymbol{h}).\end{aligned}\qquad\square$$

Theorem 1 answers the questions raised in [7, p. 422] and also settles a question in [13, p. 239] in a more general framework with regard to the intersection of the sets of pseudo and cross-variograms. It turns out that this intersection is trivial in the following sense.

Corollary 1. *Let*

$$\begin{aligned}\mathcal{P}&=\{\boldsymbol{\gamma}:\mathbb{R}^d\to\mathbb{R}^{m\times m}\mid\boldsymbol{\gamma}\ \textit{pseudo cross-variogram}\},\\\mathcal{C}&=\{\tilde{\boldsymbol{\gamma}}:\mathbb{R}^d\to\mathbb{R}^{m\times m}\mid\tilde{\boldsymbol{\gamma}}\ \textit{cross-variogram}\}.\end{aligned}$$

Then we have

$$\mathcal{P}\cap\mathcal{C}=\{\mathbf{1}_m\mathbf{1}_m^{\top}\gamma\mid\gamma:\mathbb{R}^d\to\mathbb{R}\ \textit{variogram}\}.\tag{3}$$

Proof. Let $\boldsymbol{\gamma}\in\mathcal{P}\cap\mathcal{C}$. Without loss of generality, assume $m=2$. Since $\boldsymbol{\gamma}\in\mathcal{P}\cap\mathcal{C}$, for $n=2$, $\boldsymbol{x}_{\mathbf{1}}=\boldsymbol{h}$, $\boldsymbol{x}_{\mathbf{2}}=\mathbf{0}$, $\boldsymbol{a}_{\mathbf{1}},\boldsymbol{a}_{\mathbf{2}}\in\mathbb{R}^2$ with $\mathbf{1}_{\mathbf{2}}^{\top}\sum_{k=1}^{2}\boldsymbol{a}_{\boldsymbol{k}}=0$, using the symmetry of $\boldsymbol{\gamma}$ and $\boldsymbol{\gamma}(\mathbf{0})=\mathbf{0}$ we have

$$\begin{aligned}0&\ge\sum_{i=1}^{2}\sum_{j=1}^{2}\boldsymbol{a}_i^{\top}\boldsymbol{\gamma}(\boldsymbol{x}_i-\boldsymbol{x}_j)\boldsymbol{a}_j\\&=2a_{11}a_{21}\gamma_{11}(\boldsymbol{h})+2a_{12}a_{22}\gamma_{22}(\boldsymbol{h})+2(a_{11}a_{22}+a_{12}a_{21})\gamma_{12}(\boldsymbol{h}).\end{aligned}$$

Choosing $\boldsymbol{a}_{\mathbf{1}}=(-1,0)^{\top}$, $\boldsymbol{a}_{\mathbf{2}}=(1-k,k)^{\top}$, $k\ge2$, and applying the Cauchy–Schwarz inequality due to $\boldsymbol{\gamma}\in\mathcal{C}$ gives

$$0\le\gamma_{11}(\boldsymbol{h})\le\frac{-k}{1-k}\gamma_{12}(\boldsymbol{h})\le\frac{1}{1-1/k}\sqrt{\gamma_{11}(\boldsymbol{h})}\sqrt{\gamma_{22}(\boldsymbol{h})}.\tag{4}$$

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By symmetry, we also have

$$0 \le \gamma_{22}(\boldsymbol{h}) \le \frac{-k}{1-k}\gamma_{12}(\boldsymbol{h}) \le \frac{1}{1-1/k}\sqrt{\gamma_{11}(\boldsymbol{h})}\sqrt{\gamma_{22}(\boldsymbol{h})}. \tag{5}$$

