On the Validity and Identifiability of Spatial Deformation Models for Heterogeneous Spatial Correlation Structure

Peter Guttorp   Wendy Meiring   Paul D. Sampson

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Wendy Meiring[1], Peter Guttorp[2], and Paul D. Sampson[2]

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Corresponding Author:

Dr. Wendy Meiring
Geophysical Statistics Project
National Center for Atmospheric Research
P.O. Box 3000
Boulder, CO, 80307-3000
USA

Phone: (303) 497-1375
Fax: (303) 497 1333
Email: meiring@ucar.edu

[1]Geophysical Statistics Project, National Center for Atmospheric Research, Boulder, Colorado, USA

[2]Department of Statistics, University of Washington, Seattle, Washington, USA

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Abstract

Many environmental processes are heterogeneous in space (spatially non-stationary), due to factors such as topography, local pollutant emissions, and meteorology. Much of the commonly used spatial statistical methodology depends on simplifying assumptions such as spatial isotropy. Violations of these assumptions can cause problems, including incorrect error assessment of spatial estimates. This paper demonstrates important properties of the spatial deformation model of Sampson and Guttorp (1992) and Guttorp and Sampson (1994) for heterogeneous anisotropic spatial correlation structure.

The modeling approach utilizes a deformation of the geographic coordinate space into a new coordinate system (known as the D-space, or D-plane in two dimensions) where isotropic spatial correlation structure is modeled. We provide proofs of two fundamental properties of the model: validity and invariance of the modeled correlations to translating, scaling and rotating operations on a D-space representation. We also prove two identifiability results. We prove first that two non-trivial variograms, and two corresponding affine transformations of the geographic coordinate system yield the same modeled dispersions between all pairs of locations in a region if and only if the variogram models and affine mappings are identical. Second we prove that two strictly increasing D-space variograms and corresponding bijective transformations of the geographic coordinate system yield the same modeled dispersions between all pairs of locations in a region if and only if the variogram models and deformation mappings are identical.

Keywords: Anisotropy, Non-stationary environmental processes, Variogram

1 Introduction

Spatial interpolation techniques are used widely in the geosciences to estimate values of a spatial process at unmonitored locations, or to interpolate data onto a regular grid of points for use in subsequent analyses. Several spatial interpolation techniques assume a known second-order spatial structure. In practice, this structure generally is unknown, and must be estimated. Empirical estimates of a finite number of spatial correlations do not provide a means for estimating the correlation between unmonitored sites, so spatial correlation models in continuous space are needed for this purpose.

In order to model the second order spatial structure, simplifying assumptions are often made (Cressie, 1993, chapter 2). These include the assumption of spatial stationarity or homogeneity, where the second order association between pairs of sites is assumed to depend only on the spatial difference, including direction, 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 modeling heterogeneous (spatially non-stationary) second order structure. Guttorp and Sampson (1994) reviews several approaches for modeling such structure. These include an approach which was initially introduced in Sampson (1986), further developed in Sampson and Guttorp (1992) and Guttorp and Sampson (1994), and for which the estimation methodology continues to evolve. This approach models second order spatial correlation structure as a function of Euclidean distance between sites in a bijective deformation of the geographic space, as described in section 2.

Consider a spatio-temporal process with value $Z(x, t)$ at site x and time t. We model spatial association between any two geographic locations x and y in terms of the variance of the spatial

increments $D_v(x, y)$, which we call the spatial dispersion function,

$$D_v(x, y) = \text{var}[Z(x, t) - Z(y, t)].$$

In most of the geostatistical literature, $D_v(x, y)$ is known as the *variogram* when homogeneity or intrinsic stationarity is assumed (see for example, Cressie, 1993, section 2.3.1, which includes references to terminology used in other areas of study). In this paper we will use the terminology *variogram* only when we are referring to isotropic dispersion models, which depend only on the Euclidean distance between sites. For simplicity in this paper we assume that the observations at monitoring sites are independent in time, but correlated in space, and that the spatial dispersion does not vary in time. The case of strong temporal correlation, common in many environmental applications, is discussed further in section 7.

