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IDENTIFIABILITY FOR NON-STATIONARY SPATIAL STRUCTURE

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Abstract

For modelling non-stationary spatial random fields $Z = \{Z(x) : x \in \mathbb{R}^n, n \geq 2\}$ a recent method has been proposed to deform bijectively the index space so that the spatial dispersion $D(x, y) = var[Z(x) - Z(y)]$, $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$, depends only on the Euclidean distance in the deformed space through a stationary and isotropic variogram γ. We prove uniqueness of this model in two different cases: *(i)* γ is strictly increasing; *(ii)* $\gamma(u)$ is differentiable for $u > 0$.

BIJECTIVE SPACE DEFORMATION; DISPERSION FUNCTION; ISOTROPY; STATIONARITY; UNIQUENESS; VARIOGRAM

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1. Introduction

Spatial interpolation or smoothing techniques are used widely in the environmental sciences to estimate a spatial random field at un-monitored locations, or to interpolate data onto a regular grid of points for use in subsequent analyses. Many of these techniques require spatial variogram models in continuous space. Such models are based often on simplifying assumptions (see [3], Chapter 2, for instance), including spatial stationarity or homogeneity where the second order association between pairs of sites is assumed to depend only on the spatial distance between these sites. In environmental applications, factors such as topography, local pollutant emissions, and meteorological influences may cause such assumptions to be violated. This has led to research into modelling heterogeneous (spatially non-stationary) second order structure, as reviewed in [7].

We consider identifiability of the heterogeneous spatial modelling approach proposed by Sampson and Guttorp [15]. They model the spatial dispersion $D(x, y) = \mathrm{var}\,[Z(x) - Z(y)]$ of the spatial random field $Z = \{Z(x) : x \in \mathbb{R}^n, n \geq 2\}$ as a function of Euclidean distance between site locations in a bijective deformation of the geographic coordinate system. The geographic coordinate system is referred to as the G-space, and the deformed coordinate system is known as the D-space, where D stands for dispersion. In the following, we identify both the G-space and the D-space

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as $\mathbb{R}^n$ for simplicity. The model is of the form

$$D(x,y)=\gamma\left(\|\Phi(y)-\Phi(x)\|\right),\ \forall(x,y)\in\mathbb{R}^n\times\mathbb{R}^n, \tag{1.1}$$

where $\|.\|$ represents the classical Euclidean norm in $\mathbb{R}^n$, Φ represents a bijective bi-continuous deformation of the G-space onto the D-space and γ a stationary and isotropic variogram which depends only on the Euclidean distance between sites. When γ is increasing, the deformation effectively stretches the G-space in regions of relatively higher spatial dispersion, while contracting it in regions of relatively lower spatial dispersion, so that a stationary and isotropic variogram can model the dispersion as a function of the distance in the D-space representation. The simplest non-trivial example is an affine bijective deformation $\Phi(x)=Ax$, where A is a regular square matrix and where the principal axes of A determine the geographic directions of greatest and weakest spatial dispersion in this stationary anisotropic model. This is called the case of geometric or elliptical anisotropy in the geostatistics literature. In this paper we use the terminology variogram only when we are referring to stationary and isotropic dispersion models.

When γ is strictly increasing and $n=2$, Meiring [9] proves the uniqueness of both the deformation Φ and the variogram γ, up to a homothetic Euclidean motion for Φ and up to a scaling for γ. Her proof is based on geometrical arguments. This result can be generalized to $n\geq 2$ as indicated in Meiring *et al.* [10]. Using topological properties of metric transforms given by Schœnberg [16], we provide a more concise proof of uniqueness of γ up to scaling, and Φ up to homothetic Euclidean motion in $\mathbb{R}^n$, $n\geq 2$, when γ is strictly increasing and continuous except possibly at the origin.