Assume first that, without loss of generality, $\gamma_{11}(\boldsymbol{h}) = 0$. Then $\gamma_{12}(\boldsymbol{h}) = 0$ and $\gamma_{22}(\boldsymbol{h}) = 0$ due to inequalities (4) and (5). Suppose now that $\gamma_{11}(\boldsymbol{h}), \gamma_{22}(\boldsymbol{h}) \ne 0$. Letting $k \to \infty$ in inequalities (4) and (5) yields $\gamma_{11}(\boldsymbol{h}) = \gamma_{22}(\boldsymbol{h})$. Inserting this into inequality (5) gives

$$\gamma_{22}(\boldsymbol{h}) \le \frac{1}{1-1/k}\gamma_{12}(\boldsymbol{h}) \le \frac{1}{1-1/k}\gamma_{22}(\boldsymbol{h})$$

and consequently the result for $k \to \infty$. □

Remark 1. Let $\boldsymbol{Z}$ be a random field on $\mathbb{R}^d$ with cross-variogram $\tilde{\boldsymbol{\gamma}} \in \mathcal{P} \cap \mathcal{C}$. Then the pseudo and cross-variogram of $\boldsymbol{Z}$ do not necessarily coincide; in fact, the pseudo cross-variogram might not even exist. For instance, let $\boldsymbol{Y}$ be a random field on $\mathbb{R}^d$ with cross-variogram $\tilde{\boldsymbol{\gamma}}$, and take $Z_i(\boldsymbol{x}) := Y_i(\boldsymbol{x}) + U_i$, for i.i.d. random variables U_i, $i = 1, \ldots, m$, without existing variance. However, if $\boldsymbol{Z}$ is a random field with existing pseudo cross-variogram of the form (3), then we have $2\gamma_{ij}(\boldsymbol{0}) = \mathrm{Var}(Z_i(\boldsymbol{x}) - Z_j(\boldsymbol{x})) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^d$, $i, j = 1, \ldots, m$. Consequently, the difference between $Z_i(\boldsymbol{x})$ and $Z_j(\boldsymbol{x})$ is almost surely constant for all $\boldsymbol{x} \in \mathbb{R}^d$, $i, j = 1, \ldots, m$, implying that cross- and pseudo cross-variogram of $\boldsymbol{Z}$ coincide in that case.

Corollary 1 can also be proved by means of a result in [21]. In fact, Theorem 1 enables us to reproduce their result, which was originally derived in a stochastic manner, by a direct proof.

Corollary 2. *Let $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m \times m}$ be a pseudo cross-variogram. Then $\boldsymbol{\gamma}$ fulfils*

$$\left(\sqrt{\gamma_{ii}(\boldsymbol{h})} - \sqrt{\gamma_{ij}(\boldsymbol{h})}\right)^2 \le \gamma_{ij}(\boldsymbol{0}), \quad \boldsymbol{h} \in \mathbb{R}^d, \quad i, j = 1, \ldots, m.$$

Proof. Without loss of generality, assume $m = 2$. We present a proof for $i = 1, j = 2$ and $\gamma_{11}(\boldsymbol{h}), \gamma_{12}(\boldsymbol{h}) > 0$. Then, for $n = 2$, $\boldsymbol{x_1} = \boldsymbol{h}$, $\boldsymbol{x_2} = \boldsymbol{0}$, $\boldsymbol{a_1}, \boldsymbol{a_2} \in \mathbb{R}^2$ with $\boldsymbol{1}_{\boldsymbol{2}}^\top \sum_{k=1}^2 \boldsymbol{a_k} = 0$, we have

$$\begin{aligned} 0 \ge\; & a_{11}a_{21}\gamma_{11}(\boldsymbol{h}) + a_{12}a_{22}\gamma_{22}(\boldsymbol{h}) \\ & + a_{11}a_{22}\gamma_{12}(\boldsymbol{h}) + a_{12}a_{21}\gamma_{21}(\boldsymbol{h}) + (a_{11}a_{12} + a_{21}a_{22})\gamma_{12}(\boldsymbol{0}). \end{aligned} \tag{6}$$