The remainder of the paper proceeds as follows. We review the deformation modeling approach in section 2. A brief discussion of estimation is provided in section 3. Sections 4 and 5 concern validity of the dispersion models and the invariance of the modeled dispersions to rotation, scale and location changes of the bijective deformation of the geographic space. (The intuitive result of section 5 was previously noted, but no proof was published.) In section 6, we prove two results about identifiability of the variogram and deformation mappings. Section 7 is a concluding discussion section.

2 Deformation-based heterogeneous spatial correlation model

We express the spatio-temporal process as

$$Z(x, t) = \mu(x, t) + E_\tau(x) + E_\epsilon(x, t),$$

where $\mu(x, t)$ is a spatio-temporal mean (assumed known in this presentation), and $E_\tau(x)$ is a zero mean component with no temporal correlation and with spatial correlation being a

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smooth function of geographic coordinates. $E_\epsilon(x, t)$ represents measurement error and small scale variability, considered independent in space and time. We assume that

$$\text{var} [\ E_\tau(x) - E_\tau(y)\ ] \rightarrow 0, \text{ as } x \rightarrow y. \quad \text{Hence } D_v(x, y) \quad \rightarrow \quad 2 \text{ var} [\ E_\epsilon(x, t)\ ] = 2\ \sigma_\epsilon^2,$$

as $x \rightarrow y$, where σ_ϵ^2 is the nugget effect, which is a measure of the small scale variability and measurement error (Cressie, 1993, section 2.3.1). In practice, we assume the existence of covariances, and we model dispersions for the variance-standardized process. The dispersions may then be written (dropping the subscript v on the standardized scale) as $D(x, y) = 2[1 - \rho_{xy}]$ where ρ_{xy} is the spatial correlation between sites x and y.

The deformation approach of Sampson and Guttorp (1992), models the spatial correlation structure as a function of Euclidean distance between site locations in a bijective transformation of the geographic coordinate system. The geographic coordinate system is referred to as the G-space, and the transformed coordinate system is known as the D-space, where D stands for dispersion. The G and D-spaces have most often be considered as two-dimensional, although the D-space may have dimension $p \geq 2$ (Guttorp and Sampson, 1994). The model is of the form

$$D(x, y) = \gamma_\theta\left(\|f(x) - f(y)\|\right) \tag{1}$$

where $f(.)$ is a bijective transformation of the G-space to the D-space, and γ_θ is a valid isotropic variogram with parameters θ. The transformation effectively stretches the G-space in regions of relatively lower spatial correlation, while contracting it in regions of relatively higher spatial correlation, so that an isotropic variogram can model the dispersions as functions of distance in the D-space representation. The simplest non-trivial example is an affine transformation, $f(x) = Ax$, where the principal axes of the matrix A determine the geographic directions of greatest and weakest spatial correlation in this homogeneous (stationary) anisotropic model. This is called the case of geometric or elliptical anisotropy in the geostatistics literature.

3 Estimation

The deformation models are fitted to empirical estimates of the pairwise spatial dispersions. Most of the applications to date have considered processes observed at T time points at each of N point monitoring sites in space, since repeated observations in time at each of the N monitoring sites clearly may be used to obtain empirical estimates d_{ij} for the dispersion $D(x_i, x_j)$ between each pair of monitoring sites x_i and x_j (c.f., Meiring et al., 1997b for references). Estimation of spatial dispersions between pairs of sites is more difficult if samples are available only from a single realization of a spatial process, or if the process is irregularly sampled in space and time. However, once empirical estimates have been obtained, the fitting of the models may be addressed in the same way.

The sample dispersions are then modeled as

$$d_{ij} \quad = \quad \gamma_\theta \left(\| f(x_i) - f(x_j) \| \right) + e_{ij}$$

where d_{ij} is the sample dispersion between geographic sites x_i and x_j, γ_θ and $f(.)$ are as defined in section 2, and e_{ij} is an error term. These errors are neither independent nor identically distributed. The form of γ_θ must be chosen — for example γ_θ might be an exponential or Gaussian variogram model with nugget — and the variogram parameters θ and the D-space coordinates must be estimated. Cressie (1993, chapter 2) provides a discussion of valid variograms.

