**ORIGINAL PAPER**

CrossMark

# Simulation of intrinsic random fields of order $k$ with a continuous spectral algorithm

Daisy Arroyo[1] · Xavier Emery[2,3]

## Abstract

Intrinsic random fields of order $k$, defined as random fields whose high-order increments (generalized increments of order $k$) are second-order stationary, are used in spatial statistics to model regionalized variables exhibiting spatial trends, a feature that is common in earth and environmental sciences applications. A continuous spectral algorithm is proposed to simulate such random fields in a $d$-dimensional Euclidean space, with given generalized covariance structure and with Gaussian generalized increments of order $k$. The only condition needed to run the algorithm is to know the spectral measure associated with the generalized covariance function (case of a scalar random field) or with the matrix of generalized direct and cross-covariances (case of a vector random field). The algorithm is applied to synthetic examples to simulate intrinsic random fields with power generalized direct and cross-covariances, as well as an intrinsic random field with power and spline generalized direct covariances and Matérn generalized cross-covariance.

**Keywords** Non-stationary random fields · Generalized direct and cross-covariances · Generalized increments of order $k$ · Spectral density

## 1 Introduction

In geostatistical applications, regionalized variables exhibiting a spatial trend may not be modeled with second-order stationary random fields, i.e., random fields whose first and second-order moments exist and are invariant through a translation in space, nor with random fields whose increments are second-order stationary (intrinsic random fields of order 0, also known as stationary intrinsic random fields). This is the case, for instance, in geothermal reservoir modeling, where the temperature and the pressure tend to increase with depth, whereas porosity and

permeability tend to decrease (Chilès and Gable 1984). In petroleum reservoir modeling, geometrical characteristics or petrophysical properties such as rock porosity often present trends that cannot be dealt with stationarity hypotheses (Chilès and Gable 1984; Dimitrakopoulos 1990). In ore body modeling, the distribution of geological properties such as rock types, mineral types or alteration types, also exhibit spatial zonations and trends, depending on the geological setting and paragenesis of the ore body, making difficult the representation of these properties with second-order stationary or intrinsic stationary random fields (Madani and Emery 2017).

The theory of intrinsic random fields of order $k$ (for short, IRF-$k$) has been introduced when the assumption of second-order stationarity is not satisfied, but generalized increments filter out the trend and fulfill the assumptions of second-order stationarity (Chilès and Delfiner 2012; Christakos 1992; Matheron 1973). These random fields have been used in the past decades for spatial prediction purposes in geothermal fields (Chilès and Gable 1984; Suárez Arriaga and Samaniego 1998), oil reservoirs (Haas and Jousselin 1976), aquifers (Dong et al. 1990; Kitanidis 1999), soil (Buttafuoco and Castrignano 2005) and

✉ Xavier Emery
  xemery@ing.uchile.cl

  Daisy Arroyo
  darroyof@udec.cl

1 Department of Statistics, University of Concepción, Concepción, Chile

2 Department of Mining Engineering, University of Chile, Santiago, Chile

3 Advanced Mining Technology Center, University of Chile, Santiago, Chile

environmental sciences (Christakos and Thesing 1993), among other applications.

Apart from prediction, there is a growing interest in quantifying the uncertainty at locations with no direct observation, or jointly over several locations, for which conditional simulation techniques have been developed (Chilès and Delfiner 2012). In this respect, several algorithms have been proposed to simulate intrinsic random fields of order $k$, under the assumption that their generalized increments have multivariate-Gaussian distributions (Arroyo and Emery 2015; Chilès and Delfiner 2012; Christakos 1992; Dimitrakopoulos 1990; Emery and Lantuéjoul 2006, 2008; Pardo-Igúzquiza and Dowd 2003). Among these algorithms, the continuous spectral and turning bands approaches have proved to be successful in accurately reproducing the spatial correlation structure of the generalized increments, while being computationally efficient. However, they are still limited to the simulation of scalar random fields and are therefore not suitable for multivariate applications. The aim of this paper is to extend the continuous spectral algorithm to the simulation of vector random fields representing co-regionalized variables.

The outline of the paper is the following: Sect. 2 is devoted to an overview of the IRF-$k$ theory, Sect. 3 introduces the spectral simulation algorithms for generating non-conditional simulations of an univariate IRF-$k$ and of a vector IRF-$k$. Section 4 is devoted to applications to synthetic case studies. Conclusions follow in Sect. 5.

## 2 Concepts and notations

In IRF-$k$ theory, the spatial trend is represented by a combination of basic drift functions $\{f^l\}_{l\in 0,\ldots,L}$ that are monomials of the spatial coordinates. The number $L$ of such basic functions depends on the degree $k$ of the drift and on the dimension $d$ of the working space.

A generalized increment of order $k$, also referred to as an authorized linear combination of order $k$ (for short, ALC-$k$), of a spatial random field $Y$ is defined as a weighted sum of the form $\sum_{i\in I} \lambda_i Y(\mathbf{x}_i)$ for a system of weights and locations $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I}$ such that, for any basic drift function $f^l$, one has

$$\sum_{i\in I} \lambda_i f^l(\mathbf{x}_i) = 0. \tag{1}$$

In the following, the set of weights and locations $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I}$ fulfilling Eq. (1) will be denoted as $\Lambda_k$ and the ALC-$k$ will be denoted as $Y(\lambda)$.

A random field defined in the $d-$dimensional Euclidean space, say $Y = \{Y(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^d\}$, is an intrinsic random field of order $k$ if its ALC-$k$ have zero mean and are second-order stationary, i.e., if the following conditions are satisfied for any $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I} \in \Lambda_k$ and $\mu = \{\mu_j, \mathbf{x}'_j\}_{j\in J} \in \Lambda_k$ (Chilès and Delfiner 2012):

(1) $E\{Y(\lambda)\} = 0$

(2) $\text{Cov}\{Y(\lambda), Y(\mu)\} = \sum_{i\in I} \sum_{j\in J} \lambda_i \mu_j \mathbf{K}(\mathbf{x}_i - \mathbf{x}'_j),$

where $\mathbf{K}$ is a generalized covariance function defined up to an even polynomial of degree less than or equal to $2k$.

A property of generalized covariances is that they are $k$-conditionally positive definite, that is, for any $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I} \in \Lambda_k$, one has

$$\sum_{i\in I} \sum_{j\in I} \lambda_i \lambda_j \mathbf{K}(\mathbf{x}_i - \mathbf{x}_j) \geq 0.$$

The generalized covariance has the following spectral representation (Chilès and Delfiner 2012):

$$\mathbf{K}(\mathbf{h}) = \int_{\mathbb{R}^d} \frac{\cos(2\pi\langle \mathbf{h}, \mathbf{u}\rangle) - \mathbf{1}_\mathbf{B}(\mathbf{u})P_k(2\pi\langle \mathbf{h}, \mathbf{u}\rangle)}{\left(4\pi^2\|\mathbf{u}\|^2\right)^{k+1}} \chi(\mathbf{du}) + Q_k(\mathbf{h}),$$

where:

$P_k$ is the Taylor expansion of the cosine up to order $2k$, that is

$$P_k(x) = 1 - \frac{x^2}{2!} + \cdots + (-1)^k \frac{x^{2k}}{(2k)!}, \quad x \in \mathbb{R}$$

$\mathbf{1}_\mathbf{B}(\mathbf{u})$ is the indicator function of an arbitrary neighborhood $\mathbf{B}$ of $\mathbf{u}_0 = \mathbf{0}$

$\chi(\mathbf{du})$ is a positive symmetric measure, with no atom at the origin (that is, $\chi(\{\mathbf{0}\}) = 0$) and satisfying

$$\int_{\mathbb{R}^d} \frac{\chi(\mathbf{du})}{\left(1 + 4\pi^2\|\mathbf{u}\|^2\right)^{k+1}} < \infty$$

$Q_k$ is an arbitrary even polynomial of degree $\leq 2k$.

Without loss of generality, one can choose $\mathbf{B} = \mathbb{R}^d$ and $Q_k = 0$, which simplifies the spectral representation as follows:

$$\mathbf{K}(\mathbf{h}) = \int_{\mathbb{R}^d} \frac{\cos(2\pi\langle \mathbf{h}, \mathbf{u}\rangle) - P_k(2\pi\langle \mathbf{h}, \mathbf{u}\rangle)}{\left(4\pi^2\|\mathbf{u}\|^2\right)^{k+1}} \chi(\mathbf{du}). \tag{2}$$

This representation is the generalization of Bochner's theorem (Bochner 1933) according to which a continuous function is positive definite (thus, an ordinary covariance function) if and only if it is the Fourier transform of a positive bounded symmetric measure. A representation similar to Eq. (2) exists for the variogram of a stationary intrinsic random field, which corresponds to the case of an IRF-0 ($k = 0$ and $P_k = 1$) (Chilès and Delfiner 2012).