Many isotropic variogram models are not strictly increasing, including the hole-effect models [3]. Perrin and Senoussi [14] consider deformation models of non-stationary spatial correlation of the form

$$r(x,y)=\rho(\|\Phi(y)-\Phi(x)\|),\ \forall(x,y)\in\mathbb{R}^n\times\mathbb{R}^n, \tag{1.2}$$

where $r(x,y)$ is the spatial correlation between points x and y, and ρ is a stationary and isotropic correlation model which is not necessarily strictly increasing. Under smoothness assumptions on Φ and ρ, they show uniqueness of ρ up to scaling, and Φ up to a homothetic Euclidean motion in $\mathbb{R}^n$, $n\geq 2$. Their proof also is valid if written for spatial dispersion models which may exist when correlations do not. We show that one of the assumptions of [14] is redundant, and thus prove the result of [14] for spatial dispersion models under fewer assumptions. Many commonly used variograms, including the linear, spherical, exponential, Gaussian, power, and hole-effect models described in [3], satisfy the smoothness assumptions. For $n=1$ we refer to Perrin [12] and Perrin and Senoussi [13].

2. Uniqueness

We endow $\mathbb{R}^n$, $n\geq 2$, with the classical Euclidean norm $\|.\|$. Let $\mathcal{G}_n$ be the group of the orthogonal matrices G of dimension n and let $\mathcal{H}_n$ be the group of homothetic Euclidean motions H

$$\mathcal{H}_n=\{H: H(x)=\lambda Gx+b,\ \forall x\in\mathbb{R}^n \text{ with } \lambda>0, G\in\mathcal{G}_n, b\in\mathbb{R}^n\}.$$

When $n = 2$, $\mathcal{H}_n$ is composed with translations, rotations, reflections about a line and homothetic transformations, or any composition of these transformations. Concerning identification of model (1.1) we have the first result.

Proposition 2.1 If (Φ_1, γ_1) *is a solution to (1.1), then for any* H *in* $\mathcal{H}_n$, (Φ_2, γ_2) *with* $\Phi_2 = H \circ \Phi_1$ *and* $\gamma_2(u) = \gamma_1(u/\lambda)$ *is a solution as well.*

Thus, uniqueness of (Φ, γ) can only be discussed at least up to a scaling for γ and up to a homothetic Euclidean motion for Φ. The practical implications of this result are that we can fix the homothetic Euclidean motions of the D-space prior to identifying the D-space coordinates and associated variogram. For $\mathbb{R}^2 \longrightarrow \mathbb{R}^2$ deformations, fixing four coordinates in the G-space will fix translations, homothetic transformations and rotations up to reflections about a line. In higher dimensions, additional constraints are required. For instance, in $\mathbb{R}^3$ we fix two points and constrain a third point to lie in a fixed plane.

We will prove the reverse of proposition 2.1, that is, uniqueness holds exactly up to a scaling for γ and up to a homothetic Euclidean motion for Φ, in two different cases: *(i)* γ is strictly increasing; *(ii)* $\gamma(u)$ is differentiable for $u > 0$.

2.1. *Monotonic case.* We introduce first two definitions drawn from Schœnberg [16] and Von Neumann and Schœnberg [17].

Definition 2.1 A set Ω *endowed with a function* $\delta(x, y)$ *satisfying the following properties for all* $(x, y) \in \Omega^2$

$$\delta(x,y) = \delta(y,x) \geq 0 \quad \textit{and} \quad \delta(x,y) = 0 \Longleftrightarrow x = y$$

is called a semi-metric space.

Consider a continuous function $\tau : \mathbb{R}^+ \to \mathbb{R}^+$ satisfying

$$\textbf{(A)} \quad \tau(u) = 0 \Longleftrightarrow u = 0$$

and define $\delta_\tau(x, y) = \tau(\|y - x\|)$. Therefore according to definition 2.1, $\mathbb{R}^n$ endowed with δ_τ is a semi-metric space. Following Blumenthal [1] we say that

Definition 2.2 $(\mathbb{R}^n, \delta_\tau)$ *is isometrically embeddable in* $\mathbb{R}^m$, $n \leq m < \infty$, *if there is a continuous function* $\Phi : \mathbb{R}^n \to \mathbb{R}^m$ *such that for all* $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$

$$\tau(\|y - x\|) = \|\Phi(y) - \Phi(x)\|.$$

The following theorem in Schœnberg [16] gives the form of τ.

