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**Abstract**

This paper concerns the second order marginals of biphased random media. We give discriminating necessary conditions for a bivariate function to be such a valid marginal, and illustrate our study with two practical applications: (1) the spherical variograms are valid indicator variograms if and only if they are multiplied by a sufficiently small constant, which upper bound is estimated, and (2) not every covariance/indicator variogram can be obtained with a Gaussian level set. The theoretical results backing this study are contained in a companion paper.

## 1 Introduction

A random geometric structure is sometimes modelled as a bi-phased medium in the euclidean space. Its low order characteristics, such as fraction volume, variogram, or covariance, although far from containing a total description of the model, provide interesting features on the microscopic regularity of the set boundary, as well as on its long range dependency. Characterising the class of second order marginals is an old problem going back to the 50's, with applications in telecommunications, materials sciences, geostatistics, and marginal problems in general are present under different occurrences in fields as various as quantum mechanics, computer science, game theory; see the surveys [20] or [4] . Experts from these fields have contributed valuable necessary or sufficient conditions for a function to be admissible, still a deep understanding of the problem is unavailable. Our purpose is to provide improvements to the existing methods for checking the admissibility of a second-order characteristic, and illustrate it with practical examples. Related theoretical results are proved in [9].

The two point covering function of a random set $X$ contained in an ambient space $E$ is defined as

$$p^X_{x,y} = \mathbf{P}(x, y \in X), \quad x, y \in E.$$

If $E = \mathbb{R}^d$ and $X$ is *stationary*, meaning its law is invariant under the action of translations, the covariance can be factorized

$$p^X_{x,y} =: \bar{p}^X_{x-y} = \mathbf{P}(0, x - y \in X), \quad x, y \in E.$$

The precise notion of a random set, evasive in most of the applied literature, is of no importance in this paper because we are only interested in combinatorial properties of the marginals, and leave aside regularity issues. Thus we call random set here a Borel random element of the subsets of $E$, endowed with the pointwise convergence topology. Most of the study is conducted in a discrete, or even finite, ambient set $E$. The indicator function of a random set is a $\{0,1\}$-valued random field, sometimes referred to as a *binary field*. Any other sufficiently rich framework (e.g. random closed sets, see [17], or random measurable sets, see for instance [6]), would do.

The central question here is the inverse *realisability* problem, given a bivariate function $\{p_{x,y}\}$ in the class $\mathscr{F}_E$ of symmetric functions on $E$, whether it can be realised by some random set $X$ ( i.e. $p = p^X$), or the equivalent problem if one is interested in another second order marginal, such as the *covariance*, the *geometric variogram*, the *indicator variogram*, or the *unit covariance* (see below); it is for instance necessary that $p$ is semi-definite positive, but insufficient. Since $p^X_{x,y} = \mathbf{E}\mathbf{1}_{\{x\in X\}}\mathbf{1}_{\{y\in X\}}$, the problems of characterising covariances and two point covering functions are closely related, therefore both these problems are referred to as the *covariance realisability problem*. The problem is also called the $S^2$ problem in materials science. This study can serve many purposes, especially in modelisation; one needs to know admissibility conditions to propose and use new models of covariances. In reconstruction and estimation, one should test whether the estimated/reconstructed covariance indeed corresponds to a random structure (see [8]).

The *realisability* problem seems to have deep combinatorial roots, which substance remains elusive after several decades. In a recent paper [10] and the forthcoming paper [7], it is made clear that this problem can be uncoupled in two independent problems, referred to as the *positivity problem*, and the *regularity problem*. The regularity problem, treated for random sets in [7], is not addressed here. The positivity problem, central in this paper, is about the compatibility of a candidate $p$ with the algebraic properties of a set covariance, and is of combinatorial nature.

This problem has been posed by McMillan [16] in the field of telecommunications. It is more or less implicit in many articles, and has been to the author's knowledge first addressed directly by Shepp [19], and more recently by Quintanilla [18]. A series of works by Torquato and his coauthors (see [8] and [20, Sec. 2.2] and references therein), in the field of materials science, gather known necessary conditions and illustrate them in many 2D and 3D theoretical models. This question was developed alongside in the field of geostatistics; Matheron [15] has found via arithmetic considerations a wide class of necessary conditions, that he has proven to be sufficient if $E$ has cardinality less or equal to 5, and he has conjectured these conditions to be sufficient for any finite $E$. This conjecture is disproved in the companion paper [9]. Other authors do not attack frontally this question, but address the realisability problem within some particular classes of models, e.g. Gaussian, mosaic, or boolean model (see [1, 3, 11, 14]).

Depending on the community, the problem has different formulations, in function of the second order marginal of interest. Section 2 recalls the relations between those marginals. Section 3 focuses on the mathematical problem of testing a candidate second order marginal, giving an algorithm able to efficiently discard non-valid marginals. The method is illustrated in Section 4 with the Gaussian model and the spherical variograms.

# 2 Formulations of the problem

Let $E$ be a set and endow the class of its subsets with the $\sigma$-algebra generated by the mappings $A \subset E \mapsto \mathbf{1}_{\{x \in A\}}, x \in E$. An important part of the paper focuses on finite $E = [N] = \{1, \dots, N\}$ for some $N \geq 1$. Denote by $\tilde{X} : x \mapsto \mathbf{1}_{\{x \in X\}}$ the random indicator function of $X$. The two point covering function $p^X$ of $X$ is also defined as

$$p^X_{x,y} = \mathbf{E}\tilde{X}_x\tilde{X}_y.$$

Function $p^X$ lives in the space $\mathscr{F}_E$ of symmetric functions on $E$. Call $\mathscr{C}_E = \{p^X; X \subseteq E \text{ random set}\} \subset \mathscr{F}_E$ the class of realisable functions.