If $\chi(\mathrm{d}\mathbf{u})$ is absolutely continuous, the previous representation can be rewritten as follows:

$$\mathbf{K}(\mathbf{h}) = \int [\cos(2\pi\langle\mathbf{h},\mathbf{u}\rangle) - P_k(2\pi\langle\mathbf{h},\mathbf{u}\rangle)]f(\mathbf{u})\,\mathrm{d}\mathbf{u}, \qquad (3)$$

with

$$f(\mathbf{u})\,\mathrm{d}\mathbf{u} = \frac{\chi(\mathrm{d}\mathbf{u})}{\left(4\pi^2\|\mathbf{u}\|^2\right)^{k+1}} \geq 0.$$

In the following, $f$ will be referred to as the spectral density of the generalized covariance $\mathbf{K}$. Unless $Y$ is a second-order stationary random field (i.e., $\mathbf{K}$ is an ordinary covariance function), $f$ is not integrable, so it is not a genuine probability density function.

Another tool used for modeling the spatial structure of an intrinsic random field of order $k$ is the generalized variogram of order $k$, defined as (Chilès and Delfiner 2012)

$$\Upsilon(\mathbf{h}) = \frac{1}{M_k}\mathrm{Var}\left[\Delta_{\mathbf{h}}^{k+1}Y(\mathbf{x})\right] \qquad (4)$$

with,

$$M_k = \binom{2k+2}{k+1}$$

$$\Delta_{\mathbf{h}}^{k+1}Y(\mathbf{x}) = (-1)^{k+1}\sum_{q=0}^{k+1}(-1)^q\binom{k+1}{q}Y(\mathbf{x}+q\mathbf{h}).$$

$\Delta_{\mathbf{h}}^{k+1}Y(\mathbf{x})$ is the generalization of the forward finite difference $Y(\mathbf{x}+\mathbf{h}) - Y(\mathbf{x})$.

In the same way that the variogram is related to the covariance in the case of second-order stationary random fields, the generalized variogram of order $k$ is related to the generalized covariance of order $k$, as follows (Chilès and Delfiner 2012):

$$\Upsilon(\mathbf{h}) = \frac{1}{M_k}\sum_{q=-(k+1)}^{k+1}(-1)^q\binom{2k+2}{k+1+q}\mathbf{K}(q\mathbf{h}). \qquad (5)$$

# 3 Non-conditional simulation

This section focuses on the non-conditional simulation of intrinsic scalar and vector random fields of order $k$. In the presence of conditioning data, any non-conditional realization can be converted into a conditional one (i.e., a realization that reproduces the conditioning data, in addition to the desired generalized covariance model) by means of a post-processing step based on intrinsic kriging (univariate case) or cokriging (multivariate case) with the same generalized covariance model and basic drift functions (Chilès and Delfiner 2012; de Fouquet 1994; Emery 2010).

## 3.1 Univariate case

To simulate an intrinsic scalar random field of order $k$ (denoted as $Y$) with a generalized covariance function $\mathbf{K}$ associated with the spectral density $f$, let us consider a random field $Y_S$ defined as

$$\forall \mathbf{x} \in \mathbb{R}^d, \, Y_S(\mathbf{x}) = \sqrt{\frac{2f(\mathbf{U})}{g(\mathbf{U})}}\cos(2\pi\langle\mathbf{x},\mathbf{U}\rangle + \phi), \qquad (6)$$

where $\langle\,,\rangle$ represents the inner product in $\mathbb{R}^d$, $\mathbf{U}$ is a random vector (frequency) with probability density $g : \mathbb{R}^d \rightarrow \mathbb{R}_+$ with a support containing that of $f$ and $\phi$ is a random scalar (phase) uniformly distributed over the interval $[0, 2\pi)$. The demonstration that $Y_S$ is an IRF-$k$ with $\mathbf{K}$ as its generalized covariance function of order $k$ is deferred to the next subsection, which addresses the more general case of intrinsic vector random fields.

Based on the central limit theorem, to obtain an intrinsic random field of order $k$ with the same generalized covariance $\mathbf{K}$ and approximately Gaussian generalized increments of order $k$, it suffices to add and to rescale many of such independent random fields:

$$\forall \mathbf{x} \in \mathbb{R}^d, \, \mathbf{Y}_S(\mathbf{x}) = \frac{1}{\sqrt{N}}\sum_{n=1}^N \sqrt{\frac{2f(\mathbf{U}_n)}{g(\mathbf{U}_n)}}\cos(2\pi\langle\mathbf{x},\mathbf{U}_n\rangle + \phi_n), \qquad (7)$$

where $N$ is a large integer, $\{\mathbf{U}_n : n = 1,\ldots,N\}$ are mutually independent random vectors with probability density $g$ and $\{\phi_n : n = 1,\ldots,N\}$ are mutually independent random variables uniformly distributed in $[0, 2\pi)$, independent of $\{\mathbf{U}_n : n = 1,\ldots,N\}$. Without loss of generality, one can also shift the random field by a constant, so that its value is zero at the origin $\mathbf{x} = \mathbf{0}$:

$$\forall \mathbf{x} \in \mathbb{R}^d, \, \mathbf{Y}_S(\mathbf{x}) = \frac{1}{\sqrt{N}}\sum_{n=1}^N \sqrt{\frac{2f(\mathbf{U}_n)}{g(\mathbf{U}_n)}}[\cos(2\pi\langle\mathbf{x},\mathbf{U}_n\rangle + \phi_n) - \cos(\phi_n)]. \qquad (8)$$

A particular case of this algorithm has been proposed in Emery and Lantuéjoul (2008) for simulating IRF-$k$ with power or spline generalized covariances. In contrast, the algorithm presented here (Eq. 8) is applicable to any generalized covariance model whose spectral density is absolutely continuous.

## 3.2 Multivariate case

One can extend the previous spectral algorithm to the simulation of an intrinsic vector random field of order $k$ (denoted as $\mathbf{Y}$) with $P$ cross-correlated scalar components, by considering a $P \times P$ matrix of spectral densities $\mathbf{f}$ (a

Hermitian, positive semi-definite matrix) instead of a scalar spectral density $f$. In the case when this matrix is real-valued, it is associated with a $P \times P$ matrix $\mathbf{K}$ containing the generalized direct and cross-covariances of the components of $\mathbf{Y}$, in a way similar to Eq. (3) (Cassiani and Christakos 1998; Chilès and Delfiner 2012; Christakos 1992), that is:

$$\mathbf{K}(\mathbf{h}) = \int_{\mathbb{R}^d} [\cos(2\pi\langle\mathbf{h},\mathbf{u}\rangle) - P_k(2\pi\langle\mathbf{h},\mathbf{u}\rangle)]\mathbf{f}(\mathbf{u})\mathrm{d}\mathbf{u}, \qquad (9)$$

where $P_k$ is the Taylor expansion of the cosine up to order $2k$.

Specifically, let us define a vector random field as follows:

$$\mathbf{Y}_S(\mathbf{x}) = \sum_{p=1}^{P} \alpha_p(\mathbf{U}_p)\cos(2\pi\langle\mathbf{x},\mathbf{U}_p\rangle + \phi_p), \qquad (10)$$

where $\{\mathbf{U}_p : p = 1,\ldots,P\}$ are mutually independent random vectors with probability density $g : \mathbb{R}^d \to \mathbb{R}_+$, $\{\phi_p : p = 1,\ldots,P\}$ are mutually independent random variables uniformly distributed over the interval $[0, 2\pi)$, independent of the $\mathbf{U}_p$, and $\{\alpha_p : p = 1,\ldots,P\}$ are vector-valued mappings (to be determined) with $P$ real-valued components.