Theorem 2.1 If $(\mathbb{R}^n, \delta_\tau)$, $n \geq 2$, *is isometrically embeddable in* $\mathbb{R}^m$, $n \leq m < +\infty$, *then necessarily*

$$\tau(u) = u/\lambda, \ \lambda > 0, \ \textit{unless} \ \tau(u) \equiv 0.$$

We can now state our first main result about the identification of model (1.1).

Theorem 2.2 If two continuous variograms, γ_1 and γ_2, with γ_1 strictly increasing, and two bijective bi-continuous deformations, Φ_1 and Φ_2, from $\mathbb{R}^n$ onto $\mathbb{R}^n$ give the same dispersion, i.e. if

$$\gamma_1\left(\|\Phi_1(y)-\Phi_1(x)\|\right)=\gamma_2\left(\|\Phi_2(y)-\Phi_2(x)\|\right),\ \forall(x,y)\in\mathbb{R}^n\times\mathbb{R}^n, \tag{2.1}$$

then the variograms are identical up to a scaling, as are the deformations up to a homothetic Euclidean motion.

Proof. Suppose (Φ_1,γ_1) and (Φ_2,γ_2) satisfy (2.1). Setting $\gamma=\gamma_1^{-1}\circ\gamma_2$ and $\Phi=\Phi_1\circ\Phi_2^{-1}$, (2.1) is equivalent to

$$\gamma(\|y-x\|)=\|\Phi(y)-\Phi(x)\|,\ \forall(x,y)\in\mathbb{R}^n\times\mathbb{R}^n. \tag{2.2}$$

It follows from the properties of γ_1 and γ_2 that γ is positive, continuous and meets the condition **(A)**. Therefore Schœnberg's theorem applies and gives $\gamma(u)=u/\lambda$ for some $\lambda>0$. To fix homothetic transformations we may impose $\lambda=1$. So we get $\gamma_1=\gamma_2$ and (2.2) becomes

$$\|y-x\|=\|\Phi(y)-\Phi(y)\|,\ \forall(x,y)\in\mathbb{R}^n\times\mathbb{R}^n.$$

Therefore, Φ is an isometric transformation of the Euclidean space $\mathbb{R}^n$. Thus, there is an orthogonal matrix G and a vector b such that $\Phi(x)=Gx+b$. To fix Euclidean motions we may impose $G\equiv$ *identity* and $b=0$ so that we get $\Phi_1=\Phi_2$.

□

Corollary 2.1 Consider all variograms which are the sum of a continuous variogram and a nugget. If two variograms from this class, γ_1 and γ_2, with γ_1 strictly increasing, and two bijective bi-continuous deformations, Φ_1 and Φ_2, from $\mathbb{R}^n$ onto $\mathbb{R}^n$ give the same dispersion, i.e. if (2.1) holds, then the variograms are identical up to a scaling, as are the deformations up to a homothetic Euclidean motion.

Proof. γ_1 and γ_2 satisfy $\lim_{u\to 0}\gamma_1(u)=\alpha_1\geq 0$ and $\lim_{u\to 0}\gamma_2(u)=\alpha_2\geq 0$. Letting $x\to y$ in (2.1) we obtain $\alpha_1=\alpha_2=\alpha$. Now define $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$ by $\tilde{\gamma}_1(u)=\gamma_1(u)-\alpha$ and $\tilde{\gamma}_2(u)=\gamma_2(u)-\alpha$ for $u>0$, and set $\tilde{\gamma}_1(0)=\tilde{\gamma}_2(0)=0$. Then $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$ are continuous for $u\geq 0$. Therefore, according to theorem 2.2 $\tilde{\gamma}_1=\tilde{\gamma}_2$, so that $\gamma_1=\gamma_2$, and $\Phi_1=\Phi_2$.