**Remark 2.1.** It is clear, as $p^X$ is the two point covering function of a random process, that $\mathscr{C}_E \subset \mathscr{P}_E \subset \mathscr{F}_E$, where $\mathscr{P}_E$ is the convex cone of semi-definite positive functions, meaning

$$\sum_{i,j=1}^{q} p^X_{x_i,x_j} h_i h_j \geq 0$$

for every $q \geq 1$, $q-$tuple of points $(x_1, \dots, x_q)$ of $E$, and vector $h \in \mathbb{R}^q$. Thus an example of a necessary condition for a function $p_{x,y}$ to be realisable is its semi-definite positiveness.

## 2.1 Second order marginals

Other second order characteristics of random sets can be found in the literature. With the same notation define for $x, y \in E$

$$\begin{aligned} \gamma^X_{x,y} &= \frac{1}{2}\mathbf{E}(\tilde{X}_x - \tilde{X}_y)^2 = \frac{1}{2}\mathbf{P}(\tilde{X}_x \neq \tilde{X}_y) \quad \text{the } \textit{indicator variogram} \text{ of } X, \\ \rho^X_{x,y} &= 1 - 4\gamma^X_{x,y} \quad \text{the } \textit{unit covariance} \text{ of } X. \end{aligned} \tag{2.1}$$

The function $\rho^X$ takes on a special combinatorial interest because, if one defines the random field

$$Y^X_x = \begin{cases} 1 \text{ if } x \in X, \\ -1 \text{ if } x \notin X, \end{cases} = 2\tilde{X}_x - 1,$$

$\rho^X_{x,y} = \mathbf{E}Y^X_x Y^X_y$. Defining $\mathscr{F}^c_E = \{f \in \mathscr{F} : f(x,x) = c; x \in E\}$ for $c = 0$ or 1, the class $\mathscr{V}_E$ of realisable variograms is contained in $\mathscr{F}^0_E$, the class $\mathscr{U}_E$ of realisable unit covariances is contained in $\mathscr{F}^1_E$. An alternative definition of $\mathscr{U}_E$ is as the class of the covariances of random functions taking values in $\{-1,1\}$; it implies that $\mathscr{U}_E$, like $\mathscr{C}_E$, is contained in $\mathscr{P}_E$.

The two problems are fundamentally the same, and some geostatisticians seek to determine which functions $\{\gamma_x\}$ are valid models of indicator variograms. The "unit field formulation" is preferred in [15, 18, 19]. The natural symmetry of the set $\{-1,1\}$ confers to this version a more handy combinatorial structure, and is exploited in the companion paper [9] to give theoretical realisability results, transferred in this paper to other marginals.

**Remark 2.2** (centred marginals)**.** Other versions of these functionals where the first order marginal is subtracted are also used, such as the proper covariance $\mathbf{E}(\tilde{X}_x - \mathbf{E}\tilde{X}_x)(\tilde{X}_y - \mathbf{E}\tilde{X}_y)$, but they only complicate the already difficult realisability problem, and our findings can be passed on to centred marginals.

In the light of (2.1), the class of indicator variograms can be paired up with that of unit covariances, while two point covering functions, covariances and geometric variograms (see Sec. 4) form another group in the literature treating of second order marginals. The relations between these two families are precised below. There is a one-to-one mapping

$$\begin{aligned}\Phi_{\mathscr{V}\to\mathscr{U}} : \mathscr{F}_E^0 &\mapsto \mathscr{F}_E^1\\ \gamma &\mapsto \rho = 1 - 4\gamma\end{aligned}$$

that maps indicator variograms to unit covariances. The relation with the covariances is more subtle. Since for a random set $X$, $\rho^X_{x,y} = \mathbf{E}Y_xY_y$ where $Y = 2\tilde{X} - 1$, it is clear that the two point covering function of $X$ and its unit covariance are related through

$$\rho^X_{x,y} = 4p^X_{x,y} - 2(p^X_{x,x} + p^X_{yy}) + 1.$$

It is on the converse not possible to pass directly from $\rho^X$ to $p^X$. This can be understood by noting that $\rho^X = \rho^{X^c}$ but $p^X \neq p^{X^c}$ where $X^c$ is the complementary of $X$, thus a given unit covariance might correspond to different covariances. There is no canonical way to pass from two point covering functions to unit covariances, so we give below the method proposed in [15]. We introduce an exterior point $x_0 \notin E$ and put $E' = E \cup \{x_0\}$.

Let $X$ be a random set, and $p^X \in \mathscr{C}_E$ its two point covering function. Define $X' = \{x_0\} \cup X$. The unit covariance $\rho^{X'}$ of $X'$ is

$$\rho^{X'}_{x,y} = \Phi_{\mathscr{C}\to\mathscr{U}}(p^X)_{x,y} := \begin{cases} 4p^X_{x,y} - 2(p^X_{x,x} + p^X_{y,y}) + 1 \text{ if } x, y \neq x_0 \\ 2p^X_{yy} - 1, \text{ if } x = x_0, y \in E \\ 1 \text{ if } x = y = x_0. \end{cases} \tag{2.2}$$