Considering $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I} \in \Lambda_k$, one can define an ALC-$k$ of the simulated vector random field $\mathbf{Y_S}(\lambda)$ as follows:

$$\mathbf{Y_S}(\lambda) = \sum_{\mathbf{i}\in\mathbf{I}} \lambda_{\mathbf{i}} \sum_{\mathbf{p}=1}^{\mathbf{P}} \alpha_{\mathbf{p}}(\mathbf{U_p})\cos(2\pi\langle\mathbf{x_i},\mathbf{U_p}\rangle + \phi_{\mathbf{p}}). \qquad (11)$$

Accounting for the fact that $\{\phi_p : p = 1,\ldots,P\}$ are independent and uniformly distributed in $[0, 2\pi)$, the conditional expectation of $\mathbf{Y}_S(\lambda)$ given $\mathbf{U}_p = \mathbf{u}_p$ is

$$\mathbb{E}\big[\mathbf{Y}_S(\lambda)|\mathbf{U}_p = \mathbf{u}_p\big] = \mathbf{0}.$$

Therefore, the prior expectation is

$$\begin{aligned}\mathbb{E}[\mathbf{Y}_S(\lambda)] &= \mathbb{E}\big\{\mathbb{E}\big[\mathbf{Y}_S(\lambda)|\mathbf{U}_p\big]\big\}\\ &= \mathbf{0}.\end{aligned}$$

Now, consider $\lambda = \{\lambda_i, \mathbf{x}_i\}_{i\in I} \in \Lambda_k$ and $\mu = \{\mu_j, \mathbf{x}'_j\}_{j\in J} \in \Lambda_k$. If it exists, the matrix of direct and cross-covariances between $\mathbf{Y}_S(\lambda)$ and $\mathbf{Y}_S(\mu)$ is

$$\begin{aligned}\mathbb{E}[\mathbf{Y}_S(\lambda)\mathbf{Y}_S(\mu)] &= \mathbb{E}\Big[\sum_{i\in I}\sum_{j\in J}\sum_{p=1}^{P}\sum_{q=1}^{P}\lambda_i\mu_j\alpha_p(\mathbf{U}_p)\alpha_q^{\mathrm{T}}(\mathbf{U}_q)\cos(2\pi\langle\mathbf{x}_i,\mathbf{U}_p\rangle\\ &\quad + \phi_p)\cos(2\pi\langle\mathbf{x}'_j,\mathbf{U}_q\rangle + \phi_q)\Big]\\ &= \mathbb{E}\Big[\sum_{i\in I}\sum_{j\in J}\sum_{p=1}^{P}\sum_{q=1}^{P}\lambda_i\mu_j\alpha_p(\mathbf{U}_p)\alpha_q^{\mathrm{T}}(\mathbf{U}_q)\\ &\quad \times \frac{1}{2}\Big[\cos(2\pi\langle\mathbf{x}_i,\mathbf{U}_p\rangle + 2\pi\langle\mathbf{x}'_j,\mathbf{U}_q\rangle + \phi_p + \phi_q)\\ &\quad + \cos(2\pi\langle\mathbf{x}_i,\mathbf{U}_p\rangle - 2\pi\langle\mathbf{x}'_j,\mathbf{U}_q\rangle + \phi_p - \phi_q)\Big]\Big].\end{aligned}$$

Accounting for the fact the phases $\{\phi_p, p = 1,\ldots,P\}$ are independent and uniformly distributed in $[0, 2\pi)$, all the cosine terms have a zero expectation except when $p = q$, so that the previous equation simplifies into

$$\begin{aligned}\mathbb{E}[\mathbf{Y}_S(\lambda)\mathbf{Y}_S(\mu)] &= \frac{1}{2}\mathbb{E}\Big[\sum_{i\in I}\sum_{j\in J}\sum_{p=1}^{P}\lambda_i\mu_j\alpha_p(\mathbf{U}_p)\alpha_p^{\mathrm{T}}(\mathbf{U}_p)\\ &\quad \times \Big[\cos(2\pi\langle\mathbf{x}_i + \mathbf{x}'_j,\mathbf{U}_p\rangle + 2\phi_p) + \cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{U}_p\rangle)\Big]\Big].\end{aligned}$$
$$(12)$$

The first cosine term has a zero expectation because $\phi_p$ is uniform on $[0, 2\pi)$ and is independent of $\mathbf{U}_p$, for all $p = 1,\ldots,P$. Therefore, Eq. (12) reduces to

$$\begin{aligned}&\mathbb{E}[\mathbf{Y}_S(\lambda)\mathbf{Y}_S(\mu)]\\ &= \mathbb{E}\Big[\sum_{i\in I}\sum_{j\in J}\lambda_i\mu_j\sum_{p=1}^{P}\alpha_p(\mathbf{U}_p)\alpha_p^{\mathrm{T}}(\mathbf{U}_p)\frac{\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{U}_p\rangle)}{2}\Big]\\ &= \int_{\mathbb{R}^d}\sum_{i\in I}\sum_{j\in J}\lambda_i\mu_j\sum_{p=1}^{P}\alpha_p(\mathbf{u})\alpha_p^{\mathrm{T}}(\mathbf{u})\frac{\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle)}{2}g(\mathbf{u})\,\mathrm{d}\mathbf{u}\\ &= \int_{\mathbb{R}^d}\sum_{i\in I}\sum_{j\in J}\lambda_i\mu_j\frac{\mathbf{A}(\mathbf{u})\mathbf{A}^{\mathrm{T}}(\mathbf{u})}{2}\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle)g(\mathbf{u})\,\mathrm{d}\mathbf{u},\end{aligned}$$

where $\mathbf{A}(\mathbf{u})$ is the $P \times P$ matrix whose $p$-th column is $\alpha_p(\mathbf{u})$.

Since the weights $\{\lambda_i\}_{i\in I}$ and $\{\mu_j\}_{j\in J}$ filter out the polynomials of degree less than or equal to $2k$ (Eq. 1), one can subtract the Taylor expansion $P_k$ of the cosine without modifying the integrand, as follows:

$$\begin{aligned}\mathbb{E}[\mathbf{Y}_S(\lambda)\mathbf{Y}_S(\mu)] &= \int_{\mathbb{R}^d}\sum_{i\in I}\sum_{j\in J}\lambda_i\mu_j\frac{\mathbf{A}(\mathbf{u})\mathbf{A}^{\mathrm{T}}(\mathbf{u})}{2}\\ &\quad \times \Big[\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle) - P_k(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle)\Big]g(\mathbf{u})\,\mathrm{d}\mathbf{u}.\end{aligned}$$
$$(13)$$

For the simulated vector random field $\mathbf{Y}_S$ to be an intrinsic vector random field of order $k$ with a matrix of generalized direct and cross-covariances $\mathbf{K}$ associated with the spectral density matrix $\mathbf{f}$ (Eq. 9), it suffices that the following condition is satisfied for any frequency vector $\mathbf{u}$:

$$\frac{\mathbf{A}(\mathbf{u})\mathbf{A}^{\mathrm{T}}(\mathbf{u})}{2}g(\mathbf{u}) = \mathbf{f}(\mathbf{u}),$$

or, equivalently,

$$\mathbf{A}(\mathbf{u})\mathbf{A}^{\mathrm{T}}(\mathbf{u}) = \frac{2\mathbf{f}(\mathbf{u})}{g(\mathbf{u})}. \qquad (14)$$

This condition, which is analogous to that found for the simulation of intrinsic vector random fields of order 0 (Arroyo and Emery 2017), ensures that the improper integral

$$\frac{\mathbf{A}(\mathbf{u})\mathbf{A}^{\mathrm{T}}(\mathbf{u})}{2}\int_{\mathbb{R}^d}\Big[\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle) - P_k(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j,\mathbf{u}\rangle)\Big]g(\mathbf{u})\,\mathrm{d}\mathbf{u}$$

is convergent, insofar as it coincides with the spectral representation of the generalized covariance $\mathbf{K}(\mathbf{x}_i - \mathbf{x}'_j)$.

The summations and integral signs in Eq. (13) can therefore be permuted, which yields

$$
\begin{aligned}
\mathbb{E}[\mathbf{Y}_S(\lambda)\mathbf{Y}_S(\mu)] &= \sum_{i \in I}\sum_{j \in J}\lambda_i\mu_j\frac{\mathbf{A}(\mathbf{u})\mathbf{A}^\mathrm{T}(\mathbf{u})}{2} \\
&\quad \times \int_{\mathbb{R}^d}\Big[\cos(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j, \mathbf{u}\rangle) - P_k(2\pi\langle\mathbf{x}_i - \mathbf{x}'_j, \mathbf{u}\rangle)\Big]g(\mathbf{u})\,\mathrm{d}\mathbf{u} \\
&= \sum_{i \in I}\sum_{j \in J}\lambda_i\mu_j\mathbf{K}(\mathbf{x}_i - \mathbf{x}'_j).
\end{aligned}
$$

For instance, $\mathbf{A}(\mathbf{u})$ can be chosen as the principal square root matrix of $\frac{2\mathbf{f}(\mathbf{u})}{g(\mathbf{u})}$. The knowledge of $\mathbf{A}(\mathbf{u})$ determines the vector-valued mappings $\{\alpha_p : p = 1, \ldots, P\}$ to be used in Equation (10), which completes the specification of the algorithm.