Once a particular isotropic variogram model γ_θ has been chosen, the D-space locations for the monitoring sites and the parameters of the D-space variogram are estimated by minimizing a goodness-of-fit criterion. We currently use a penalized weighted least squares procedure based on a representation of $f()$ in terms of thin-plate splines, although other approaches have been suggested. The penalty is on the degree of bending of the deformation. Estimation is not the topic of this paper, and the reader is referred to Guttorp et al. (1994), Meiring (1995), Smith

(1996), and Meiring et al. (1997a, 1997b) for discussion of recent estimation approaches, as well as the form of the G-space to D-space mappings and computational issues. The proofs provided in this paper do not concern the optimization criterion or the form of the deformation mapping.

4   Validity of the dispersion model

Proposition 4.1 *The deformation model (1) results in a positive definite spatial covariance structure, assuming the existence of covariances.*

Proof of proposition 4.1:

It follows from Bochner's Theorem (Bochner, 1955), that a function is a valid correlation model *iff* it is positive definite. (See Cressie, 1993, section 2.5.1 for details.) Consider any geographic sites $x_1, \ldots, x_M$, and corresponding D-space coordinates $f(x_1), \ldots, f(x_M)$ for any $M \in \{2, \ldots, \infty\}$. Let $C_G(x_i, x_j)$ denote the correlation between geographic sites x_i and x_j. Under model (1) we can write $C_D(\|f(x_i) - f(x_j)\|) = C_G(x_i, x_j)$ for the correlation in the D-space. Then

$$\sum_{i=1}^{M} \sum_{j=1}^{M} a_i a_j C_G(x_i, x_j) \;\; = \;\; \sum_{i=1}^{M} \sum_{j=1}^{M} a_i a_j C_D(\|f(x_i) - f(x_j)\|) \;\; \geq \;\; 0$$

for all $\{a_1, \ldots, a_M \mid a_i \in \Re \}$, since the deformation approach fits a valid isotropic variogram (and hence correlation structure, assuming the existence of covariances), as a function of the D-space coordinates. Thus C_G is valid as a function of the geographic coordinates. $\square$

The heuristic motivation of the deformation modeling approach suggests that the dispersions should be a function of distance between points in a smooth, continuous, one-to-one $(x \neq y$ *iff.* $f(x) \neq f(y))$ deformation of the geographic coordinate system. The previous argument shows

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that we obtain a valid spatial correlation structure as a function of the G-space coordinates even if the mapping is not one-to-one.

Validity is not the only question of interest though. We must also ask whether the correlation model makes sense scientifically. In the simple case of $\Re^2 \to \Re^2$ mappings, a continuous mapping that is not one-to-one, will fold. If the mapping folds, any two geographic sites that are mapped onto the same D-plane location will have a modeled correlation of 1, which will not be reasonable for most environmental monitoring applications. Due to local emissions and reactions, sites some distance apart in certain environmental monitoring problems, may be more closely correlated than sites which are geographically "in between" these sites. If one considers only strictly increasing D-space variograms, the spatial correlation model may not be physically reasonable for a non-folding map. In these applications it will be necessary to consider higher-dimensional models mapping $\Re^p \to \Re^d$ with $d > p$, or alternatively to use non-monotone D-space variograms. We are investigating properties of the model for higher-dimensional mappings.

5 Location, scale and rotation of D-space representation

Guttorp et al. (1994) note that the same modeled dispersions may be obtained for any shifted, scaled and rotated version of a D-space representation. No proof was included at that stage; it is presented here for completeness.

The practical implications of this result are that we can fix the location, scale and rotation of the D-space prior to estimating the D-space coordinates and associated variogram parameters. For $\Re^2 \to \Re^2$ mappings, fixing four parameters in the optimization problem will fix the rotation, scale and location up to reflection of the plane. We commonly fix the D-plane locations of two

sites at their geographic locations. In higher dimensions, additional constraints are required. For example, in $\Re^3$, we fix two points and constrain a third point to lie in a fixed plane. The following proposition shows that the dispersion model is invariant to the choice of the fixed sites. However, numerical problems may be encountered in fitting the model when fixing certain combinations of sites, as discussed briefly in chapter 4 of Meiring (1995).