Assuming $a_{12} = 0$, $a_{22} > 0$ and $a_{11} + a_{22} = -a_{21} > 0$, inequality (6) simplifies to

$$\begin{aligned} \gamma_{12}(\boldsymbol{0}) &\ge -\frac{a_{11}}{a_{22}}\gamma_{11}(\boldsymbol{h}) + \frac{a_{11}}{a_{11} + a_{22}}\gamma_{12}(\boldsymbol{h}) \\ &= -x\gamma_{11}(\boldsymbol{h}) + \frac{x}{1+x}\gamma_{12}(\boldsymbol{h}) \end{aligned} \tag{7}$$

for $x := a_{11}/a_{22}$. Maximization of the function

$$x \mapsto -x\gamma_{11}(\boldsymbol{h}) + \frac{x}{1+x}\gamma_{12}(\boldsymbol{h}), \quad x > -1,$$

leads to

$$x^* = \sqrt{\frac{\gamma_{12}(\boldsymbol{h})}{\gamma_{11}(\boldsymbol{h})}} - 1.$$

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Inserting x^* into (7) gives

$$\gamma_{12}(\mathbf{0}) \geq -\left(\sqrt{\frac{\gamma_{12}(\boldsymbol{h})}{\gamma_{11}(\boldsymbol{h})}}-1\right)\gamma_{11}(\boldsymbol{h}) + \left(\frac{\sqrt{\frac{\gamma_{12}(\boldsymbol{h})}{\gamma_{11}(\boldsymbol{h})}}-1}{1+\sqrt{\frac{\gamma_{12}(\boldsymbol{h})}{\gamma_{11}(\boldsymbol{h})}}-1}\right)\gamma_{12}(\boldsymbol{h})$$
$$= \left(\sqrt{\gamma_{11}(\boldsymbol{h})} - \sqrt{\gamma_{12}(\boldsymbol{h})}\right)^2. \qquad \square$$

3. A Schoenberg-type characterization

The stochastically motivated proof of Theorem 1 contains an important relation between matrix-valued positive definite kernels and conditionally negative definite functions we have not yet emphasized. Due to its significance, we formulate it in a separate lemma. As readily seen, the assumption on the main diagonal stemming from our consideration of pseudo cross-variograms can be dropped, resulting in the matrix-valued version of Lemma 3.2.1 in [2].

Lemma 1. *Let $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ be a matrix-valued function with $\gamma_{ij}(\boldsymbol{h}) = \gamma_{ji}(-\boldsymbol{h})$, $i, j = 1, \dots, m$. Define*

$$\boldsymbol{C_k}(\boldsymbol{x}, \boldsymbol{y}) := \boldsymbol{\gamma_k}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + \mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\boldsymbol{k}}^\top(\boldsymbol{y}) - \boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y}) - \gamma_{kk}(\mathbf{0})\mathbf{1}_{\boldsymbol{m}}\mathbf{1}_{\boldsymbol{m}}^\top$$

with $\boldsymbol{\gamma_k}(\boldsymbol{h}) = (\gamma_{1k}(\boldsymbol{h}), \dots, \gamma_{mk}(\boldsymbol{h}))^\top$, $k \in \{1, \dots, m\}$. Then $\boldsymbol{C_k}$ is a positive definite matrix-valued kernel for $k \in \{1, \dots, m\}$ if and only if $\boldsymbol{\gamma}$ is conditionally negative definite. If $\gamma_{kk}(\mathbf{0}) \geq 0$ for $k = 1, \dots, m$, then

$$\tilde{\boldsymbol{C}}_{\boldsymbol{k}}(\boldsymbol{x}, \boldsymbol{y}) := \boldsymbol{\gamma_k}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + \mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\boldsymbol{k}}^\top(\boldsymbol{y}) - \boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y})$$

is a positive definite matrix-valued kernel for $k \in \{1, \dots, m\}$ if and only if $\boldsymbol{\gamma}$ is conditionally negative definite.

The kernel construction in Lemma 1 leads to a matrix-valued version of Schoenberg's theorem [2].