Let reciprocally $\rho^{X'}$ be the unit covariance of a random set $X' \subseteq E'$. Defining

$$X'' = \begin{cases} X' \text{ if } x_0 \in X' \\ (X')^c \text{ if } x_0 \notin X' \end{cases}$$

yields $\rho^{X''} = \rho^{X'}$, thus we can assume without loss of generality that $x_0 \in X'$ a.s. Define $X = X' \cap E = X' \setminus \{x_0\}$. Then the two point covering function of $X$ can be obtained by reversing (2.2), explicitly for all $x, y \in E$,

$$p^X_{x,y} = \frac{1}{4}(\rho^{X'}_{x,y} + 1 + \rho^{X'}_{x_0,y} + \rho^{X'}_{x_0,x}) = (\Phi^{-1}_{\mathscr{C}\to\mathscr{U}}(\rho^{X'}))_{xy}.$$

**Remark 2.3.** The bijection between $\mathscr{U}_{E'}$ and $\mathscr{C}_E$ corresponds to the transformation $X' = X \cup \{x_0\}$. There are many other ways to pass from covariances to unit covariances, one can for instance impose that the law of $\tilde{X}'_{x_0}$ is that of a Bernoulli variable with parameter $p$ for every $p \in [0,1]$, but the construction is slightly more complicated.

**Proposition 2.4.** *We have the following relations between $\mathscr{C}_E, \mathscr{U}_E$ and $\mathscr{V}_E$. Assume that $x_0$ is a fixed point external to $E$, and $E' = E \cup \{x_0\}$. We have*

$$\mathscr{U}_E = \Phi_{\mathscr{V}\to\mathscr{U}}(\mathscr{V}_E), \qquad \mathscr{V}_E = \Phi_{\mathscr{U}\to\mathscr{V}}(\mathscr{U}_E),$$
$$\mathscr{U}_{E'} = \Phi_{\mathscr{C}\to\mathscr{U}}(\mathscr{C}_E), \qquad \mathscr{C}_E = \Phi_{\mathscr{U}\to\mathscr{C}}(\mathscr{U}_{E'})$$

*where $\Phi_{\mathscr{V}\to\mathscr{U}} : \mathscr{F}^1_E \mapsto \mathscr{F}^0_E$ and $\Phi_{\mathscr{C}\to\mathscr{U}} : \mathscr{F}_E \mapsto \mathscr{F}^1_{E'}$ are the one-to-one affine mappings described above, and $\Phi_{\mathscr{U}\to\mathscr{V}} = \Phi^{-1}_{\mathscr{V}\to\mathscr{U}}, \Phi_{\mathscr{U}\to\mathscr{C}} = \Phi^{-1}_{\mathscr{C}\to\mathscr{U}}$. If $E = [N]$ for $N \geq 1$, identify $E' = [N+1]$.*

For $\mathsf{u}, \mathsf{v}$ two real functions on $E$, denote by $(\mathsf{u} \otimes \mathsf{v})_{x,y} = \mathsf{u}_x \mathsf{v}_y, x, y \in E$, their tensor product. Marginals of central theoretic importance are the deterministic ones, namely the $p^A = \tilde{A} \otimes \tilde{A}$ for $A \subseteq E$ deterministic, and the corresponding deterministic unit covariances $\rho^A = (2\tilde{A} - 1) \otimes (2\tilde{A} - 1)$. The deterministic variograms are the $\gamma^A = \Phi_{\mathscr{U}\to\mathscr{V}}(\rho^A) = \frac{1}{4}(1 - \rho^A) \in \mathscr{V}_E, A \subset E$.

The following theorem unveils the convex structure of the class of valid second order marginals.

**Theorem 2.5.** *(i)$\mathscr{C}_E$ (resp. $\mathscr{V}_E$) is a convex subset of $\mathscr{F}_E$ which extreme points are the deterministic two point covering functions $p^A$ for $A \subset E$ (resp. the deterministic variograms $\gamma_A, A \subset E$). (ii) If $E = [N], N \geq 1$, call $d_N = \frac{N(N+1)}{2}$. Then $\mathscr{V}_E$ has inner dimension $d_N$, and $\mathscr{C}_E$ has inner dimension $d_{N+1}$. Every valid variogram (resp. valid two point covering function) can be realised by a random set taking at most $d_N + 1$ (resp. $d_{N+1} + 1$) different values.*

*Proof.* It is proved in the companion paper [9] that $\mathscr{U}_E$ is convex, that its extreme points are the $\mathsf{u} \otimes \mathsf{u}$ for $\mathsf{u} \in \{-1, 1\}^E$, and that furthermore if $card(E) = N \geq 1$ there are exactly $2^{N-1}$ extreme points and $\mathscr{U}_N$ has inner dimension $d_N$. The isomorphisms $\Phi_{\mathscr{U}\to\mathscr{V}}$ and $\Phi_{\mathscr{U}\to\mathscr{C}}$ yield the announced conclusions for $\mathscr{V}_E$ and $\mathscr{C}_E$.

Similarly, the last statement is a direct consequence of Prop. 1.4 in [9], itself an application of the Minkowski-Carathéodory Theorem. □

**Remark 2.6.** Algorithms yielding a simplex of $d_N + 1$ points containing a realisable unit covariance $\rho$ provide a reconstruction algorithm for a structure with given unit covariance $\rho$, see [22] Sec. 1.6 and references therein. Still the obtained model completely lacks structure and geometrical meaning, and such a naive approach is probably useless for applications.

Still it is proved in the forthcoming paper [7] that one can control the mean perimeter of the obtained set via its second order marginals, giving a geometric substance to the model, therefore such a constrained reconstruction algorithm could be fruitful.

If $E$ is finite with cardinal $N \geq 1$, a function $p_{x,y}$ is sometimes identified with the $N \times N$ matrix $(p_{x_i,x_j})_{1\leq i,j\leq N}$, $\{x_i;\ 1 \leq i \leq N\}$ being an enumeration of $E$. The following theorem enlightens the way the realisability problem should be posed in a discrete setting.

