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Summary. This paper investigates the use of non-Euclidean distances to characterize isotropic spatial dependence for geostatistical related applications. A simple example is provided to demonstrate there are no guarantees that existing covariogram and variogram functions remain valid (i.e. positive definite or conditionally negative definite) when used with a non-Euclidean distance measure. Furthermore, satisfying the conditions of a metric is not sufficient to ensure the distance measure can be used with existing functions. Current literature is not clear on these topics. There are certain distance measures that when used with existing covariogram and variogram functions remain valid, an issue that is explored. No new theorems are provided, rather links between existing theorems and definitions related to the concepts of isometric embedding, conditionally negative definiteness, and positive definiteness are used to demonstrate classes of valid norm dependent isotropic covariogram and variogram functions, results most of which have yet to appear in mainstream geostatistical literature or application. These classes of functions extend the well known classes by adding a parameter to define the distance norm. In practice, this distance parameter can be set a priori to represent, for example, the Euclidean distance, or kept as a parameter to allow the data to choose the distance norm. Applications of the latter are provided for demonstration.

Key Words: Conditionally Negative Definite, Euclidean Distance, Isometric Embedding, Positive Definite, Spatial Dependence

1 Introduction

Characterizing spatial dependence of random processes via the covariogram or variogram function is cornerstone to many geostatistical related applications. Because these functions represent a second moment structure they must be of specific type, positive definite for covariograms and conditionally negative definite for variograms. Available to practitioners are parametric families of known valid covariogram and variogram functions. Under the pragmatic assumptions of stationarity and isotropy, these covariograms and variograms are provided as a function of the Euclidean inter-point distance. There is a large body of literature pertaining to the validity and mathematical characterization of covariogram and variogram functions (Schlather 1999, Christakos 1984). A topic less covered is the concept of using different (non-Euclidean) measures of inter-point distance to characterize isotropic spatial dependence. Some substantive references include Kruvoruchko and Gribov (2004), Loland and Host (2003), Kern and Higdon (2000), Dominici et al. (2000), Rathbun (1998), Cressie and Majure (1997a,b), Curriero (1996), and Cressie et al. (1990). In a related issue Banjerjee (2005) discusses distance related computations for spatial modeling on the earth's surface.

Spatial prediction (kriging) is a primary objective in geostatistical applications. Reasons to consider a non-Euclidean distance could include physical properties of how the process under study disperses or has come to exist in space or sampling non-convex spatial domains such as irregular waterways. References cited above provide some examples. Distances based on travel times is another possible consideration. In other applications focus is on regression coefficients and covariograms or variograms are commonly used to characterize residual spatial variation, which may be quite complicated, for example due to contagious agents and/or a combination of missing covariates, as well as being dependent on the spatial design of sampled locations. In practice our goal is to characterize spatial dependence as best as possible and consideration to possible non-Euclidean isotropy may prove beneficial.

The purpose of this paper is to demonstrate some of the technical details involved in using a non-Euclidean inter-point distance to characterize isotropic spatial dependence. A simple motivating example is provided to convey the following key message. There are no guarantees that existing covariogram and variogram functions will remain valid when used with a measure of distance other than Euclidean. It is therefore essential that applications involving a non-Euclidean distance provide proof that the proposed family of covariogram or variogram functions remain valid when used with an alternative distance measure.

It turns out that some norm dependent measures of distance can be used with certain covariogram and variogram functions. Links between existing theorems and definitions related to the concepts of isometric embedding, conditionally negative definiteness, and positive definiteness are used to demonstrate classes of valid norm dependent isotropic covariogram and variogram functions. These classes of functions extend the well known classes by adding a parameter to define the distance norm. In practice, this distance parameter can be set a priori to represent, for example, the Euclidean distance, or kept as a parameter to allow the data to choose the distance norm. Applications of the latter are provided for demonstration.

2 Motivating Example

As a motivating example consider a simple four point regular grid configuration in $\Re^2$ with unit spacing, points represented by (x_i, y_i), $i = 1, \ldots, 4$, and propose the city block metric, $\rho_{ij} = |x_i - x_j| + |y_i - y_j|$, as an alternative distance to the Euclidean metric. This yields the following matrix of inter-point city block distances,

$$\begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 2 & 1 \\ 1 & 2 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix},$$

which when used with the Gaussian covariogram, $20\exp(-\rho_{ij}^2/4)$, nugget, sill, and range parameters arbitrarily set at (0,20,4) respectively, results in the following proposed covariance matrix,

$$\begin{pmatrix} 20.00 & 15.58 & 15.58 & 7.36 \\ 15.58 & 20.00 & 7.36 & 15.58 \\ 15.58 & 7.36 & 20.00 & 15.58 \\ 7.36 & 15.58 & 15.58 & 20.00 \end{pmatrix}.$$

The characteristic roots of this matrix are $(58.52, 12.64, 12.64, -3.80)$, implying the Gaussian covariogram is no longer positive definite when used with the city block metric. Using the same distance matrix and parameter settings, the same conclusion can be drawn from other known covariogram functions such as the spherical, rational quadratic, and various forms from the Matern class. On the contrary, the exponential covariogram, $\tau^2 + \sigma^2 \exp(-\rho_{ij}/\phi)$ with positive parameters (τ^2, σ^2, ϕ) remains positive definite in dimensions $>= 1$ when used with the city block metric. This fact is straight forward to show since the exponential covariogram with the city block metric in $\Re^N$ reduces to the product of one dimensional exponential covariograms based on the Euclidean metric in $\Re^1$ and hence positive definite, a separable covariogram as noted by Cressie (1991, p. 68).