Theorem 2. *A function $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ is conditionally negative definite if and only if $\exp^*(-t\boldsymbol{\gamma})$, with $\exp^*(-t\boldsymbol{\gamma}(\boldsymbol{h}))_{ij} := \exp(-t\gamma_{ij}(\boldsymbol{h}))$, is positive definite for all $t > 0$.*

Remark 2. Theorem 2, in the form presented here, has recently been formulated in [9] in terms of conditionally positive definite matrix-valued functions with complex entries. Nonetheless, we present an alternative proof of the 'only if' part, which relies on the kernel construction in Lemma 1 and follows the lines of the proof of Theorem 3.2.2 in [2].

Proof of Theorem 2. Assume that $\boldsymbol{\gamma}$ is conditionally negative definite. Then

$$(\boldsymbol{x}, \boldsymbol{y}) \mapsto \boldsymbol{\gamma_1}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + \mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y}) - \boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y}) - \gamma_{11}(\mathbf{0})\mathbf{1}_{\boldsymbol{m}}\mathbf{1}_{\boldsymbol{m}}^\top$$

is a positive definite kernel due to Lemma 1. Since positive definite matrix-valued kernels are closed with regard to sums, Hadamard products, and pointwise limits (see e.g. [27]), the kernel

$$(\boldsymbol{x}, \boldsymbol{y}) \mapsto \exp^*\left(t\boldsymbol{\gamma_1}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + t\mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y}) - t\boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y}) - t\gamma_{11}(\mathbf{0})\mathbf{1}_{\boldsymbol{m}}\mathbf{1}_{\boldsymbol{m}}^\top\right)$$
$$= \exp(-t\gamma_{11}(\mathbf{0}))\exp^*\left(t\boldsymbol{\gamma_1}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top + t\mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y}) - t\boldsymbol{\gamma}(\boldsymbol{x}-\boldsymbol{y})\right)$$

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is again positive definite for all $t > 0$. The same holds true for the kernel

$$(\boldsymbol{x}, \boldsymbol{y}) \mapsto \exp^*\big(-t\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top - t\mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y})\big),$$

since

$$\exp\big(-t\boldsymbol{\gamma}_{\mathbf{1}}(\boldsymbol{x})\mathbf{1}_{\boldsymbol{m}}^\top - t\mathbf{1}_{\boldsymbol{m}}\boldsymbol{\gamma}_{\mathbf{1}}^\top(\boldsymbol{y})\big)_{ij} = \exp\left(-t\gamma_{i1}(\boldsymbol{x})\right)\exp\left(-t\gamma_{j1}(\boldsymbol{y})\right), \quad i, j = 1, \dots, m,$$

with the product separable structure implying positive definiteness. Again using the stability of positive definite kernels under Hadamard products, the first part of the assertion follows.

Assume now that $\exp^*(-t\boldsymbol{\gamma})$ is a positive definite function for all $t > 0$. Then

$$\exp\left(-t\gamma_{ij}(\boldsymbol{h})\right) = \exp\left(-t\gamma_{ji}(-\boldsymbol{h})\right),$$

and thus

$$\left(\frac{1 - \mathrm{e}^{-t\gamma_{ij}}}{t}\right)_{i,j=1,\dots,m} = \frac{\mathbf{1}_{\boldsymbol{m}}\mathbf{1}_{\boldsymbol{m}}^\top - \exp^*(-t\boldsymbol{\gamma})}{t}$$

is a conditionally negative definite function. The assertion follows for $t \to 0$. □

Combining Theorems 1 and 2, and recalling that the classes of matrix-valued positive definite functions and covariance functions for multivariate random fields coincide, we immediately get the following characterization of pseudo cross-variograms.

Corollary 3. *A function $\boldsymbol{\gamma} : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ is a pseudo cross-variogram if and only if $\exp^*(-t\boldsymbol{\gamma})$ is a matrix-valued correlation function for all $t > 0$.*

Corollary 3 establishes a direct link between matrix-valued correlation functions and pseudo cross-variograms. Together with Corollary 1, it shows that the cross-variograms for which Theorem 10 in [14] holds are necessarily of the form (3), and it explains the findings in the first part of Remark 2 in [27].