□

It follows immediately from a conjecture by Schœnberg [16], proved by Crum [4] (see for instance Gneiting and Sasvári [5]), that the assumption of continuity of the variograms in Theorem 2.2 and Corollary 2.1 (except possibly at zero distance in the Corollary 2.1) may be replaced by the assumption of measurability when second moments exist.

2.2. *Differentiable case.* The first result considers affine deformations and shows that two variograms give the same modelled dispersions for all pairs of locations if and only if the variograms and affine deformations are identical (shown in [10] and included here for completeness). The second result deals with the more general case of a bijective and bi-differentiable deformation, and a variogram γ such that $\gamma(u)$ is differentiable for $u > 0$. The latter result is proved for non-stationary deformation models of spatial correlations in Perrin and Senoussi [14] under an additional assumption, which we prove is redundant.

Lemma 2.1 If two non-constant variograms, γ_1 and γ_2, which are the sum of continuous variograms plus nuggets, and two bijective affine deformations, Φ_1 and Φ_2, give the same dispersions, i.e. if (2.1) holds, then the variograms are identical up to a scaling, as are the deformations up to a homothetic Euclidean motion.

Proof. Consider any distinct points x and y in $\mathbb{R}^n$. Then, by properties of affine mappings and by (2.1), there exists $\lambda(x,y) > 0$ such that

$$\|\Phi_1(w) - \Phi_1(v)\| = \lambda(x,y)\ \|\Phi_2(w) - \Phi_2(v)\|\,, \tag{2.3}$$

and

$$\gamma_1\left(\|\Phi_1(w) - \Phi_1(v)\|\right) = \gamma_2\left(\|\Phi_2(w) - \Phi_2(v)\|\right) = \gamma_2\left(\frac{\|\Phi_1(w) - \Phi_1(v)\|}{\lambda(x,y)}\right)$$

for all v and w collinear with x and y in $\mathbb{R}^n$. Hence, by isotropy of γ_1 and γ_2,

$$\gamma_1(u) = \gamma_2\left(\frac{u}{\lambda(x,y)}\right)$$

for all $u \geq 0$, so γ_1 and γ_2 are identical up to a scaling. Now x and y were any two distinct points, and γ_1 and γ_2 are not constant, hence $\lambda(x,y) = \lambda$ for all x, y. By (2.3), Φ_1 and Φ_2 are identical up to a homothetic Euclidean motion.

□

We suppose now that Φ is a bijective deformation from $\mathbb{R}^n$ onto $\mathbb{R}^n$ and that γ is a variogram, satisfying the following assumptions

(B1) Φ is differentiable in $\mathbb{R}^n$ as is its inverse.
(B2) $\gamma(u)$ is differentiable for $u > 0$.

For any differentiable function $f : (x,y) \in \mathbb{R}^n \times \mathbb{R}^n \longmapsto f(x,y) \in \mathbb{R}$ let J_f denote the Jacobian matrix of f and set

$$\begin{cases} \partial_x f(x,y) &= (\partial_1 f, \ldots, \partial_n f)(x,y) \\ \partial_y f(x,y) &= (\partial_{n+1} f, \ldots, \partial_{n+n} f)(x,y), \end{cases}$$

where $\partial_i f(x,y)$, $i = 1, 2, \ldots, 2n$, denotes the i^{th} first partial derivative of $f(x,y)$.

We now show that, if $\gamma(u)$ is not constant for $u > 0$, **(B1)** and **(B2)** imply linear independence of a set of derivative mapping functions, denoted **(B3)**.