Finally, based on the central limit theorem, to obtain an intrinsic vector random field with approximately Gaussian increments of order $k$ and with zero value at the origin $\mathbf{x} = \mathbf{0}$, it suffices to shift, add and rescale many of such independent random fields:

$$
\mathbf{Y}_S(\mathbf{x}) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\sum_{p=1}^{P}\alpha_p(\mathbf{U}_{n,p})\big[\cos(2\pi\langle\mathbf{x}, \mathbf{U}_{n,p}\rangle + \phi_{n,p}) - \cos(\phi_{n,p})\big],
\tag{15}
$$

where $N$ is a large integer, $\{\mathbf{U}_{n,p} : n = 1, \ldots, N; p = 1, \ldots, P\}$ are mutually independent random vectors with probability density $g$ and $\{\phi_{n,p} : n = 1, \ldots, N; p = 1, \ldots, P\}$ are mutually independent random variables uniformly distributed as $\phi_p$.

This algorithm (Eq. 15) generalizes the ones proposed in Emery et al. (2016) and in Arroyo and Emery (2017), which are restricted to the simulation of stationary and intrinsic vector random fields of order $k = 0$, respectively. The density $g$ can be chosen freely, provided that its support contains the support of each component of the spectral density matrix $\mathbf{f}$ (this necessary condition is implied by Eq. 14). Note that the spectral representation under consideration (Eq. 9) is restricted to generalized cross-covariances that are even functions of the lag vector $\mathbf{h}$. A more general representation allowing the incorporation of an odd component is presented in Chilès and Delfiner (2012) for the case when $k = 0$ and in Huang et al. (2009) for any non-negative integer $k$. The design of non-even generalized cross-covariance models together with algorithms for simulating vector IRF-$k$ with such covariance models is a topic of further research.

# 4 Examples

In this section, the proposed spectral algorithm is tested to simulate random fields on a set of 250,000 locations on a regular two-dimensional grid $G$ with a unit mesh along

each coordinate axis ($d = 2$). The simulation is performed by using $N = 500$ basic random fields in Eqs. (8) or (15). The density $g$ is chosen as the spectral density of a stationary isotropic Matérn covariance with a unit sill (Lantuéjoul 2002):

$$
\mathbf{M}(\mathbf{h}, a, v) = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\|\mathbf{h}\|}{a}\right)^{v}K_v\left(\frac{\|\mathbf{h}\|}{a}\right),
\tag{16}
$$

that is:

$$
g(\mathbf{u}, a, v) = \frac{(2\pi a)^d\,\Gamma\big(v + \frac{d}{2}\big)}{\Gamma(v)\pi^{d/2}}\frac{1}{\big(1 + (2\pi a)^2\|\mathbf{u}\|^2\big)^{v+d/2}},
\tag{17}
$$

where $\Gamma(\cdot)$ is the gamma function and $K_v(\cdot)$ is the modified Bessel function of the second kind of order $v$.

In the following, the scale parameter will be set to $a = 30$ and the shape parameter to $v = \min(\alpha_1, \alpha_2)/2$, where $\alpha_1$ and $\alpha_2$ will be defined in each example. These values of $a$ and $v$ correspond to a heuristic choice that provides a good sampling of both large and small frequencies when generating the random vectors $\{\mathbf{U}_n : n = 1, \ldots, N\}$ (Eq. 8) or $\{\mathbf{U}_{n,p} : n = 1, \ldots, N; p = 1, \ldots, P\}$ (Eq. 15). However, as proved in the previous sections, the algorithm is applicable with any other choice for these scale and shape parameters, insofar as the support of the Matérn density is the whole space $\mathbb{R}^d$.

## 4.1 Example 1: Simulating a scalar random field with power generalized covariance in $\mathbb{R}^d$

Let us consider the simulation of a scalar intrinsic random field with a power generalized covariance of the form

$$
\forall\mathbf{h} \in \mathbb{R}^d,\ \mathbf{K}(\mathbf{h}) = (-1)^{1+\lfloor\alpha/2\rfloor}\left\|\frac{\mathbf{h}}{b}\right\|^{\alpha},
$$

where $\lfloor\cdot\rfloor$ is the floor function, $b$ is a positive real number and $\alpha$ is a positive real number different from an even integer. The order of the intrinsic random field with such a generalized covariance is $k = \lfloor\alpha/2\rfloor$.

The spectral density of $\mathbf{K}(\mathbf{h})$ is (Chilès and Delfiner 2012):

$$
\forall\mathbf{u} \in \mathbb{R}^d,\ f_P(\mathbf{u}, b, \alpha) = \frac{b^d\Gamma\big(\frac{\alpha}{2} + 1\big)\Gamma\big(\frac{\alpha+d}{2}\big)}{\Gamma\big(\frac{\alpha}{2} - k\big)\Gamma\big(1 - \frac{\alpha}{2} + k\big)\pi^{\alpha+d/2}\|b\mathbf{u}\|^{\alpha+d}}.
\tag{18}
$$

As an example, Fig. 1 (left) shows the map of one realization obtained by using Eq. (8) with $\alpha = 5$ (therefore, $k = 2$) and $b = 100$. The simulated field (an IRF-2) exhibits a quadratic drift, which makes difficult to visually assess whether or not the desired spatial correlation
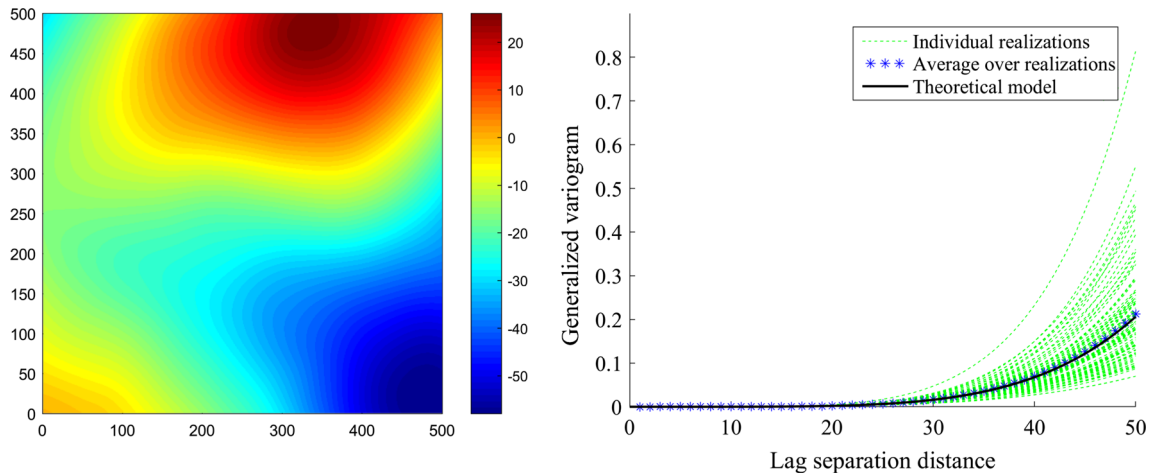
**Fig. 1** Left: map of one realization of an IRF-2 with power generalized covariance of exponent $\alpha = 5$ and scale factor $b = 100$. Right: experimental generalized variograms of order 2 of 100 realizations (green dashed lines) calculated for lag separation vectors oriented along the abscissa axis, average of experimental generalized variograms (blue stars) and theoretical generalized variogram (black solid line)

structure is accurately reproduced. Since this structure is related to the generalized increments of order 2, one option to unveil it is to focus on the generalized variogram of order 2 of the simulated field, that is (Eq. 4):

$$\Upsilon(\mathbf{h}) = \frac{1}{20} E\Big\{ [Y(\mathbf{x} + 3\mathbf{h}) - 3Y(\mathbf{x} + 2\mathbf{h}) + 3Y(\mathbf{x} + \mathbf{h}) - Y(\mathbf{x})]^2 \Big\}.$$
(19)

$\Upsilon(\mathbf{h})$ can be expressed as a function of the generalized covariance $\mathbf{K}(\mathbf{h})$ (Eq. 5). Experimentally, it can be estimated for each realization $\{y(\mathbf{x}) : \mathbf{x} \in G\}$ by replacing the expectation in the previous equation by an average of the form

$$\hat{\Upsilon}(\mathbf{h}) = \frac{1}{20} \frac{\sum_{\mathbf{x} \in G \cap G_{-\mathbf{h}} \cap G_{-2\mathbf{h}} \cap G_{-3\mathbf{h}}} [y(\mathbf{x} + 3\mathbf{h}) - 3y(\mathbf{x} + 2\mathbf{h}) + 3y(\mathbf{x} + \mathbf{h}) - y(\mathbf{x})]^2}{\text{card}\{G \cap G_{-\mathbf{h}} \cap G_{-2\mathbf{h}} \cap G_{-3\mathbf{h}}\}},$$
(20)

where $G_{-\mathbf{h}}, G_{-2\mathbf{h}}$ and $G_{-3\mathbf{h}}$ stand for the grid $G$ shifted by vector $-\mathbf{h}, -2\mathbf{h}$ and $-3\mathbf{h}$, respectively, while card$\{.\}$ indicates cardinality. Such an experimental generalized variogram is expected to fluctuate without bias around the theoretical generalized variogram (Chilès and Delfiner 2012). Accordingly, on average over a large set of realizations (so that statistical fluctuations become negligible), it is expected that the experimental generalized variogram matches the theoretical generalized variogram. This effectively happens when considering one hundred realizations (Fig. 1 right), confirming that the simulated field accurately reproduces the target power generalized covariance.