Proposition 5.1 *Let γ be an isotropic variogram model. Suppose that the dispersions between geographic sites are modeled as $D_{12} = \gamma\left(\|x_1^* - x_2^*\|\right)$ for each pair of geographic sites x_1 and x_2, where $x_1^* = f(x_1)$ and $x_2^* = f(x_2)$ are the corresponding D-space coordinates in a particular dispersion-space, denoted $\mathcal{H}$. Then the same modeled dispersions between all pairs of geographic locations, can be obtained using a rescaled (still valid) variogram defined for distances in any dispersion space obtained by translation, rotation, or scaling of $\mathcal{H}$.*

Proof of Proposition 5.1:

Denote distances between any two geographic sites x_1 and x_2 by h_{12}^* in $\mathcal{H}$ and h_{12}' in any other dispersion space obtained by translating, rotating, or scaling $\mathcal{H}$. Consider a similarity transformation so that $x_1' = b\,G\,x_1^* + \underline{c}$ for every geographic site x_1, for some constant $b > 0$, rotation matrix G, and translation vector $\underline{c}$. Then $h_{12}' = b\,h_{12}^*$. Define $\eta\left(h_{12}'\right) = \gamma\left(h_{12}'/b\right) = \gamma\left(h_{12}^*\right)$. For each integer m, for all real numbers $\{a_1, \ldots, a_m\}$, and for all spatial locations $\{x_i : i = 1, \ldots, m\}$,

$$\sum_{i=1}^m \sum_{j=1}^m a_i a_j \left[1 - \frac{\eta\left(h_{ij}'\right)}{2}\right] = \sum_{i=1}^m \sum_{j=1}^m a_i a_j \left[1 - \frac{\gamma\left(h_{ij}^*\right)}{2}\right] \geq 0,$$

since $(1 - \gamma/2)$ is positive definite. This shows that $(1 - \eta/2)$ is positive definite, and η is a valid variogram. □

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6 Identifiability of D-space variogram model

One of the fundamental issues in this modeling approach is the impact of the choice of D-space variogram model γ_θ on the final dispersion model. In this section we present two proofs (under different assumptions) of identifiability of the variogram model and deformation, assuming that the dispersion field is known for all pairs of points in the geographic space.

The first result considers affine deformations and shows that two isotropic D-space variograms give the same modeled dispersions for all pairs of locations if and only if the variograms and affine deformations are identical. The second proposition is a similar result for the more general case of bijective deformations, but restricting the class of D-space variograms to those that are strictly increasing.

Proposition 6.1 *If two isotropic variogram models γ and η, which are not pure nugget variograms, and two affine G-space to D-space mappings h and b, give the same dispersions for the entire G-space, i.e. if*

$$\gamma\left(\|h\left(x_1\right) - h\left(x_2\right)\|\right) \;\; = \;\; \eta\left(\|b\left(x_1\right) - b\left(x_2\right)\|\right) \quad \forall \text{ geographic sites } x_1 \text{ and } x_2, \qquad (2)$$

then the variograms are identical, as are the deformation mappings (up to translation, scaling, rotation — and reflection of the whole D-plane in the two-dimensional case).

Proof of Proposition 6.1: For simplicity, we present the proof for $\Re^2 \to \Re^2$ mappings. The proof for $\Re^p \to \Re^p$ mappings with $p > 2$ may be obtained by fixing the required number of coordinates in order to fix the scale, rotation and location of the D-space representations.

Suppose there exist two isotropic variogram models γ and η and two affine mappings h and b from $\Re^2$ to $\Re^2$ yielding D-space representations $\mathcal{H}$ and $\mathcal{B}$, such that (2) holds. Assume that

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the location, rotation and scale of the mappings have been fixed by mapping two sites, say x_s and x_t, to their geographic locations in both $\mathcal{H}$ and $\mathcal{B}$. $\mathcal{H}$ and $\mathcal{B}$ are each affine transformations of the geographic space $\mathcal{G}$. Hence $\mathcal{H}$ is an affine transformation of $\mathcal{B}$. It follows that points are collinear in $\mathcal{G}$ *iff* their images are collinear in $\mathcal{H}$ and $\mathcal{B}$.

Denote distances in planes $\mathcal{H}$ and $\mathcal{B}$ corresponding to each pair of geographic sites x_1 and x_2 by $h_{12} \equiv \|h(x_1) - h(x_2)\|$ and $b_{12} \equiv \|b(x_1) - b(x_2)\|$. For all points x_1 and x_2 that are collinear with x_s and x_t, $h_{12} = b_{12}$ by properties of affine transformations because we fixed $h_{st} = b_{st}$ (without loss of generality). By (2), $\gamma(h_{12}) = \eta(b_{12}) = \eta(h_{12})$. Hence, by isotropy of γ and η,

$$\gamma(h) = \eta(h) \quad \forall \ h; \tag{3}$$

ie. the variograms γ and η are identical.