*Lemma 2.2 Assume **(B1)** and **(B2)** hold. If (Φ, γ) is a solution to (1.1), such that $\gamma(u)$ is not constant for $u > 0$, then*

> ***(B3)*** *the set of functions $\{y \neq 0 \longmapsto \partial_j D(0,y), j = 1,2,\ldots,n\}$ is linearly independent.*

Proof. Without loss of generality we may impose, due to proposition 2.1, the restriction that $\Phi(0) = 0$. We denote the first derivative of γ by $\gamma^{(1)}(u)$ for $u > 0$, and let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ be any vector in $\mathbb{R}^n$. We set $\Phi = (\phi_1, \phi_2, \ldots, \phi_n)$ and $\partial_i \Phi(0) = (\partial_i \phi_1, \partial_i \phi_2, \ldots, \partial_i \phi_n)(0)$, $i = 1, 2, \ldots, n$. We have for $x = 0$ and all $y \neq 0$

$$\boldsymbol{\alpha}(\partial_x D(0,y))^t = -\frac{\gamma^{(1)}(\|\Phi(y)\|)}{\|\Phi(y)\|} \sum_{i=1}^{n} \alpha_i \partial_i \Phi(0)(\Phi(y))^t.$$

Suppose $\boldsymbol{\alpha}(\partial_x D(0,.))^t = 0$. Then $\gamma^{(1)}(.) = 0$ or $\sum_{i=1}^{n} \alpha_i \partial_i \Phi(0)(\Phi(.))^t = 0$. The equality $\gamma^{(1)}(.) = 0$ contradicts our assumption concerning γ. Therefore for all $y \neq 0$

$$\sum_{i=1}^{n} \alpha_i \partial_i \Phi(0)(\Phi(y))^t = 0$$

which is equivalent to

$$\sum_{j=1}^{n} \beta_j \phi_j(y) = 0 \tag{2.4}$$

with $\beta_j = \sum_{i=1}^{n} \alpha_i \partial_i \phi_j(0)$, $j = 1, 2, \ldots, n$. Now $J_\Phi(x)$ is nonsingular since $\Phi^{-1}(x)$ exists by **(B1)**. Hence $\{\phi_1, \ldots, \phi_n\}$ are linearly independent. Therefore (2.4) implies necessarily that $\beta_j = 0$, $j = 1, 2, \ldots, n$. For the same reason, it follows that $\alpha_i = 0$, $i = 1, 2, \ldots, n$.

□

Perrin and Senoussi [14] prove identifiability of ρ in model (1.2) up to scaling and Φ up to homothetic Euclidean motion, under the assumptions **(B1)**, and **(B2)** and **(B3)** modified for correlations by replacing γ by ρ and $D(0,y)$ by $r(0,y)$. In Lemma 2.2 we have shown that assumption **(B3)** is redundant. Under fewer assumptions, we now prove the identifiability of γ up to scaling and Φ up to homothetic Euclidean motion.

*Theorem 2.3 Assume **(B1)** and **(B2)** hold. If (Φ, γ) is a solution to (1.1), such that $\gamma(u)$ is not constant for $u > 0$, then it is unique, up to a scaling for γ and up to a homothetic Euclidean motion for Φ.*

Proof. Let (Φ_1, γ_1) and (Φ_2, γ_2) be two solutions to (1.1). Set $\Phi = \Phi_1 \circ \Phi_2^{-1}$. By an analogous argument to that of Perrin and Senoussi [14] (details are provided in the Appendix for referees), it follows that for all $x \neq y$

$$\partial_x D(x,y) J_{\Phi_2}^{-1}(x) = \partial_x D(x,y) J_{\Phi_2}^{-1}(x) J_{\Phi}^{-1}(\Phi_2(y)) J_{\Phi}(\Phi_2(x)),$$

where $J_\Phi(\Phi_2(x)) = J_{\Phi_1}(x) J_{\Phi_2}^{-1}(x)$. When $x = 0$ we obtain

$$\partial_x D(0,y) = \partial_x D(0,y) A_1 J_{\Phi}^{-1}(\Phi_2(y)) A_2, \quad y \neq 0,$$