## 4.2 Example 2: Simulating a vector random field with power generalized direct and cross-covariances

Let us now simulate an intrinsic vector random field $\mathbf{Y}$ with $P = 2$ components with the following $2 \times 2$ matrix of generalized direct and cross-covariances:

$\forall \mathbf{h} \in \mathbb{R}^d$, $\mathbf{K}(\mathbf{h})$

$$= \begin{pmatrix} (-1)^{1+\lfloor \alpha_1/2 \rfloor} \left\| \frac{\mathbf{h}}{b_1} \right\|^{\alpha_1} & \rho(-1)^{1+\lfloor \alpha_{12}/2 \rfloor} \left\| \frac{\mathbf{h}}{b_{12}} \right\|^{\alpha_{12}} \\ \rho(-1)^{1+\lfloor \alpha_{12}/2 \rfloor} \left\| \frac{\mathbf{h}}{b_{12}} \right\|^{\alpha_{12}} & (-1)^{1+\lfloor \alpha_2/2 \rfloor} \left\| \frac{\mathbf{h}}{b_2} \right\|^{\alpha_2} \end{pmatrix},$$
(21)

where $\rho \in \mathbb{R}$, $(b_1, b_2, b_{12}, \alpha_1, \alpha_2, \alpha_{12}) \in (\mathbb{R}_+^*)^6$, such that $\alpha_1$ and $\alpha_2$ are not even integers. The orders of the first and second components of the vector random field are $k_1 = \lfloor \alpha_1/2 \rfloor$ and $k_2 = \lfloor \alpha_2/2 \rfloor$, respectively, while the overall order of the intrinsic vector random field is $k = \max(k_1, k_2)$.

The corresponding spectral density matrix for a given frequency vector $\mathbf{u} \in \mathbb{R}^d$ is:

$$\mathbf{f}(\mathbf{u}) = \begin{pmatrix} f_P(\mathbf{u}, b_1, \alpha_1) & \rho f_P(\mathbf{u}, b_{12}, \alpha_{12}) \\ \rho f_P(\mathbf{u}, b_{12}, \alpha_{12}) & f_P(\mathbf{u}, b_2, \alpha_2) \end{pmatrix}. \quad (22)$$

The conditions under which this matrix is Hermitian positive semi-definite for any $\mathbf{u} \in \mathbb{R}^d$ are detailed in "Appendix 1".

As an illustration, Fig. 2 shows the map of one realization obtained by using Eq. (15) with $\alpha_1 = 2.5$ ($k_1 = 1$), $\alpha_2 = 4.5$ ($k_2 = k = 2$), $\alpha_{12} = 3.5$, $b_1 = 100$, $b_2 = 90$,
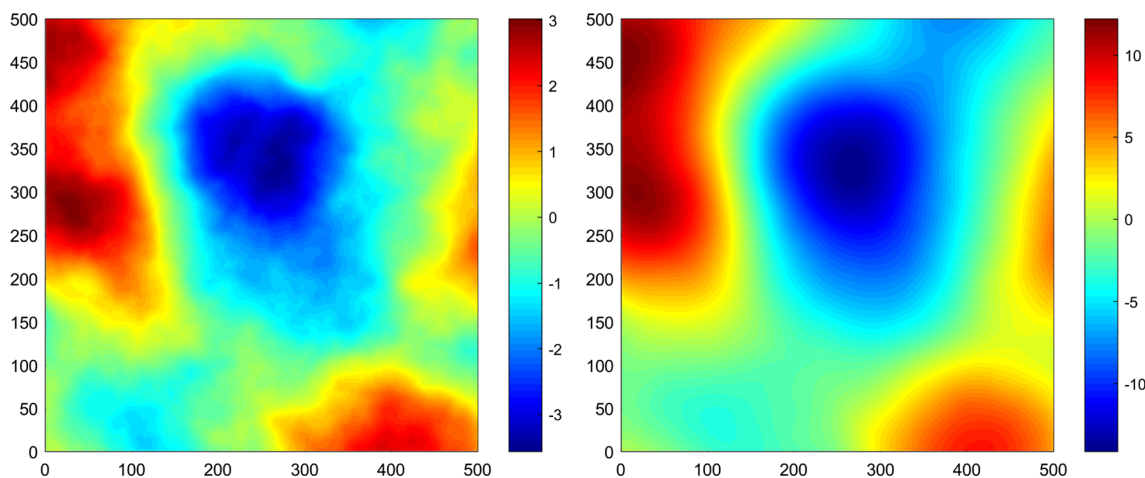
**Fig. 2** Realizations of a bivariate intrinsic random field whose first component is an IRF-1 (on the left) and the second component is an IRF-2 (on the right). Generalized direct and cross-covariances are

power models with $\alpha_1 = 2.5$ $(k_1 = 1)$, $\alpha_2 = 4.5$ $(k_2 = 2)$, $\alpha_{12} = 3.5$, $b_1 = 100$, $b_2 = 90$, $b_{12} = 70$ and $\rho = 0.4$

$b_{12} = 70$ and $\rho = 0.4$. Figure 3 compares the experimental generalized direct and cross-variograms of order 2 of one hundred realizations with the theoretical generalized direct and cross-variograms of order 2. The generalized cross-variogram is defined by substituting the covariance or the product of generalized increments for the variance (Eq. 4) or the squared value (Eqs. 19, 20) of generalized increments. As for the previous subsection, on average over the realizations, the experimental generalized variograms match the theoretical generalized variograms, which corroborates that the proposed spectral simulation algorithm accurately reproduces the spatial correlation structure of the desired vector random field.

### 4.3 Example 3: Simulating a vector random field with power and spline generalized direct covariances and Matérn generalized cross-covariance

Let us now simulate an intrinsic vector random field of order $k$, $\mathbf{Y}$, with $P = 2$ components by using the following $2 \times 2$ matrix of generalized direct and cross-covariances:

$$\forall \mathbf{h} \in \mathbb{R}^d, \mathbf{K}(\mathbf{h})$$
$$= \begin{pmatrix} (-1)^{1+\lfloor \alpha_1/2 \rfloor} \left\| \frac{\mathbf{h}}{b_1} \right\|^{\alpha_1} & \rho \, \mathbf{M}(\mathbf{h}, a_{12}, v_{12}) \\ \rho \, \mathbf{M}(\mathbf{h}, a_{12}, v_{12}) & (-1)^{1+k_2} \left\| \frac{\mathbf{h}}{b_2} \right\|^{\alpha_2} \ln\left( \left\| \frac{\mathbf{h}}{b_2} \right\| \right) \end{pmatrix},$$
$$\tag{23}$$

where $\rho \in \mathbb{R}$, $(b_1, b_2, \alpha_1, a_{12}, v_{12}) \in (\mathbb{R}_+^*)^5$ such that $\alpha_1$ is not an even integer, $k_2 \in \mathbb{N}^*$ and $\alpha_2 = 2k_2$. The orders of the first and second components of the vector random field are $k_1 = \lfloor \alpha_1/2 \rfloor$ and $k_2$, respectively, while the overall order of the intrinsic vector random field is $k = \max(k_1, k_2)$.

$\mathbf{M}(\mathbf{h}, a_{12}, v_{12})$ is the stationary Matérn covariance with sill $\rho$, scale parameter $a_{12}$ and shape parameter $v_{12}$ (Lantuéjoul 2002); therefore, this is also a valid generalized covariance for any order $k$ (Chilès and Delfiner 2012).