**Theorem 2.7.** *Let $N \geq 1$. Given a $N \times N$ matrix $\Sigma$ with only 0's on the diagonal, for $s > 0$ sufficiently small, $I + s\Sigma \in \mathscr{U}_N$ is realisable in $E = [N]$ as a unit covariance, and $-s\Sigma \in \mathscr{V}_N$ is realisable as a variogram. Calling $s_c(\Sigma) > 0$ the critical value such that $I + s\Sigma \in \mathscr{U}_N$ and $\frac{-s}{4}\Sigma \in \mathscr{V}_N$ if and only if $s \leq s_c(\Sigma)$, we have $s_c(\Sigma) \geq \frac{2}{\pi}\|\Sigma\|_2^{-1}$, where $\|\cdot\|_2$ is the Euclidean norm for matrices.*

*Proof.* It is proved in Prop. 4.2 that if $\Lambda$ is a semi-definite positive matrix with 1's on the diagonal and entries in $[-1, 1]$,

$$\rho_{x,y} = \frac{2}{\pi}\arcsin(\Lambda_{x,y}), x, y \in E$$

is a realisable unit covariance (realised by the 0 level set of a centred Gaussian process on $E$ with covariance $\Lambda$). Given $\Sigma$ semi-definite positive, the strategy here is to write

$$I + s\Sigma = \frac{2}{\pi}\arcsin(\Lambda)$$

for some such $\Lambda$, hence verifying for $x, y \in E$,

$$\Lambda_{x,y} = \begin{cases} 1 \text{ if } x = y \\ \sin(\frac{\pi}{2}s\Sigma_{x,y}) \text{ otherwise.} \end{cases}$$

Let us prove that for $s$ small, $\Lambda$ so defined is semi-definite positive. We have for any vector $h = (h_x)_{x\in E}$

$$\begin{aligned}\sum_{x,y\in E}\Lambda_{x,y}h_xh_y &= \sum_{x\in E}h_x^2 + \sum_{x\neq y}\Lambda_{x,y}h_xh_y \geq \sum_{x\in E}h_x^2 - \sqrt{\sum_{x\neq y}\Lambda_{x,y}^2}\sqrt{\sum_{x\neq y}h_x^2h_y^2} \\ &\geq \sum_{x\in E}h_x^2 - \sqrt{\sum_{x\neq y}\sin\left(\frac{\pi}{2}s\Sigma_{x,y}\right)^2}\sum_{x\in E}h_x^2 \geq \sum_{x\in E}h_x^2\left(1 - s\frac{\pi}{2}\sqrt{\sum_{x\neq y}\Sigma_{x,y}^2}\right)\end{aligned}$$

by the Cauchy-Schwarz inequality. Hence if $s \leq \frac{2}{\pi}\|\Sigma\|_2^{-1}$, $\Lambda$ is semi-definite positive, and therefore $I + s\Sigma$ is a valid unit covariance, and in virtue of (2.1), $\frac{1}{4}(I - (I + s\Sigma)) = \frac{-s}{4}\Sigma$ is a valid indicator variogram.

$\square$

Finding precisely this value is not possible in general because one cannot characterise completely $\mathscr{U}_N$, but we give in Section 3 a heuristic procedure to estimate it, and illustrate it in Section 4 on the spherical variograms.

## 2.2 Stationarity and Isotropy

In most of the literature about random structures, models are assumed to be stationary and/or isotropic. If $X$ is a random subset of $\mathbb{R}^d$, $X$ is said to be stationary - or homogeneous - if its law is invariant under translations, and isotropic it its law is invariant under rotations. A second order marginal $\{\alpha_{x,y}^X\}$ of $X$ (covariance, indicator variogram, or two point covering function) then factorizes to a simpler form denoted $\bar{\alpha}^X$ on a smaller space $H$ :

$$\begin{aligned} \overline{\alpha}_x^X &= \alpha_{0,x}^X, x \in H = \mathbb{R}^d, \text{ if } X \text{ is stationary, with } \alpha_{x,y}^X = \overline{\alpha}_{x-y}^X, \\ \overline{\alpha}_r^X &= \alpha_{0,ru}^X, r \in H = \mathbb{R}_+, \text{ if } X \text{ is stationary and isotropic, with } \alpha_{x,y} = \overline{\alpha}_{\|x-y\|}, \end{aligned} \tag{2.3}$$

where $u$ is some unit vector of $\mathbb{R}^d$. The realisability problem is therefore posed in this terms for $\bar{\alpha}$.

**Theorem 2.8.** *A function $\overline{\alpha}$ on $H$ is the reduced covariance of a stationary (and/or isotropic) random set if and only if $\alpha$ defined by (2.3) is realisable.*

The proof of Th. 2.8, as well as more general statements, can be derived from Th. 2.13 in [10]. Under this form, the problem of characterising numerically stationary covariances is the same without stationarity. Nevertheless it might be possible to take advantage of the special Toeplitz form of stationary field covariances to make efficient computations, for instance by imbedding it in a circulant matrix, as it has been made in [21, 2]. For the same reasons, the numerical complexity of the problem reduces since the dimension of the space where live stationary covariances is smaller, but the combinatorial symmetry is lost, thus there is no gain on the theoretical point of view.