where $A_1 = J_{\Phi_2}^{-1}(0)$ and $A_2 = J_{\Phi_1}(0)$ are two regular square matrices. It follows from lemma 2.2 that $J_\Phi(\Phi_2(y)) = A = A_2 A_1$ for all $y \neq 0$, *i.e.* $\Phi_1 = A\Phi_2 + b$, where $b \in \mathbb{R}^n$. Without loss of generality we may impose, due to proposition 2.1, the restriction that $\Phi_1(0) = \Phi_2(0) = 0$, that is $b = 0$. Thus, $\Phi = A$ and it follows that $\gamma_2(\|v - u\|) = \gamma_1(\|A(v - u)\|)$ for all $(u, v) \in \mathbb{R}^n \times \mathbb{R}^n$. Therefore, we obtain from lemma 2.1 that necessarily $A = \lambda G$ where $\lambda > 0$ and G is an orthogonal matrix. Consequently, the variograms γ_1 and γ_2 are identical up to a scaling, as are the deformations Φ_1 and Φ_2 up to a homothetic Euclidean motion.

□

3. Discussion

Deformation models for non-stationary spatial second order structure have found application in a number of areas [11], including spatial estimation in air pollution studies [2], monitoring network design [8], and the investigation of the regional representativeness of monitoring locations in terms of second order structure [6]. Practical questions remain regarding identifiability of spatial dispersion models (1.1) fitted to data from finite monitoring networks. However our results suggest asymptotic identifiability of such models when fitted to data from increasingly dense networks of monitoring sites, or to observations from remote sensing studies with increasing spatial resolution. The importance of spatial estimation in environmental studies motivates strongly for further theoretical study of the properties of deformation models and for a characterization of situations when non-stationary spatial dispersion models improve spatial estimation and variability assessment.

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Appendix

In the paper we omit selected steps from the proof of Theorem 2.3, since they are very similar to those in [14] which is submitted for publication elsewhere. These steps are included here to aid the referees of our paper, and would not appear in the final paper.

The notation is different from [14] since we consider spatial dispersions, which may exist even when the spatial correlations considered by [14] do not.

*Theorem 2.3 Assume **(B1)** and **(B2)** hold. If (Φ, γ) is a solution to (1.1), such that $\gamma(u)$ is not constant for $u > 0$, then it is unique, up to a scaling for γ and up to a homothetic Euclidean motion for Φ.*

Proof. Let (Φ_1, γ_1) and (Φ_2, γ_2) be two solutions to (1.1). Set $\Phi = \Phi_1 \circ \Phi_2^{-1}$, and $\Gamma(u,v) = D(\Phi_2^{-1}(u), \Phi_2^{-1}(v))$. Then

$$\Gamma(u,v) = \gamma_2(\|v-u\|) = \gamma_1(\|\Phi(v) - \Phi(u)\|). \tag{3.1}$$

It follows that the following relations hold for all $u \neq v$

$$\begin{cases} \partial_u \Gamma(u,v) & = & -\partial_v \Gamma(u,v) \\ \partial_u \Gamma(u,v) & = & -\partial_v \Gamma(u,v) J_\Phi^{-1}(v) J_\Phi(u), \end{cases}$$

from which we deduce $\partial_u \Gamma(u,v) = \partial_u \Gamma(u,v) J_\Phi^{-1}(v) J_\Phi(u)$. Set $x = \Phi_2^{-1}(u)$ and $y = \Phi_2^{-1}(v)$. Then for all $x \neq y$

$$\partial_x D(x,y) J_{\Phi_2}^{-1}(x) = \partial_x D(x,y) J_{\Phi_2}^{-1}(x) J_\Phi^{-1}(\Phi_2(y)) J_\Phi(\Phi_2(x)),$$

and $J_\Phi(\Phi_2(x)) = J_{\Phi_1}(x) J_{\Phi_2}^{-1}(x)$.

Our proof now continues as provided in the paper, making use of Lemmas 2.1 and 2.2, unlike Perrin and Senoussi who use the result of Lemma 2.2 as an assumption.

□