The corresponding spectral density matrix for a given frequency vector $\mathbf{u} \in \mathbb{R}^d$ is:

$$\mathbf{f}(\mathbf{u}) = \begin{pmatrix} f_P(\mathbf{u}, b_1, \alpha_1) & \rho \, g(\mathbf{u}, a_{12}, v_{12}) \\ \rho \, g(\mathbf{u}, a_{12}, v_{12}) & f_S(\mathbf{u}, b_2, k_2) \end{pmatrix}, \tag{24}$$

where $f_S(\mathbf{u}, b_2, k_2)$ is the spectral density of the spline generalized covariance $(-1)^{1+k_2} \left\| \frac{\mathbf{h}}{b_2} \right\|^{2k_2} \ln\left( \left\| \frac{\mathbf{h}}{b_2} \right\| \right)$. The expression of this spectral density can be obtained by considering the spline generalized covariance as the limit, as $\epsilon$ tends to zero, of a power generalized covariance of exponent $2k_2 + \epsilon$ divided by $\epsilon$ (Emery and Lantuéjoul 2008). This implies

$$\forall \mathbf{u} \in \mathbb{R}^d, f_S(\mathbf{u}, b_2, k_2) = \lim_{\epsilon \to 0} \left( \frac{f_P(\mathbf{u}, b_2, 2k_2 + \epsilon)}{\epsilon} \right)$$
$$= \frac{b_2^d \Gamma(k_2 + 1) \Gamma\left(\frac{2k_2+d}{2}\right)}{2\pi^{2k_2+d/2} \| b_2 \mathbf{u} \|^{2k_2+d}}. \tag{25}$$

The conditions under which the spectral density matrix in Eq. (24) is Hermitian positive semi-definite for any $\mathbf{u} \in \mathbb{R}^d$ (therefore, the defined generalized direct and cross-covariances constitute a valid model) are indicated in "Appendix 2".

As an illustration, Fig. 4 shows the map of one realization obtained by using Eq. (15) with $\alpha_1 = 3$ $(k_1 = 1)$, $\alpha_2 = 2$ $(k_2 = 1)$, $b_1 = 180$, $b_2 = 100$, $a_{12} = 80$, $v_{12} = 1.25$ and $\rho = 0.55$. Figure 5 compares the experimental generalized direct and cross-variograms of order 1 of one hundred realizations with the theoretical generalized direct and cross-variograms of order 1. On average over the
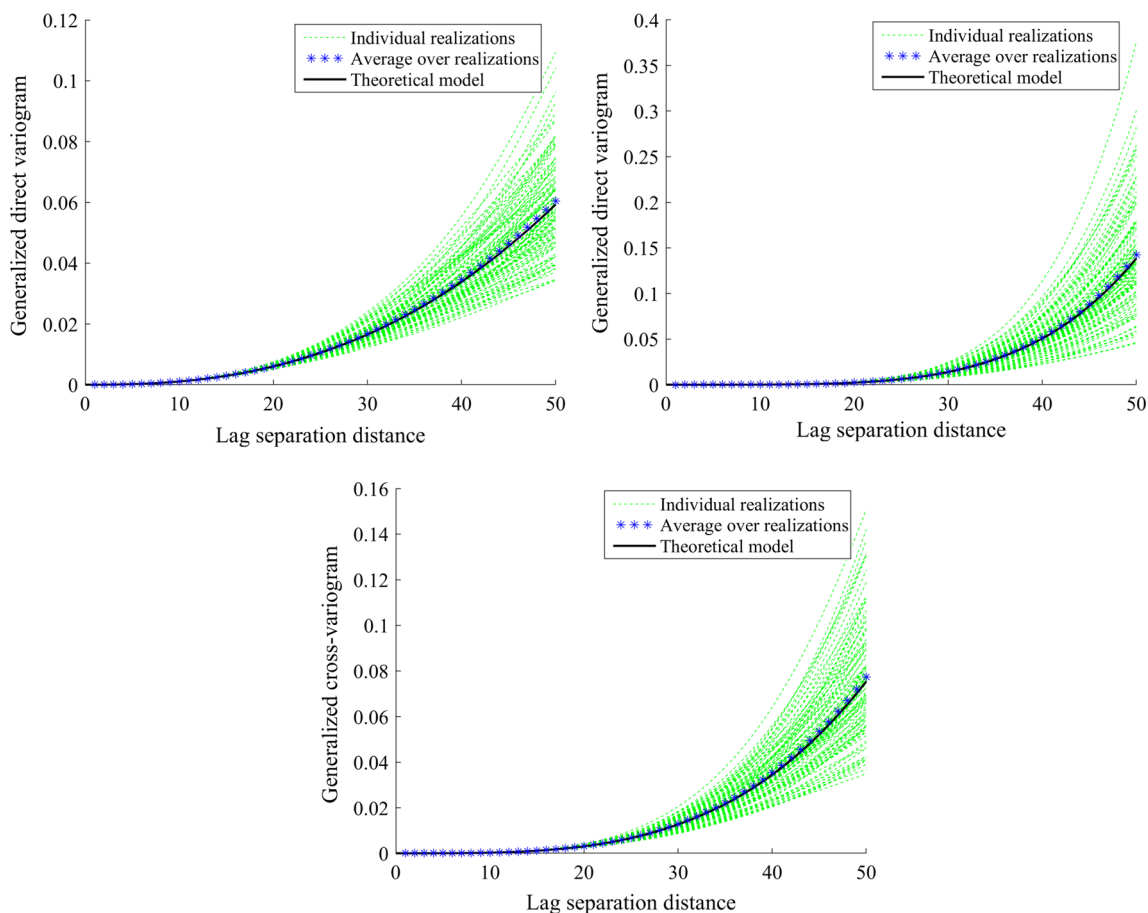
**Fig. 3** Experimental generalized variograms of order 2 for 100 realizations (green dashed lines) calculated for lag separation vectors oriented along the abscissa axis, average of experimental generalized variograms (blue stars) and theoretical models (black solid lines). From left to r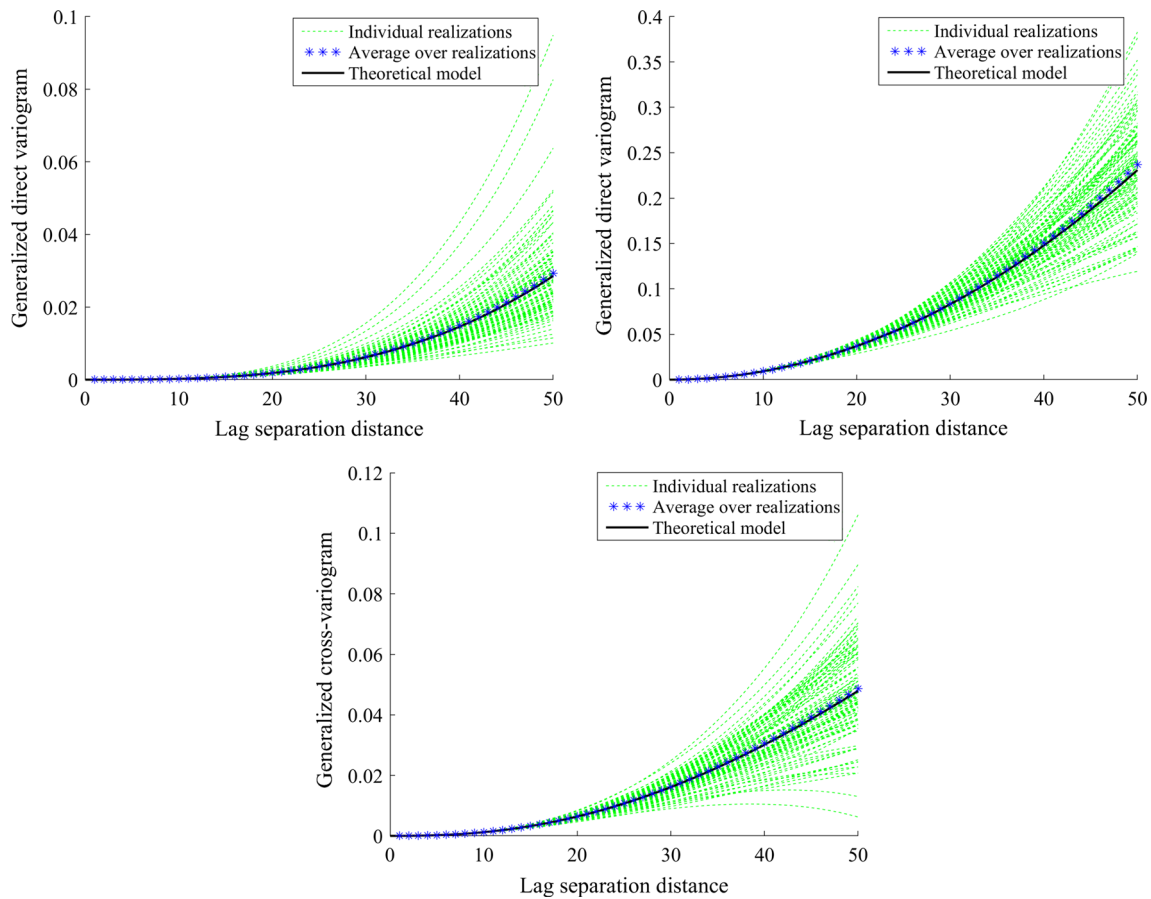ight and top to bottom: generalized direct variograms for first component, generalized direct variograms for second component, and generalized cross-variograms. Generalized direct and cross-covariances are power models with $\alpha_1 = 2.5$ ($k_1 = 1$), $\alpha_2 = 4.5$ ($k_2 = 2$), $\alpha_{12} = 3.5$, $b_1 = 100$, $b_2 = 90$, $b_{12} = 70$ and $\rho = 0.4$
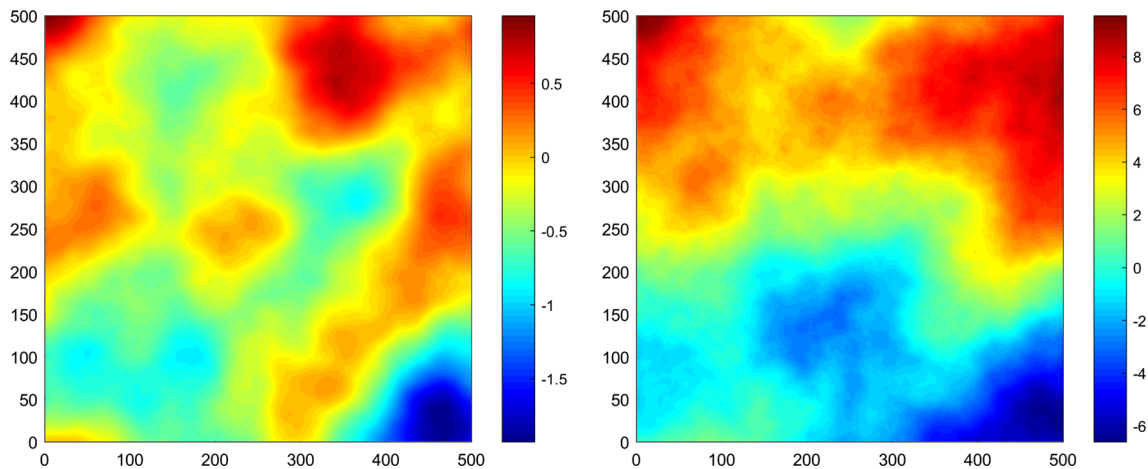