# 3 Checking realisability numerically and Matheron's conjecture

## 3.1 A heuristic for checking Matheron's conditions

Matheron formulated necessary conditions for an indicator variogram $\gamma$ on $E$ to be admissible, namely $\gamma$ must satisfy

$$\sum_{i,j=1}^{q} \varepsilon_i \varepsilon_j \gamma_{x_i,x_j} \leq 0 \tag{3.1}$$

for every $\varepsilon \in \{-1,0,1\}^N$ such that $\sum_i \varepsilon_i = 1$, and $x_1, \ldots, x_q \in E$. It is acknowledged in the literature that they are hard to check in practice (see [8] for a heuristic approach). The unique condition used in practice for proving the non-validity of some indicator variogram is the so-called *triangular inequality*

$$\gamma_{x,z} \leq \gamma_{x,y} + \gamma_{y,z}, \quad x, y, z \in E,$$

that arises from (3.1) by specialising for $q = 3, (x_1, x_2, x_3) = (x, y, z), \varepsilon = (1, -1, 1)$. See Markov [13] for a discussion of this inequality and its consequences. This condition implies for instance that a valid variogram in a continuous medium must have a cusp at the origin (see [11, 8]). Authors have been able to discard for instance the *Gaussian variogram* $\gamma_{x,y} = 1 - \exp(-\|x - y\|^2)$ ([11] p. 27) as a valid indicator variogram. We claim here that in a discrete setting it is more convenient to characterise realisability in terms of the unit covariance $\rho = 1 - 4\gamma$. Assume that $N = card(E) < \infty$ and call *unitary vector* some $\mathsf{e} \in \mathbb{Z}^N$ such that there exists $\mathsf{u} \in \{-1, 1\}^N$ satisfying $\sum_i \mathsf{e}_i \mathsf{u}_i = 1$. Call $\mathcal{E}_N$ the class of unitary vectors. It is proved in the companion paper (with numeric computations) that the conditions

$$\sum_{i,j} \rho_{x_i,x_j} \mathsf{e}_i \mathsf{e}_j \geq 1 \qquad \mathsf{e} \in \mathcal{E}_N, \tag{3.2}$$

are necessary for the realisability of $\rho$ (and hence of $\gamma$), and sufficient if $N \leq 6$. The advantage of using instead the conditions (3.2) is twofold:

1. Due to spectral considerations, it is easier to check than (3.1) (see Th. 3.1 and the heuristic below).

2. Conditions (3.2) are more discriminant. Indeed, conditions (3.1) only characterise the positive convex cone generated by 0 in $\mathscr{V}_N$, while (3.1) delimit a compact convex set. The new conditions involve the $\mathsf{e}$ such that $\sum_i \mathsf{u}_i \mathsf{e}_i = 1$ for unitary $\mathsf{e}$ such that $\sum_i \mathsf{e}_i \neq 1$.

**Theorem 3.1.** *Take $\rho \in \mathscr{F}_N^1$ a non-singular symmetric matrix. If $\rho$ is not definite positive, then it is not realisable. Otherwise, call $\lambda > 0$ its smallest eigenvalue. Then $\rho$ verifies (3.2) for every $\mathsf{e} \in \mathcal{E}_N$ if and only if it satisfies them only for $\mathsf{e} \in \mathcal{E}_N$ such that*

$$\sum_i \mathsf{e}_i^2 < \lambda^{-1}. \tag{3.3}$$

*Proof.* For any $\mathsf{e} \in \mathbb{Z}^N$, we have

$$\sum_{ij} \rho_{ij} \mathsf{e}_i \mathsf{e}_j \geq \lambda \|\mathsf{e}\|_2^2.$$

Thus (3.2) is automatically fulfilled if $\|\mathsf{e}\|^2 \geq \lambda^{-1}$. □

At this stage the number of conditions to effectively check in (3.2) for a non-singular symmetric matrix is finite, even though the number depends on the smallest eigenvalue $\lambda$ of

$\rho$. Still if $\lambda$ is very small, this number might explode. The heuristic procedure below can help find $\mathsf{e}$ more likely to fail (3.2). Real data more often concerns non-singular matrices; still the singular case is treated in Th. 3.2 .

**Theorem 3.2.** *Assume $\rho \in \mathscr{F}_N^1$ has rank $r < N$, and let $\sigma \in \mathscr{F}_r^1$and $I \subseteq [N]$ with $card(I) = r$ be such that $\sigma = (\rho_{ij})_{ij \in I}$ is non-singular. Then for $k \notin I$, the $k$-th line $L_k$ of $\rho$ can be written as a linear combination*

$$L_k = \sum_{i \in I} \alpha_i^k L_i$$

*of the lines $L_i, i \in I$. Then $\rho$ satisfies conditions (3.2) if and only if $\sigma$ satisfies them with $N = r$ and for $i, j \in [N]$*

$$\rho_{ij} = \sum_{k,q \in I} \alpha_k^i \alpha_q^j \rho_{kq}. \tag{3.4}$$

*where $\alpha_k^i := \delta_{k=i}$ if $k \in I$.*

*Proof.* Assume that $\rho$ is realisable by a random field $Y \in \{-1, 1\}^N$. Then $\sigma$ is realisable as the covariance of the unit field $Y_I = \{Y_i;\, i \in I\}$ that furthermore satisfies for $k \notin I, j \in [N]$,

$$\mathbf{E} Y_j (Y_k - \sum_{i \in I} \alpha_i^k Y_i) = \rho_{kj} - \sum_{i \in I} \alpha_i^k \rho_{ij} = 0,$$

summing up with the proper coefficients yields

$$\mathbf{E}(Y_k - \sum_{i \in I} \alpha_i^k Y_i)^2 = 0$$

and $Y_k = \sum_{i=1}^N \alpha_i^k Y_i$ a.s., $k \notin I$. Condition (3.4) follows easily.