Remark 3. The correspondence of the proofs of the matrix-valued and real-valued versions of Schoenberg's theorem (Theorem 2 here and Theorem 3.2.2 in [2]) is no coincidence. Since [2] does not impose any assumption on the underlying domain X of the negative definite function there, we could also choose $X = \mathbb{R}^d \times \{1, \dots, m\}$, which translates into Theorem 2. The same holds true for Lemma 1. With this 'dimension expansion view', it is no surprise that the pseudo cross-variogram turns out to be the natural multivariate analogue of the variogram from a theoretical standpoint. Due to our interest in pseudo cross-variograms, we chose a stochastically/pseudo cross-variogram driven derivation of Lemma 1 and Theorem 2.

As demonstrated in Theorem 3.2.3 in [2], Schoenberg's theorem can be further generalized for conditionally negative definite functions with non-negative components in terms of componentwise Laplace transforms. Here we present the corresponding matrix-valued version explicitly for clarity, and combine it with our previous results concerning pseudo cross-variograms. With regard to Remark 3, and since we have already presented the matrix-valued proof of Theorem 2, we omit the proof here.

Theorem 3. *Let μ be a probability measure on $[0, \infty)$ such that*

$$0 < \int_0^\infty s \,\mathrm{d}\mu(s) < \infty.$$

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Let $\mathcal{L}$ denote its Laplace transform, that is,

$$\mathcal{L}\mu(x) = \int_0^\infty \exp(-sx)\,\mathrm{d}\mu(s), \qquad x \in [0, \infty).$$

Then $\boldsymbol{\gamma} : \mathbb{R}^d \to [0, \infty)^{m\times m}$ is conditionally negative definite if and only if $(\mathcal{L}\mu(t\gamma_{ij}))_{i,j=1,\ldots,m}$ is positive definite for all $t > 0$. In particular, $\boldsymbol{\gamma}$ is a pseudo cross-variogram if and only if $(\mathcal{L}\mu(t\gamma_{ij}))_{i,j=1,\ldots,m}$ is an m-variate correlation function for all $t > 0$.

Corollary 4. *Let $\boldsymbol{\gamma} : \mathbb{R}^d \to [0, \infty)^{m\times m}$ be a matrix-valued function. If $\boldsymbol{\gamma}$ is a pseudo cross-variogram, then for all $\lambda > 0$, the function $C : \mathbb{R}^d \to \mathbb{R}^{m\times m}$ with*

$$C(\boldsymbol{h}) = \big((1 + t\gamma_{ij}(\boldsymbol{h}))^{-\lambda}\big)_{i,j=1,\ldots,m}, \qquad \boldsymbol{h} \in \mathbb{R}^d, \tag{8}$$

is a correlation function of an m-variate random field for all $t > 0$. Conversely, if a $\lambda > 0$ exists such that $C_{ii}(\mathbf{0}) = 1$, $i = 1, \ldots, m$, and such that C is positive definite for all $t > 0$, then $\boldsymbol{\gamma}$ is a pseudo cross-variogram.

Proof. Choose

$$\mu(\mathrm{d}s) = \frac{1}{\Gamma(\lambda)} \exp(-s) s^{\lambda-1} \mathbb{1}_{(0,\infty)}(s)\,\mathrm{d}s$$

in Theorem 3. □

Similarly to Theorem 3, we can translate the 'univariate' result that Bernstein functions operate on real-valued conditionally negative definite functions [2] to the matrix-valued case, which can thus be used to derive novel pseudo cross-variograms from known ones. Again, we omit the proof for the reasons given above.