**Fig. 4** Realizations of a bivariate intrinsic random field whose components are IRF-1 (first component on the left, second component on the right). Generalized direct and cross-covariances are power, spline and Matérn models with $\alpha_1 = 3$ ($k_1 = 1$), $\alpha_2 = 2$ ($k_2 = 1$), $b_1 = 180$, $b_2 = 100$, $a_{12} = 80$, $v_{12} = 1.25$ and $\rho = 0.55$

**Fig. 5** Experimental generalized variograms of order 1 for 100 realizations (green dashed lines) calculated for lag separation vectors oriented along the abscissa axis, average of experimental generalized variograms (blue stars) and theoretical models (black solid lines). From left to right and top to bottom: generalized direct variograms for first component, generalized direct variograms for second component, and generalized cross-variograms. Generalized direct and cross-covariances are power, spline and Matérn models with $\alpha_1 = 3$ ($k_1 = 1$), $\alpha_2 = 2$ ($k_2 = 1$), $b_1 = 180$, $b_2 = 100$, $a_{12} = 80$, $v_{12} = 1.25$ and $\rho = 0.55$

realizations, the experimental generalized variograms match the theoretical generalized variograms, corroborating that the spatial correlation structure of the target vector random field is accurately reproduced.

## 5 Conclusions

This paper presented an algorithm for simulating intrinsic vector random fields of order $k$ with given generalized direct and cross-covariances and multivariate Gaussian generalized increments. The algorithm relies on the spectral decomposition of the generalized covariances, in order to reproduce the spatial correlation structure of the desired random field, and on the central limit theorem, in order to obtain generalized increments whose finite-dimensional distributions are approximately Gaussian.

The implementation of the algorithm is straightforward, with no restriction on the number of components of the vector random field, space dimension, number and positions of the locations targeted for simulation, or number of desired realizations, other than hardware and software capacities. The presented examples show the versatility of the algorithm and its applicability to simulate random fields with a complex covariance structure.

## Appendix 1: Existence conditions for Example 2

The spectral density matrix $\mathbf{f}(\mathbf{u})$ defined in Eq. (22) is Hermitian since it is real-valued and symmetric, with positive diagonal entries. It is positive semi-definite for any $\mathbf{u} \in \mathbb{R}^d$ (therefore, the associated generalized direct and

cross-covariances constitute a valid model) if and only if its determinant is non-negative, that is:

$$f_P(\mathbf{u}, b_1, \alpha_1) \cdot f_P(\mathbf{u}, b_2, \alpha_2) \geq \rho^2 f_P^2(\mathbf{u}, b_{12}, \alpha_{12}),$$

with $f_P$ the spectral density of the power generalized covariance (Eq. 18).

Now, if $\rho$ is different from zero, the determinant is negative for large $\|\mathbf{u}\|$ if $\alpha_{12} < \frac{\alpha_1 + \alpha_2}{2}$ and for small $\|\mathbf{u}\|$ if $\alpha_{12} > \frac{\alpha_1 + \alpha_2}{2}$; a necessary condition for positive semi-definiteness is therefore that the exponent of the cross-covariance is the arithmetic average of the exponents of the direct covariances, i.e., $\alpha_{12} = \frac{\alpha_1 + \alpha_2}{2}$. Under this condition, the sign of the determinant is the same as the sign of

$$\frac{\Gamma\left(\frac{\alpha_1}{2}+1\right)\Gamma\left(\frac{\alpha_1+d}{2}\right)}{\Gamma\left(\frac{\alpha_1}{2}-\lfloor\alpha_1/2\rfloor\right)\Gamma\left(1-\frac{\alpha_1}{2}+\lfloor\alpha_1/2\rfloor\right)b_1^{\alpha_1}}\frac{\Gamma\left(\frac{\alpha_2}{2}+1\right)\Gamma\left(\frac{\alpha_2+d}{2}\right)}{\Gamma\left(\frac{\alpha_2}{2}-\lfloor\alpha_2/2\rfloor\right)\Gamma\left(1-\frac{\alpha_2}{2}+\lfloor\alpha_2/2\rfloor\right)b_2^{\alpha_2}}$$
$$-\left(\rho\frac{\Gamma\left(\frac{\alpha_{12}}{2}+1\right)\Gamma\left(\frac{\alpha_{12}+d}{2}\right)}{\Gamma\left(\frac{\alpha_{12}}{2}-\lfloor\alpha_{12}/2\rfloor\right)\Gamma\left(1-\frac{\alpha_{12}}{2}+\lfloor\alpha_{12}/2\rfloor\right)b_{12}^{\alpha_{12}}}\right)^2.$$

Accordingly, positive semi-definiteness is ensured if, and only if, either $\rho = 0$ or the two following constraints are fulfilled:

1. $\alpha_{12} = \dfrac{\alpha_1 + \alpha_2}{2}$
2. 

$$\rho^2 \leq \frac{b_{12}^{2\alpha_{12}}\Gamma^2\left(\frac{\alpha_{12}}{2}-\lfloor\alpha_{12}/2\rfloor\right)\Gamma^2\left(1-\frac{\alpha_{12}}{2}+\lfloor\alpha_{12}/2\rfloor\right)\Gamma\left(\frac{\alpha_1}{2}+1\right)\Gamma\left(\frac{\alpha_2}{2}+1\right)\Gamma\left(\frac{\alpha_1+d}{2}\right)\Gamma\left(\frac{\alpha_2+d}{2}\right)}{b_1^{\alpha_1}b_2^{\alpha_2}\Gamma^2\left(\frac{\alpha_{12}}{2}+1\right)\Gamma^2\left(\frac{\alpha_{12}}{2}+\frac{d}{2}\right)\Gamma\left(\frac{\alpha_1}{2}-\lfloor\alpha_1/2\rfloor\right)\Gamma\left(\frac{\alpha_2}{2}-\lfloor\alpha_2/2\rfloor\right)\Gamma\left(1-\frac{\alpha_1}{2}+\lfloor\alpha_1/2\rfloor\right)\Gamma\left(1-\frac{\alpha_2}{2}+\lfloor\alpha_2/2\rfloor\right)}$$

$$\kappa = \frac{\Gamma\left(\frac{\alpha_1}{2}+1\right)\Gamma\left(\frac{\alpha_1+d}{2}\right)\Gamma(k_2+1)\Gamma\left(\frac{2k_2+d}{2}\right)\Gamma^2(v_{12})}{2b_1^{\alpha_1}b_2^{2k_2}\pi^{\alpha_1+2k_2}\Gamma\left(\frac{\alpha_1}{2}-\lfloor\alpha_1/2\rfloor\right)\Gamma\left(1-\frac{\alpha_1}{2}+\lfloor\alpha_1/2\rfloor\right)\Gamma^2\left(v_{12}+\frac{d}{2}\right)}.$$