Consider any two points x_1 and x_2 in $\mathcal{G}$. As $\mathcal{H}$ and $\mathcal{B}$ are affine transformations, there exists a constant $a_{12} \neq 0$ such that $h_{34} = a_{12} b_{34}$ for all x_3 and x_4 collinear with x_1 and x_2. Hence

$$\gamma(h_{34}) = \eta\left(\frac{1}{a_{12}} h_{34}\right) \quad \text{for all } x_3 \text{ and } x_4 \text{ collinear with } x_1 \text{ and } x_2. \tag{4}$$

By (3), (4), and isotropy, $\gamma(h) = \gamma\left(\frac{1}{a_{12}} h\right)$ for every h. Hence, either γ is constant for $h > 0$ (a nugget variogram), or $a_{12} = 1$. If $a_{12} = 1$, then the D-planes $\mathcal{H}$ and $\mathcal{B}$ are identical up to reflection of the whole D-plane, since x_1 and x_2 may be any two sites in $\mathcal{G}$. $\qquad\square$

Proposition 6.2 *If two strictly increasing isotropic variogram models γ and η, and two corresponding bijective G-space to D-space mappings h and b, give the same dispersions for the entire G-space, i.e. if*

$$\gamma\left(\|h\left(x_1\right) - h\left(x_2\right)\|\right) \quad = \quad \eta\left(\|b\left(x_1\right) - b\left(x_2\right)\|\right) \quad \forall \text{ geographic sites } x_1 \text{ and } x_2, \tag{5}$$

then the variograms are identical, as are the deformation mappings (up to rotation, translation, scaling — and reflection of the whole D-plane in the two-dimensional case).

Proof of Proposition 6.2:   For simplicity we present the proof for $\Re^2 \to \Re^2$ mappings. The proof for $\Re^p \to \Re^p$ mappings with $p > 2$ is analogous, replacing G-plane by G-space, D-plane by D-space, circle by p-dimensional sphere, and without loss of generality by fixing the required number of coordinates in order to fix the rotation, scale and location of the D-space representation (proposition 5.1).

Consider two strictly increasing isotropic variogram models γ and η and two bijective mappings h and b from $\Re^2$ to $\Re^2$ yielding D-plane representations $\mathcal{H}$ and $\mathcal{B}$, such that (5) holds. Denote distances between each pair of geographic sites x_1 and x_2 by $h_{12} \equiv \|h\left(x_1\right) - h\left(x_2\right)\|$ in $\mathcal{H}$ and $b_{12} \equiv \|b\left(x_1\right) - b\left(x_2\right)\|$ in $\mathcal{B}$. Assume that the location, rotation and scale of the mappings have been determined by mapping two sites, say x_s and x_t, to their geographic locations in $\mathcal{H}$ and $\mathcal{B}$. Writing $\|x_s - x_t\| = m$, we have $\gamma\left(h_{st}\right) = \gamma\left(m\right) = M$, say, and likewise $\eta\left(b_{st}\right) = M$.

In Appendix A we show that the rank order of intersite distances in $\mathcal{H}$ is the same as the rank order of the intersite distances in $\mathcal{B}$ (lemma A.1), and that points mapped onto a circle or line in $\mathcal{H}$ also lie on a circle or a line, respectively, in $\mathcal{B}$ (lemma A.2). Let x_1 and x_2 be any two geographic locations. We now show that $h_{12} = b_{12}$.

Consider the line in $\mathcal{H}$ from $h(x_1)$ to $h(x_2)$ of length $h_{12} \equiv c$. There are three cases.

1. $c < m$:

   Extend the line between $h(x_1)$ and $h(x_2)$ to a point $h(x_3)$ such that $h_{13} = m$, and $h(x_2)$

   is on the line joining $h(x_1)$ and $h(x_3)$. Divide the line from $h(x_1)$ to $h(x_2)$ into $c(m-c)$

   line segments each of length $\frac{1}{(m-c)}$. Divide the line from $h(x_2)$ to $h(x_3)$ into $(m-c)^2$ line

   segments of length $\frac{1}{(m-c)}$.