Proposition 1. *Let $\boldsymbol{\gamma} : \mathbb{R}^d \to [0, \infty)^{m\times m}$ be conditionally negative definite. Let $g : [0, \infty) \to [0, \infty)$ denote the continuous extension of a Bernstein function. Then $\boldsymbol{g} \circ \boldsymbol{\gamma}$ with $((\boldsymbol{g} \circ \boldsymbol{\gamma})(\boldsymbol{h}))_{ij} := (g \circ \gamma_{ij})(\boldsymbol{h})$, $i, j = 1, \ldots, m$, is conditionally negative definite. In particular, if $g(0) = 0$ and $\boldsymbol{\gamma}$ is a pseudo cross-variogram, then $\boldsymbol{g} \circ \boldsymbol{\gamma}$ is again a pseudo cross-variogram.*

4. Multivariate versions of Gneiting's space–time model

Schoenberg's result is often an integral part of proving the validity of univariate covariance models. Here we use its matrix-valued counterparts derived in the previous section to naturally extend covariance models of Gneiting type to the multivariate case.

Gneiting's original space–time model is a univariate covariance function on $\mathbb{R}^d \times \mathbb{R}$ defined via

$$G(\boldsymbol{h}, u) = \frac{1}{\psi(|u|^2)^{d/2}} \varphi\left(\frac{\|\boldsymbol{h}\|^2}{\psi(|u|^2)}\right), \qquad (\boldsymbol{h}, u) \in \mathbb{R}^d \times \mathbb{R}, \tag{9}$$

where $\psi : 0, \infty) \to (0, \infty)$ is the continuous extension of a Bernstein function, and $\varphi : [0, \infty) \to [0, \infty)$ is the continuous extension of a bounded completely monotone function [10]. For convenience, we simply speak of bounded completely monotone functions henceforth. Model (9) is very popular in practice due to its versatility and ability to model space–time interactions; see [24] for a list of several applications. Its special structure has attracted and still attracts interest from a theoretical perspective as well, resulting in several extensions and

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refinements of the original model (9); see e.g. [17], [18], [23], [25], [32]. Only recently, specific simulation methods have been proposed [1] for the so-called extended Gneiting class, a special case of [32, Theorem 2.1],

$$G(\boldsymbol{h}, \boldsymbol{u}) = \frac{1}{(1+\gamma(\boldsymbol{u}))^{d/2}}\varphi\left(\frac{\|\boldsymbol{h}\|^2}{1+\gamma(\boldsymbol{u})}\right), \quad (\boldsymbol{h}, \boldsymbol{u}) \in \mathbb{R}^d \times \mathbb{R}^l,$$

with γ denoting a continuous variogram. One of these methods is based on an explicit construction of a random field, where the continuity assumption on γ is not needed [1], and which can be directly transferred to the multivariate case via pseudo cross-variograms.

Theorem 4. *Let R be a non-negative random variable with distribution μ, $\boldsymbol{\Omega} \sim N(\boldsymbol{0}, \boldsymbol{1}_{d\times d})$ with $\boldsymbol{1}_{d\times d} \in \mathbb{R}^{d\times d}$ denoting the identity matrix, $U \sim U(0, 1)$, $\Phi \sim U(0, 2\pi)$, and let $\boldsymbol{W}$ be a centred, m-variate Gaussian random field on $\mathbb{R}^l$ with pseudo cross-variogram $\boldsymbol{\gamma}$, all independent. Then the m-variate random field $\boldsymbol{Z}$ on $\mathbb{R}^d \times \mathbb{R}^l$ defined via*

$$Z_i(\boldsymbol{x}, \boldsymbol{t}) = \sqrt{-2\log(U)}\cos\left(\sqrt{2R}\langle\boldsymbol{\Omega}, \boldsymbol{x}\rangle + \frac{\|\boldsymbol{\Omega}\|}{\sqrt{2}}W_i(\boldsymbol{t}) + \Phi\right), \quad (\boldsymbol{x}, \boldsymbol{t}) \in \mathbb{R}^d \times \mathbb{R}^l, \quad i = 1, \ldots, m,$$

has the extended Gneiting-type covariance function

$$G_{ij}(\boldsymbol{h}, \boldsymbol{u}) = \frac{1}{(1+\gamma_{ij}(\boldsymbol{u}))^{d/2}}\varphi\left(\frac{\|\boldsymbol{h}\|^2}{1+\gamma_{ij}(\boldsymbol{u})}\right), \quad (\boldsymbol{h}, \boldsymbol{u}) \in \mathbb{R}^d \times \mathbb{R}^l, \quad i, j = 1, \ldots, m, \tag{10}$$

where φ denotes a bounded completely monotone function.