The mapping $\varphi : \mathbb{R}_+ \to \mathbb{R}$ is unbounded if $\alpha_1 + 2k_2 > 4v_{12}$, in which case inequality (26) cannot be satisfied. In the converse case ($\alpha_1 + 2k_2 \leq 4v_{12}$), the maximum of $\varphi$ is

$$\varphi_{\max} = \frac{(\alpha_1 + 2k_2 + 2d)^{(\alpha_1+2k_2)/2+d}(4v_{12} - \alpha_1 - 2k_2)^{2v_{12}-(\alpha_1+2k_2)/2}}{(4v_{12} + 2d)^{2v_{12}+d}(2\pi a_{12})^{\alpha_1+2k_2}}.$$

Therefore, when $\rho \neq 0$, the following two necessary and sufficient conditions must be fulfilled for the spectral density matrix $\mathbf{f}(\mathbf{u})$ to be positive semi-definite for all $\mathbf{u} \in \mathbb{R}^d$:

1. $\alpha_1 + 2k_2 \leq 4v_{12}$
2. $\rho^2 \leq \rho_{\max}^2 = \dfrac{\kappa}{\varphi_{\max}}$.

In the specific case when $\alpha_1 + 2k_2 = 4v_{12}$, $\varphi_{\max} = (2\pi a_{12})^{-(\alpha_1+2k_2)}$ and the upper bound of $\rho^2$ is given by

$$\rho^2 \leq \frac{\Gamma^2\left(\frac{\alpha_1+2k_2}{4}\right)}{\Gamma^2\left(\frac{\alpha_1+2k_2}{4}+\frac{d}{2}\right)}\left(\frac{2a_{12}}{b_1}\right)^{\alpha_1}\left(\frac{2a_{12}}{b_2}\right)^{2k_2}$$
$$\times \frac{\Gamma\left(\frac{\alpha_1}{2}+1\right)\Gamma(k_2+1)\Gamma\left(\frac{\alpha_1+d}{2}\right)\Gamma\left(\frac{2k_2+d}{2}\right)}{2\Gamma\left(\frac{\alpha_1}{2}-\lfloor\alpha_1/2\rfloor\right)\Gamma\left(1-\frac{\alpha_1}{2}+\lfloor\alpha_1/2\rfloor\right)}.$$

The above bivariate model and conditions of validity bear a resemblance to the non-stationary models proposed in Arroyo and Emery (2017) and in Maleki and Emery (2017), in which the spline generalized direct covariance is replaced by a power or by a Matérn covariance, and, to a lesser extent, to the stationary bivariate Matérn covariance model (Gneiting et al. 2010; Apanasovich et al. 2012).

## Appendix 2: Existence conditions for Example 3

As for the previous example, the spectral density matrix $\mathbf{f}(\mathbf{u})$ defined in Eq. (24) is positive semi-definite if and only if its determinant is non-negative, i.e.:

$$f_P(\mathbf{u}, b_1, \alpha_1) \cdot f_S(\mathbf{u}, b_2, k_2) \geq \rho^2 g^2(\mathbf{u}, a_{12}, v_{12}),$$

where $f_P$ and $f_S$ are the spectral densities of the power and spline generalized covariances, respectively. When $\rho = 0$, the positivity condition is fulfilled irrespective of the values of $b_1$, $\alpha_1$, $b_2$ and $k_2$. In contrast, when $\rho \neq 0$, the following necessary and sufficient condition is found:

$$\varphi(\|\mathbf{u}\|) := \frac{(2\pi a_{12})^{2d}\|\mathbf{u}\|^{\alpha_1+2k_2+2d}}{\left(1 + (2\pi a_{12})^2\|\mathbf{u}\|^2\right)^{2v_{12}+d}} \leq \frac{\kappa}{\rho^2}, \quad (26)$$

with

## References

Apanasovich TV, Genton MG, Sun Y (2012) A valid Matérn class of cross-covariance functions for multivariate random fields with any number of components. J Am Stat Assoc 107(497):180–193

Arroyo D, Emery X (2015) Simulation of intrinsic random fields of order $k$ with Gaussian generalized increments by Gibbs sampling. Math Geosci 47(8):955–974

Arroyo D, Emery X (2017) Spectral simulation of vector random fields with stationary Gaussian increments in $d$-dimensional Euclidean spaces. Stoch Environ Res Risk Assess 31(7):1583–1592

Bochner S (1933) Monotone Funktionen Stieljessche Integrale and Harmonische Analyse. Math Ann 108:378–410

Buttafuoco G, Castrignano A (2005) Study of the spatio-temporal variation of soil moisture under forest using intrinsic random functions of order $k$. Geoderma 128(3–4):208–220

Cassiani G, Christakos G (1998) Analysis and estimation of natural processes with nonhomogeneous spatial variation using secondary information. Math Geol 30(1):57–76

Chilès JP, Delfiner P (2012) Geostatistics: modeling spatial uncertainty, 2nd edn. Wiley, New York

Chilès JP, Gable R (1984) Three-dimensional modelling of a geothermal field. In: Verly G, David M, Journel AG, Maréchal A (eds) Geostatistics for natural resources characterization. Reidel, Dordrecht, pp 587–598

Christakos G (1992) Random field models in earth sciences. Academic, San Diego

Christakos G, Thesing GA (1993) The intrinsic random-field model in the study of sulfate deposition processes. Atmos Environ Part A Gen Top 27(10):1521–1540

de Fouquet C (1994) Reminders on the conditioning kriging. In: Armstrong M, Dowd PA (eds) Geostatistical simulations. Kluwer, Dordrecht, pp 131–145

Dimitrakopoulos R (1990) Conditional simulation of intrinsic random functions of order $k$. Math Geol 22(3):361–380

Dong A, Ahmed S, Marsily G de (1990) Development of geostatistical methods dealing with the boundary conditions problem encountered in fluid mechanics of porous media. In: Guérillot D, Guillon O (eds) 2nd European conference on the mathematics of oil recovery. Edition Technip, Paris, pp 21–30

Emery X (2010) Multi-Gaussian kriging and simulation in the presence of an uncertain mean value. Stoch Environ Res Risk Assess 24(2):211–219

Emery X, Arroyo D, Porcu E (2016) An improved spectral turning-bands algorithm for simulating stationary vector Gaussian random fields. Stoch Environ Res Risk Assess 30(7):1863–1873

Emery X, Lantuéjoul C (2006) TBSIM: a computer program for conditional simulation of three-dimensional Gaussian random fields via the turning bands method. Comput Geosci 32(10):1615–1628

Emery X, Lantuéjoul C (2008) A spectral approach to simulating intrinsic random fields with power and spline generalized covariances. Comput Geosci 12(1):121–132

Gneiting T, Kleiber W, Schlather M (2010) Matérn cross-covariance functions for multivariate random fields. J Am Stat Assoc 105(491):1167–1177

Haas A, Jousselin C (1976) Geostatistics in petroleum industry. In: Guarascio M, David M, Huijbregts C (eds) Advanced geostatistics in the mining industry. Springer, Dordrecht, pp 333–347

Huang C, Yao Y, Cressie N, Hsing T (2009) Multivariate intrinsic random functions for cokriging. Math Geosci 41(8):887–904

Kitanidis PK (1999) Generalized covariance functions associated with the Laplace equation and their use in interpolation and inverse problems. Water Resour Res 35(5):1361–1367

Lantuéjoul C (2002) Geostatistical simulation: models and algorithms. Springer, Berlin

Madani N, Emery X (2017) Plurigaussian modeling of geological domains based on the truncation of non-stationary Gaussian random fields. Stoch Environ Res Risk Assess 31:893–913

Maleki M, Emery X (2017) Joint simulation of stationary grade and non-stationary rock type for quantifying geological uncertainty in a copper deposit. Comput Geosci 109:258–267

Matheron G (1973) The intrinsic random functions and their applications. Adv Appl Probab 5:439–468

Pardo-Igúzquiza E, Dowd PA (2003) IRFK2D: a computer program for simulating intrinsic random functions of order $k$. Comput Geosci 29(6):753–759

Suárez Arriaga MC, Samaniego F (1998) Intrinsic random functions of high order and their application to the modeling of non-stationary geothermal parameters. In: Twenty-third workshop on geothermal reservoir engineering. Technical report SGP-TR-158, Stanford University, Stanford, pp 169–175