   The line of length m in $\mathcal{H}$ has now been divided into $m(m-c)$ equal but disjoint (except

   for endpoints where adjacent) line segments. Each of these line segments can be considered

   as the diameter of a circle of diameter $\frac{1}{(m-c)}$, as shown in figure 1.

   ... Figure 1 about here ...

   Circles in $\mathcal{H}$ correspond to circles in $\mathcal{B}$, and

   $$\gamma\left(\frac{1}{m-c}\right) = \eta(r_l) \qquad \forall\, l \in \{1, \ldots, m(m-c)\}, \tag{6}$$

   where r_l is the diameter of the circle in $\mathcal{B}$ corresponding to the lth circle in $\mathcal{H}$ as one moves

   along the line from $h(x_1)$ to $h(x_3)$. (By lemma A.1, the order of the sites on the line in

   $\mathcal{B}$ is the same as that in $\mathcal{H}$ since the rank ordering of distances is the same.)

   Since γ and η are strictly increasing, (6) implies $r_l \equiv r$, for all $l \in \{1, \ldots, m(m-c)\}$.

   Lines in $\mathcal{H}$ are transformed to lines in $\mathcal{B}$ (lemma A.2), so the line from $h(x_1)$ to $h(x_3)$ in

   $\mathcal{H}$ corresponds to a line from $b(x_1)$ to $b(x_3)$ in $\mathcal{B}$. Now

   $$m \quad = \quad \|h(x_1) - h(x_3)\|$$

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$$= m(m-c) * \text{diameter of circles in } \mathcal{H}$$

$$= m(m-c) \frac{1}{(m-c)}$$

and, since $h_{13} = m$ iff $b_{13} = m$ (shown in Lemma A.1),

$$m = \|b(x_1) - b(x_3)\|$$

$$= m(m-c) * \text{diameter of circles in } \mathcal{B}$$

$$= m(m-c) r.$$

Hence $r = \frac{1}{(m-c)}$. It follows that the line between $b(x_1)$ and $b(x_2)$ is of length

$$b_{12} = c(m-c) * r = c = h_{12},$$

concluding the argument for the case $c < m$.

2. $c > m$:

Locate a point $h(x_3)$ on the line between $h(x_1)$ and $h(x_2)$ such that $h_{13} = m$.

Divide the line from $h(x_1)$ to $h(x_3)$ into mc line segments each of length $\frac{1}{c}$, and the line

from $h(x_3)$ to $h(x_2)$ into $c(c-m)$ line segments each of length $\frac{1}{c}$. Use a similar argument

to that given for the case $c < m$ to show that $b_{12} = h_{12}$.

3. $c = m$:

By (5) and since $h_{12} = m = h_{st} = b_{st}$, it follows that $\eta(b_{12}) = \gamma(h_{12}) = \eta(b_{st})$. Hence, by

isotropy of η, $b_{12} = b_{st} = h_{12}$.

Since $h_{12} = b_{12}$ for all geographic sites x_1 and x_2, and since sites x_s and x_t were fixed at their

geographic locations; it follows that the deformation maps are the same up to reflection of the

entire D-plane.

Finally, since γ and η are both strictly increasing variograms, and $h_{12} = b_{12}$ for all geographic sites x_1 and x_2, by (5) we have $\gamma = \eta$, concluding the proof. $\square$

7   Discussion

The previous section demonstrates identifiability of the D-space variogram model and bijective transformation when the dispersions between all pairs of geographic locations are known. This suggests asymptotic identifiability for an increasingly dense network of monitoring sites, but leaves open practical questions of identifiability for models fitted to data from finite monitoring networks. Currently we can not demonstrate theoretical results about identifiability based on finite samples from spatial-temporal processes, although we have addressed questions regarding the deformation models that we fit to these observations.

Indeed, even without consideration of deformation, it is well recognized that, for example, a Gaussian variogram with nugget may give similar modeled dispersions between all pairs of monitoring sites, to those provided by an exponential variogram with nugget for small networks of monitoring sites not including pairs with "very small" intersite distances. Differences may be substantial in the fitted nugget effect representing small scale variability and measurement error. This may result in substantial differences in estimated variances at unmonitored sites for different D-space variograms. The results of this paper thus are relevant for monitoring network design. When economically feasible, it is highly desirable to locate a few monitoring sites close together geographically, in order to obtain a better estimate of the small scale variability and measurement error (c.f. Laslett, 1994), and thus aid in the choice of D-space variogram model.