Proof. The proof follows the lines of the proof of Theorem 3 in [1]. In the multivariate case, the cross-covariance function reads

$$\mathrm{Cov}(Z_i(\boldsymbol{x}, \boldsymbol{t}), Z_j(\boldsymbol{y}, \boldsymbol{s})) = \mathbb{E}\cos\left(\sqrt{2R}\langle\boldsymbol{\Omega}, \boldsymbol{x}-\boldsymbol{y}\rangle + \frac{\|\boldsymbol{\Omega}\|}{\sqrt{2}}(W_i(\boldsymbol{t}) - W_j(\boldsymbol{s}))\right),$$

$(\boldsymbol{x}, \boldsymbol{t}), (\boldsymbol{y}, \boldsymbol{s}) \in \mathbb{R}^d \times \mathbb{R}^l$, $i, j = 1, \ldots, m$. Due to the assumptions, $W_i(\boldsymbol{t}) - W_j(\boldsymbol{s})$ is a Gaussian random variable with mean zero and variance $2\gamma_{ij}(\boldsymbol{t}-\boldsymbol{s})$. Proceeding further as in [1] gives the result. □

Theorem 4 provides a multivariate extension of the extended Gneiting class, and lays the foundations for a simulation algorithm for an approximately Gaussian random field with the respective cross-covariance function; see [1]. The existence of a Gaussian random field with a preset pseudo cross-variogram $\boldsymbol{\gamma}$ and the possibility of sampling from it are ensured by Theorem 1 and Lemma 1, respectively.

Due to our results in previous sections, Theorem 4 can easily be generalized further, replacing $d/2$ in the denominator in equation (10) with a general parameter $r \geq d/2$.

Corollary 5. *Let $\boldsymbol{\gamma} : \mathbb{R}^l \to \mathbb{R}^{m\times m}$ be a pseudo cross-variogram. Then the function $\boldsymbol{G} : \mathbb{R}^d \times \mathbb{R}^l \to \mathbb{R}^{m\times m}$ with*

$$G_{ij}(\boldsymbol{h}, \boldsymbol{u}) = \frac{1}{(1+\gamma_{ij}(\boldsymbol{u}))^{r}}\varphi\left(\frac{\|\boldsymbol{h}\|^2}{1+\gamma_{ij}(\boldsymbol{u})}\right), \quad (\boldsymbol{h}, \boldsymbol{u}) \in \mathbb{R}^d \times \mathbb{R}^l, \quad i, j = 1, \ldots, m, \tag{11}$$

is positive definite for $r \geq d/2$ and a bounded completely monotone function φ.

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Proof. We proved the assertion for $r = d/2$ in Theorem 4. Now let $\lambda > 0$ and $r = \lambda + d/2$. Then the matrix-valued function (11) is the componentwise product of positive definite functions of the form (8) and (10), and consequently positive definite itself. □

Even further refinements of Corollary 5 are possible. We can replace $\mathbf{1}_m\mathbf{1}_m^\top + \boldsymbol{\gamma}$ in (11) with general conditionally negative definite matrix-valued functions, but for a subclass of completely monotone functions, the so-called generalized Stieltjes functions of order λ. This leads to a multivariate version of a result in [17]. A bounded generalized Stieltjes function $S : (0, \infty) \to [0, \infty)$ of order $\lambda > 0$ has a representation

$$S(x) = a + \int_0^\infty \frac{1}{(x+v)^\lambda}\, \mathrm{d}\mu(v), \qquad x > 0,$$

where $a \geq 0$ and the so-called Stieltjes measure μ is a positive measure on $(0, \infty)$, such that $\int_{(0,\infty)} v^{-\lambda}\, \mathrm{d}\mu(v) < \infty$ [17]. As for completely monotone functions, in the following we do not distinguish between a generalized Stieltjes function and its continuous extension. Several examples of generalized Stieltjes functions can be found in [3] and [17].