If conversely $\sigma$ is realisable by a unit field $Y_I \in \{-1, 1\}^I$, then if one defines

$$Y_k = \sum_{i \in I} \alpha_k^i Y_i$$

for $k \notin I$, $\rho_{kj}$ defined by (3.4) satisfies $\rho_{kj} = \mathbf{E} Y_k Y_j$ for $k, j \in [N]$. □

## 3.2 Heuristic algorithm

The following algorithm can be used to apply (3.2) to a potential unit covariance $\rho$. Its complexity explodes quickly with $N$, the strategy used in Section 4 is to test the realisability of a bidimensional data by sampling a low dimensional restriction $\rho$ and applying the following procedure.

1. If $\rho$ is not singular, extract a singular matrix $\sigma$ of $\rho$ with maximal rank $r$ and check that $\rho$ and $\sigma$ satisfy the assumptions of Th. 3.2. Then continue the algorithm with $N = r, \rho = \sigma$.

2. Define a cut-off value $\mu > 0$ and compute the $q$ smallest eigenvalues $\lambda = \lambda_1 \leq \cdots \leq \lambda_q \leq \mu$.
3. Introduce the $q$-dimensional space $V_\mu$ spanned by eigenvectors associated to $\lambda_1, \ldots, \lambda_q$. Find by optimisation procedures the unitary vectors $\mathsf{e} \in \mathcal{E}_N$ as close of $V_\lambda$ as possible, and such that $\sum_i \mathsf{e}_i^2$ is small (at least smaller than $\lambda^{-1}$).
4. If one of those $\mathsf{e}$ fails (3.2), then $\rho$ is not realisable.

We know that for $v \in V_\mu$, we have

$$\lambda_1 \leq \frac{v\rho v^T}{\|v\|_2^2} \leq \mu.$$

In view of (3.3), the cut-off value $\mu$ need not be taken larger than 1/4 because $\sum_i \mathsf{e}_i^2 < 4$ implies that $\mathsf{e} \in \mathcal{E}_N$ has at most three non-zero components; in this case (3.2) is reduced to the triangular inequality, which can be checked by other means (see for instance [13]). This heuristic is illustrated in Section 4 to study the realisability of the circular variogram.

# 4 Spherical variograms and Gaussian level sets

This section focuses on two particular models widely used in the literature; the Gaussian level sets and the spherical variograms. We apply the work of the previous sections to establish two facts: (1) the circular and spherical variograms are not valid indicator variograms if multiplied by a too large constant, for which we give an upper bound, and (2) some admissible covariances and indicator variograms cannot be realised by Gaussian models.

## 4.1 Spherical variograms

Spherical variograms are among the most popular models used to fit experimental samples of geostatistical data. It is a recurrent question to know wether such a variogram can be used as a valid indicator variogram for a stationary model (see [11], p. 28). Emery [3] proved that indicator variograms of the most popular families of geometric models (boolean models, Gaussian models, Poisson mosaics) do not in general provide an indicator variogram under the spherical form. It does not discard a priori the spherical variograms as admissible variograms. Our study is not model-dependant as we estimate the critical value of the constant by which one can multiply a spherical variogram so that it is realisable at all. Our computations rely on the realisability conditions of Th. 3.1 and the subsequent heuristic.

For $d \geq 1$, denote by $K_d(r)$ the geometric spherical covariogram,

$$K_d(r) = \ell(B_d \cap (B_d + ru)), 0 \leq r \leq 1.$$

where $B_d$ is a ball of $\mathbb{R}^d$ with diameter 1, and $u$ is some unitary vector of $\mathbb{R}^d$. For instance for $d = 2$,

$$K_2(r) = \frac{1}{2}(\arccos(r) - r\sqrt{1-r^2}).$$

Define the spherical variogram by

$$\bar{\gamma}_r^d = \frac{K_d(0) - K_d(r)}{K_d(0)}.$$

For $d = 1$, $\bar{\gamma}^d$ is called the *triangular variogram*, for $d = 2$ the *circular variogram*, and for $d = 3$ the *spherical variogram*. Their expressions can be found in [1] pp. 81-82.

A recurring question in geostatistics [11, 1, 3] is the admissibility of $\bar{\gamma}_d$, up to some multiplicative constant, as the (reduced) indicator variogramof a (stationary) random set. Does there exists a random binary field $\tilde{X} \subseteq \mathbb{R}^d$ such that

$$s\bar{\gamma}_r^d = P(\tilde{X}_0 \neq \tilde{X}_{ru}), r \in [0,1]$$

for every unitary $u$ in $\mathbb{R}^d$, and some constant $s \in [0,1]$ called the *sill*? As is usual in this paper we prefer to study the corresponding unit covariance

$$\bar{\rho}_r^d = 1 - 2s\bar{\gamma}_r^d \in [-1,1].$$

We call $s_{c,d} \geq 0$ the *critical sill* such that $\bar{\rho}_d$ is realisable if and only if $s \leq s_{c,d}$. We have for $r \in [0,1]$

$$\begin{aligned}
\bar{\rho}_r^1 &= 1 - 2sr \\
\bar{\rho}_r^2 &= 1 - \frac{4s}{\pi}\left(\frac{\pi}{2} - \arccos(r) + r\sqrt{1-r^2}\right) \\
\bar{\rho}_r^3 &= 1 - s\left(3r - r^3\right).
\end{aligned}$$

The case of the triangular variogram is quickly settled as for $s = 1$, $\sin(\pi\rho_1(r)/2) = \cos(\pi r)$ is a semi-definite positive function. It follows by (4.4) that the triangular variogram is the indicator variogram of the centred stationary Gaussian field $W$ with covariance $\mathbf{E}W_xW_y = \cos(\pi|x-y|)$ thresholded at the level 0. Therefore $s_{c,1} = 1$.