In this paper we made the simplifying assumption that the spatial realizations of the process

were uncorrelated and identically distributed in time. This assumption is frequently violated in atmospheric and hydrological processes. Guttorp et al. (1994) and Sampson et al. (1994) use deformation modeling in a space-time framework. The first of these papers uses temporal pre-whitening followed by deformation modeling of non-stationary spatial correlation in the residuals. The second paper extends the linear model of coregionalization of Rouhani and Wackernagel (1990), applying the deformation on different temporal scales. Estimation approaches for deformation models of non-stationary and non-separable spatio-temporal correlation are currently under development for processes which are irregularly sampled in space and time. The theorems of this paper hold for space-time correlation, considering time as an additional dimension. The type of deformation should take into account the unidirectional attributes of time, and may build on time deformation results from econometrics (see for example Stock, 1988).

Theoretical questions related to bias and consistency remain to be answered in two and higher dimensions. Simulation studies have proved useful in studying the variance-bias trade-off in specific applications (Meiring et al., 1997b). Perrin (1997) has recently addressed consistency questions in one dimension, and also obtained a characterization of non-stationary one-dimensional spatial correlation structures which can be reduced to stationarity through a bijective one-dimensional deformation. A similar characterization has yet to be developed in two and higher dimensions.

Acknowledgements:

A   Appendix: Two Lemmas for proposition 6.2

The following two lemmas are part of proposition 6.2 and rely on the definitions of γ, η, $\mathcal{H}$, $\mathcal{B}$, h_{12}, b_{12}, M, m, x_s and x_t provided there.

Lemma A.1 *The rank order of intersite distances are the same in $\mathcal{H}$ and $\mathcal{B}$.*

Proof of Lemma A.1: Suppose there exist geographic sites x_1 and x_2 such that $h_{12} < m \leq b_{12}$. Then

$$\gamma(h_{12}) < \gamma(m) = M = \eta(m) \leq \eta(b_{12}),$$

since γ and η are strictly increasing. This contradicts (5), so if $h_{12} < m$, then $b_{12} < m$. By this, and analogous arguments,

$$h_{12} < m \ \ iff \ \ b_{12} < m, \qquad h_{12} = m \ \ iff \ \ b_{12} = m, \qquad \text{and} \qquad h_{12} > m \ \ iff \ \ b_{12} > m. \qquad (7)$$

Now consider sites $x_1, \ldots, x_4$ with $h_{12} < h_{34}$. By (7), if $h_{12} < m < h_{34}$, then $b_{12} < m < b_{34}$, Consider now the case where $h_{12} < h_{34} < m$, then (7) implies that $b_{12} < m$ and $b_{34} < m$. Suppose $b_{34} \leq b_{12} < m$. Since both γ and η are strictly increasing, we must have

$$M - \gamma(h_{12}) > M - \gamma(h_{34}) \quad \text{and} \quad M - \eta(b_{12}) \leq M - \eta(b_{34}). \qquad (8)$$

By (5),

$$M - \gamma(h_{12}) = M - \eta(b_{12}) \quad \text{and} \quad M - \gamma(h_{34}) = M - \eta(b_{34}).$$

This contradicts (8), so $h_{12} < h_{34} < m$ implies $b_{12} < b_{34} < m$. By analogous arguments $b_{12} < b_{34} < m$ implies $h_{12} < h_{34} < m$, and $m < h_{12} < h_{34}$ iff $m < b_{12} < b_{34}$. Thus, for any four sites, the rank order of the intersite distances in $\mathcal{H}$ is the same as the rank order of the intersite distances in $\mathcal{B}$. □

Lemma A.2 *Points mapped onto a circle or line in $\mathcal{H}$ also lie on a circle or a line, respectively, in $\mathcal{B}$.*

Proof of Lemma A.2:

Consider any site x_1 and distance α. By isotropy and (5), $\eta(b_{1r}) = \gamma(h_{1r}) = c_{1\alpha}$ for all geographic sites x_r such that $h_{1r} = \alpha$. Hence, since η is strictly increasing and isotropic, $b_{1r} = b_\alpha$, say. This shows that points mapped onto a circle in $\mathcal{H}$ are mapped also onto a circle in $\mathcal{B}$.