Theorem 5. *Let S_{ij}, $i, j = 1, \ldots, m$, be generalized Stieltjes functions of order $\lambda > 0$. Let the associated Stieltjes measures have densities φ_{ij} such that $(\varphi_{ij}(v))_{i,j=1,\ldots,m}$ is a symmetric positive semidefinite matrix for all $v > 0$. Let*

$$\boldsymbol{g} : \mathbb{R}^d \to [0, \infty)^{m\times m}, \quad \boldsymbol{f} : \mathbb{R}^l \to (0, \infty)^{m\times m}$$

be conditionally negative definite functions. Then the function $\boldsymbol{G} : \mathbb{R}^d \times \mathbb{R}^l \to \mathbb{R}^{m\times m}$ with

$$G_{ij}(\boldsymbol{h}, \boldsymbol{u}) = \frac{1}{f_{ij}(\boldsymbol{u})^r} S_{ij}\left(\frac{g_{ij}(\boldsymbol{h})}{f_{ij}(\boldsymbol{u})}\right), \quad (\boldsymbol{h}, \boldsymbol{u}) \in \mathbb{R}^d \times \mathbb{R}^l, \quad i, j = 1, \ldots, m,$$

is an m-variate covariance function for $r \geq \lambda$.

Proof. We follow the proof in [17]. It holds that

$$G_{ij}(\boldsymbol{h}, \boldsymbol{u}) = \frac{a}{f_{ij}(\boldsymbol{u})^r} + \frac{1}{f_{ij}(\boldsymbol{u})^{r-\lambda}} \int_0^\infty \frac{1}{(g_{ij}(\boldsymbol{h}) + v f_{ij}(\boldsymbol{u}))^\lambda} \varphi_{ij}(v)\, \mathrm{d}v.$$

The function $x \mapsto 1/x^\alpha$ is completely monotone for $\alpha \geq 0$ and thus the Laplace transform of a measure on $[0, \infty)$ [26, Theorem 1.4]. Therefore $(1/f_{ij}^r)_{i,j=1,\ldots,m}$ and $(1/f_{ij}^{r-\lambda})_{i,j=1,\ldots,m}$ are positive definite functions due to Theorem 2 as mixtures of positive definite functions. Furthermore, we have

$$\frac{1}{(g_{ij}(\boldsymbol{h}) + v f_{ij}(\boldsymbol{u}))^\lambda} = \frac{1}{\Gamma(\lambda)} \int_0^\infty \mathrm{e}^{-s g_{ij}(\boldsymbol{h})} \mathrm{e}^{-s v f_{ij}(\boldsymbol{u})} s^{\lambda-1}\, \mathrm{d}s.$$

The functions $\left(\mathrm{e}^{-s g_{ij}(\boldsymbol{h})}\right)_{i,j=1,\ldots,m}$ and $\left(\mathrm{e}^{-s v f_{ij}(\boldsymbol{u})}\right)_{i,j=1,\ldots,m}$ are again positive definite due to Theorem 2 for all $s, v > 0$, and so is their componentwise product. Since positive definite functions are closed under integration,

$$\left(\frac{1}{(g_{ij}(\boldsymbol{h}) + v f_{ij}(\boldsymbol{u}))^\lambda}\right)_{i,j=1,\ldots,m}$$

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is positive definite for all $v > 0$. Therefore the function

$$\left(\frac{1}{(g_{ij}(\boldsymbol{h}) + vf_{ij}(\boldsymbol{u}))^{\lambda}}\varphi_{ij}(v)\right)_{i,j=1,\ldots,m}$$

is also positive definite for all $v > 0$. Combining and applying the above arguments shows our claim. □

Theorem 5 provides a very flexible model. In a space–time framework, it allows for different cross-covariance structures in both space and time, and it does not require assumptions such as continuity of the conditionally negative definite functions involved, or isotropy, which distinguishes it from the multivariate Gneiting-type models presented in [4] and [12], respectively.

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