For higher dimensions, to study numerically the realisability of $\rho^d$, we study for $N \geq 1$ the realisability of its $N^d \times N^d$ restriction matrix

$$\rho_{i,j}^{d,N} = \bar{\rho}^d_{\|x_i - x_j\|}, \quad i \in [N]^d, j \in [N]^d$$

where

$$x_i = ((i_1 - 1)/N, \ldots, (i_N - 1)/N), \quad i \in [N]^d.$$

If $d = 2$ the heuristic described at Section 3 gave the following results.

1. For $s = 0.72$, with $N = 3$, and

$$\mathsf{v} = [1 \quad 0 \quad 1 \quad 0 \quad -1 \quad 0 \quad 1 \quad 0 \quad 1],$$

   we have

$$v\rho^{d,N}v^T = \sum_{i,j=1}^{N} \rho_{i,j}\mathsf{v}_i\mathsf{v}_j < 0,987 < 1,$$

   contradicting (3.2). It implies that $\rho^{2,N}$, and thus $\bar{\rho}^2$, is not a valid indicator variogram.

2. for $s = 0.7$ and $N = 3$, the smallest eigenvalue is $\lambda \sim 0.2370$, meaning finding $\mathsf{e} \in \mathbb{Z}^N$ with odd sum such that $\sum_i e_i^2 \leq [1/\lambda] = 4$ not satisfying (3.2) might turn up difficult.

Thus we have $s_{c,2} < 0.72$ and point 2. might lead us to think that $s_{c,2}$ should not be far from 0.7. At this stage, the only possible way to ensure realisability is to provide directly a model realising $\rho$.

**Remark 4.1.** The uniform sampling scheme $\{x_i;\, i \in [N]^d\}$ is arbitrary. Even though the efficiency of the method should increase as the smallest eigenvalue of $\rho_N$ decreases (letting theoretically the possibility for more vectors $\mathsf{e} \in \mathcal{E}_N$ to be tested), choosing the $x_{i,j}$ more concentrated instead of equally spaced did not give good results.

For $d = 3$, $\rho^{3,8}$ is not of positive type for $s > 0.58$, thus Theorem (3.1) enables us to say that $s_{c,3} \leq 0.58$.

## 4.2 Gaussian level sets covariances

When confronted to a symmetric function $p$ that might be the second order characteristic of some random set, the default strategy is sometimes to associate it with a Gaussian structure, in general a Gaussian process thresholded at a given value (see [3, 11, 20]). This approach might not be successful, therefore a legitimate question is whether it is realisable at all. In other words, are there realisable second-order characteristics that cannot be realised by a Gaussian level set? The aim of this section is to prove that the answer is yes unless $E$ is pathologically small.

A *standard Gaussian field* on $E$ is a collection of random variables $\{W_x;\, x \in E\}$ any linear combination of which is Gaussian and such that $\mathbf{E}W_x = 0$ and $\mathbf{E}W_x^2 = 1$ for $x \in E$ (see [11] or [12] for more details on Gaussian fields) . The covariance function of $W$

$$\Sigma_{x,y} = \mathbf{E}W_xW_y,\ x, y \in E$$

is semi-definite positive. Bochner's theorem states that conversely, given $\Sigma \in \mathscr{F}_E^1 \cap \mathscr{P}$ of positive type, there exists a unique (in law) standard Gaussian field $W^\Sigma$ with covariance $\Sigma$. In this section we consider the random set obtained by thresholding $W^\Sigma$ at some level $z \in \mathbb{R}$

$$X^{\Sigma,z} = \{x \in E : W_x^\Sigma \geq z\}. \tag{4.1}$$

The second order marginals of $X^{\Sigma,z}$ can be found in the literature, see for instance [11].

**Proposition 4.2.** *Let $\Sigma \in \mathscr{P} \cap \mathscr{F}_E^1, z \in \mathbb{R}$. The indicator variogram of $X^{\Sigma,z}$ is*

$$\gamma_{x,y}^{\Sigma,z} := \frac{1}{2\pi} \int_{\Sigma_{x,y}}^{1} \frac{1}{\sqrt{1-r^2}} \exp\left(-\frac{z^2}{1+r}\right) dr, \quad x, y \in E, \tag{4.2}$$

*The two point covering function of $X^{\Sigma,z}$ is*

$$p_{x,y}^{\Sigma,z} := \Phi(z)^2 + \frac{1}{2\pi} \int_{0}^{\Sigma_{x,y}} \frac{1}{\sqrt{1-r^2}} \exp\left(-\frac{z^2}{1+r}\right) dr, \quad x, y \in E, \tag{4.3}$$

*where $\Phi(z) = \int_z^{-\infty} \frac{e^{-r^2/2} dr}{\sqrt{2\pi}}$ is the Gaussian tail function.*

We have in particular a compact expression of the unit covariance if $z = 0$:

$$\rho_{x,y}^{\Sigma,0} := 1 - 4\gamma_{x,y}^{\Sigma,0} = \frac{2}{\pi} \arcsin(\Sigma_{x,y}), \quad x, y \in E. \tag{4.4}$$

*Proof.* Let us call $f_r(u,v), u, v \in \mathbb{R}^2$ the density of a Gaussian vector of $\mathbb{R}^2$ with covariance $r \in [-1, 1]$. Direct computations yield

$$\frac{\partial f_r(u,v)}{\partial r} = \frac{\partial^2 f_r(u,v)}{\partial u \partial v}.$$