$\mathcal{H}$ and $\mathcal{B}$ are bijective mappings, thus for any three geographic sites x_1, x_2 and x_3 such that $h(x_2)$ lies on the line between $h(x_1)$ and $h(x_3)$ in $\mathcal{H}$, $b(x_2)$ is the only point of intersection of two circles centered at $b(x_1)$ and $b(x_3)$ in $\mathcal{B}$ of radius b_{12} and b_{23} respectively. Hence $b(x_1)$, $b(x_2)$ and $b(x_3)$ are collinear in $\mathcal{B}$. $\qquad\square$

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References

[1] Bochner, S., 1955, Harmonic analysis and the theory of probability: Berkeley, University of California Press, 176 p.

[2] Cressie, N.A.C., 1993, Statistics for Spatial Data, Revised Edition: Wiley-Interscience, John Wiley and Sons, Inc., 900 p.

[3] Guttorp, P., Meiring, W., and Sampson, P. D., 1994, A space-time analysis of ground-level ozone data: Environmetrics, v. 5, p. 241-254.

[4] Guttorp, P., and Sampson, P. D., 1994, Methods for Estimating Heterogeneous Spatial Covariance Functions with Environmental Applications, *in* Patil, G.P. and C.R. Rao, C. R., eds., Handbook of Statistics XII: Environmental Statistics: Elsevier/North Holland, New York, p. 663-690.

[5] Laslett, G. M., 1994, Kriging and Splines: An Empirical Comparison of Their Predictive Performance in Some Applications, (With discussion): Journal of the American Statistical Association, v. 89, p. 391-409.

[6] Meiring, W., 1995, Estimation of Heterogeneous Space-Time Covariance: Ph.D. Dissertation, University of Washington, Seattle, 192 p.

[7] Meiring, W., Guttorp, P., and Sampson, P. D., 1997a, Computational Issues in Fitting Spatial Deformation Models for Heterogeneous Spatial Correlation: *To appear*, Proceedings of the 29th Symposium on the Interface: Computing Science and Statistics.

[8] Meiring, W., Monestiez, P., Sampson, P. D., and Guttorp, P., 1997b, Developments in the modelling of nonstationary spatial covariance structure from space-time monitoring data: *in* Baafi, E. Y., and Schofield, N., eds., Geostatistics Wollongong '96, vol.1, Kluwer Academic Publishers, p. 162-173.

[9] Perrin, O., 1997, Modèle de covariance d'un processus non-stationnaire par défomation de l'espace et statistique: Ph.D. dissertation, Université de Paris I Panthéon-Sorbonne, 186 p.

[10] Rouhani, S., and Wackernagel, H., 1990, Multivariate Geostatistical Approach to Space-Time Data Analysis: Water Resources Research, v. 26, no. 4, p. 585-591.

[11] Sampson, P.D., 1986, Spatial covariance estimation by scaled-metric scaling and biorthogonal grids: Technical Report No. 91, Department of Statistics, University of Washington, and SIMS Technical Report No. 102, Department of Statistics, University of British Columbia.

[12] Sampson, P.D., and Guttorp, P., 1992, Nonparametric estimation of nonstationary spatial covariance structure: Journal of the American Statistical Association, vol. 87, p. 108-119.

[13] Sampson, P.D., Guttorp, P., and Meiring, W., 1994, Spatio-temporal analysis of regional ozone data for operational evaluation of an air quality model: 1994 Proceedings of the Section on Statistics and the Environment, American Statistical Association, Alexandria: American Statistical Association, p. 46-55.

[14] Smith, R.L., 1996, Estimating nonstationary spatial correlations: Preliminary version: on the Spatial Statistics Preprint Service at
http://hp2.niss.rti.org/organization/personnel/granville/list.html

[15] Stock, J.H., 1988, Estimating continuous-time processes subject to time deformation: An application to postwar U.S. GNP: Journal of the American Statistical Association, vol. 83, p. 77-85.

Figure 1: Division of line from $h(x_1)$ to $h(x_3)$ into line segments of equal length which are disjoint except possibly for their endpoints, and which may be viewed as the diagonals of circles.

Figure 1:

$h\left(x_1\right)$ ... ... $h\left(x_2\right)$ ... $h\left(x_3\right)$

$1/(\text{m - c})$

c

$m - c$