We have

$$\begin{aligned}
\gamma_{x,y}^{\Sigma,z} &= \mathbf{P}(W(x) \geq z, W(y) \leq z) = \int_z^{\infty} \int_{-\infty}^{z} f_{\Sigma_{x,y}}(u,v) du dv \\
&= \int_z^{\infty} \int_{-\infty}^{z} \left( f_1(u,v) + \int_{\Sigma_{x,y}}^{1} \frac{\partial f_r(u,v)}{\partial r} dr \right) du dv = 0 + \int_{\Sigma_{x,y}}^{1} \int_z^{\infty} \int_{-\infty}^{z} \frac{\partial^2 f_r(u,v)}{\partial u \partial v} du dv dr \\
&= \int_{\Sigma_{x,y}}^{1} f_r(z,z) dr,
\end{aligned}$$

which proves relation (4.2). (4.3) is obtained in an exactly similar fashion and can also be found as Prop. 16.1.1 in [11]. One can also note that $p_{x,y}^{\Sigma,z} = \mathbf{P}(x, y \in X^{\Sigma,z}) - \gamma_{x,y}^{\Sigma,z} = \Phi(z) - \gamma_{x,y}^{\Sigma,z}$. $\square$

**Theorem 4.3.** *If $card(E) \geq 4$, there exists $p \in \mathscr{C}_N$ that cannot be obtained by thresholding a standard Gaussian field, i.e. that is not under the form (4.3) for some definite positive function $\{\Sigma_{x,y}\}$ and some level $z \in \mathbb{R}$.*

*Proof.* The strategy is to prove that the class of all Gaussian two point covering functions for $card(E) = N = 4$ is not convex, and therefore does not coincide with $\mathscr{C}_E$. The result follows with a restriction argument for $E$ with a larger cardinality. Take $\Sigma^0 \neq \Sigma^1 \in \mathscr{F}_E^1 \cap \mathscr{P}$ the covariances of two standard Gaussian fields, resp. $W^0, W^1$, and consider the random fields $\tilde{X}_0 := \tilde{X}^{\Sigma_0,0}$ and $\tilde{X}_1 := \tilde{X}^{\Sigma_1,0}$ obtained by thresholding resp. $W^0$ and $W^1$ at the level

0. Call $p^i$ the two point covering function of the binary field $\tilde{X}_i$, for $i = 1, 2$. We claim that if $\Sigma^0$ and $\Sigma^1$ have been chosen judiciously, the two point covering function

$$p := \frac{1}{2}(p^1 + p^2) \tag{4.5}$$

is not the two point covering function of a Gaussian level set of the form (4.1). On the other hand, it is the two point covering function of a random set because $\mathscr{U}_E$ is convex. If $X$ is a random set such that $p = p_X$, then $p_{x,x} = p^0_{x,x} = p^1_{x,x} = 1/2$. Thus $p_{x,y} = 1/4 + \frac{1}{2\pi}\arcsin(\Sigma_{x,y})$ for some semi-definite positive matrix $\Sigma$. (4.5) imposes also

$$\arcsin(\Sigma_{x,y}) = \frac{1}{2}\left(\arcsin(\Sigma^0_{x,y}) + \arcsin(\Sigma^1_{x,y})\right).$$

The conclusion follows directly from the following lemma:

**Lemma 4.4.** *It is possible to choose $\Sigma^0, \Sigma^1 \in \mathscr{P} \cap \mathscr{F}^1_4$ such that*

$$\Sigma_{x,y} = \sin\left(\frac{1}{2}(\arcsin(\Sigma^0_{x,y}) + \arcsin(\Sigma^1_{x,y}))\right), x, y \in E,$$

*is not semi-definite positive.*

*Proof.* Defining the Toeplitz matrices

$$\Sigma^0 = \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix} \quad \Sigma^1 = \begin{pmatrix} 1 & \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ \frac{\sqrt{3}}{2} & 1 & \frac{\sqrt{3}}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 1 & \frac{\sqrt{3}}{2} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & 1 \end{pmatrix}$$

gives

$$\Sigma = \begin{pmatrix} 1 & \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} & 1 \end{pmatrix}.$$

which is not of positive type (counter example provided by the user Robert Israel on the mathematical forum mathoverflow.com ).

□

Thus $\Sigma$ cannot be the covariance of a Gaussian field. □

For variograms and unit covariances, one does not have direct access to the first order marginal through the diagonal elements, thus the situation is more subtle but the result still holds if we enlarge $E$ with two elements.

**Theorem 4.5.** *For $N \geq 6$, there exists $\gamma \in \mathscr{V}_N$ such that $\gamma$ is not the indicator variogram of any Gaussian field thresholded at some level $z \in \mathbb{R}$.*

*Proof.* Consider two block-matrices covariances of the form

$$\Lambda^0 = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \Sigma^1 \end{pmatrix}, \quad \Lambda^1 = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \Sigma^2 \end{pmatrix}$$

where $\Sigma^i$ are given by lemma 4.4, and put $\gamma^i = \gamma^{\Lambda_i,0}$. Then $\frac{1}{2}(\gamma^0 + \gamma^1)$ is the variogram of a binary field $X$ such that $\tilde{X}_1 \neq \tilde{X}_2$ a.s.. If $X$ was the level set of a standard Gaussian field $W = W^\Sigma$ at a level $z \in \mathbb{R}$, we would have $W_x > z$ if and only if $W_y < z$ with probability 1, whence necessarily $\Sigma_{1,2} = -1$ and $z = 0$. Then $\Lambda_{x,y} = \sin((1/2)(\arcsin(\Lambda^1_{x,y}) + \arcsin(\Lambda^2_{x,y}))), x, y \in E$, is not semi-definite positive but still it is the covariance matrix of $\Sigma$. Contradiction. □

A similar result holds of course for unit covariances.

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