The message from this example is clear, there are no guarantees that the common set of positive definite functions used in geostatistical related applications to represent covariances will remain positive definite (and hence valid) when used with distance measures other than the Euclidean metric. Furthermore, alternative distance measures satisfying properties of a metric (defined subsequently), is not sufficient to ensure resulting covariograms remain positive definite. This message also pertains to the pool of known valid Euclidean isotropic variogram functions (see subsequent text).

The water distance used in Cressie and Majure (1997a,b) is actually calculated as though the process was an irregular one dimensional transect by assuming the winding streams have negligible width for their application. In some instances, distances calculated along such a structure can be shown to be equivalent to Euclidean distances along a corresponding regular "stretched out" one dimensional transect (isometric embedding). However, this representation is lost if the original winding stream structure branches off as it appears to do in their application. The water distance used in Rathbun (1998), who incorrectly cites a test proving positive definiteness, is calculated via a computer algorithm and accounts for water body width. The water distance used in Kern and Higdon (2000) is incorrectly justified since it hinges on satisfying conditions of a metric, which is demonstrated above as not being sufficient. The use of a water distance measure in geostatistics appears to substantiate the idea for considering non-Euclidean isotropy and a proof and/or development of valid functions to characterize such spatial dependence or good approximate methods would certainly contribute to the field.

Gneiting (1999a) discusses results that justify the great-arc distance used in Cressie et al. (1990). The non-Euclidean distance used in Dominici et al. (2000) is binary, locations within a common geographic region are given a distance one and infinity otherwise. The consequence being that spatial correlation is constant within geographic regions and zero between regions. Such binary distances can always be represented as Euclidean distances between points in some higher dimension (isometric embedding), and thus are valid to use provided the correlation function is valid in the embedding dimension, a concept that is further explored here.

3 Definitions and Notation

Let the spatial process be represented by the random field

$$\{Z(\mathbf{s}) : \mathbf{s} \in D \subset \Re^N\},$$

where $\mathbf{s} \in \Re^N$ is a generic spatial location varying continuously over a region D. Characterizing the second moment structure of such processes plays a key role in statistical inference and is usually carried out with the covariogram or variogram function, which represents the $Cov(Z(\mathbf{s}_i), Z(\mathbf{s}_j))$ and the $Var(Z(\mathbf{s}_i) - Z(\mathbf{s}_j))$, respectively, $\forall\, \mathbf{s}_i, \mathbf{s}_j \in D$. It is well known that these functions must be of a specific type, positive definite for covariograms and conditionally negative definite for variograms. Probably less well known is the connection between these definitions and the concept of isometric embedding (Wells and Williams 1970). Some general definitions regarding distance measures are provided before reviewing these connections.

Let $\mathbf{S}$ represent an arbitrary collection of objects, such as spatial locations $\mathbf{s} \in \Re^N$, and define the real valued function $\rho(\cdot, \cdot)$ to represent a distance function operating on $\mathbf{S} \times \mathbf{S}$ such that $\rho : \mathbf{S} \times \mathbf{S} \rightarrow [0, \infty)$. The distance function ρ is said to satisfy the conditions of a *metric* if:

$$\begin{array}{l} \rho(\mathbf{s}_i, \mathbf{s}_j) \geq 0 \text{ and } \rho(\mathbf{s}_i, \mathbf{s}_j) = 0 \text{ iff } \mathbf{s}_i = \mathbf{s}_j, \\ \rho(\mathbf{s}_i, \mathbf{s}_j) = \rho(\mathbf{s}_j, \mathbf{s}_i), \text{ and} \\ \rho(\mathbf{s}_i, \mathbf{s}_j) \leq \rho(\mathbf{s}_i, \mathbf{s}_k) + \rho(\mathbf{s}_k, \mathbf{s}_j) \text{ (Triangle inequality)} \end{array}$$

for all $\mathbf{s}_i, \mathbf{s}_j, \mathbf{s}_k \in \mathbf{S}$. A *vector norm* is a function $f : \Re^N \rightarrow [0, \infty)$ that satisfies the following properties:

$$\begin{array}{lll} f(\mathbf{h}) \geq 0 & \mathbf{h} \in \Re^N & (f(\mathbf{h}) = 0 \text{ iff } \mathbf{h} = 0) \\ f(\mathbf{h} + \mathbf{h}^*) \leq f(\mathbf{h}) + f(\mathbf{h}^*) & \mathbf{h}, \mathbf{h}^* \in \Re^N & \\ f(\alpha \mathbf{h}) = |\alpha| f(\mathbf{h}) & \alpha \in \Re,\ \mathbf{h} \in \Re^N. & \end{array}$$

The common α-norms for $\alpha \geq 1$ are defined as

$$||\mathbf{h}||_\alpha = (|h_1|^\alpha + |h_2|^\alpha + \cdots |h_N|^\alpha)^{1/\alpha},$$

where $\mathbf{h} = (h_1, \ldots, h_N)'$. When α =1, 2, and ∞, for example, we have

$$\begin{array}{ll} \|\mathbf{h}\|_1 = |h_1| + |h_2| + \cdots |h_N| & \text{(Manhattan or City Block)} \\ \|\mathbf{h}\|_2 = (h_1^2 + h_2^2 + \cdots h_N^2)^{1/2} & \text{(Euclidean)} \\ \|\mathbf{h}\|_\infty = \text{Max}|h_i| & \text{(Dominating).} \end{array}$$

A vector norm becomes a metric by defining $\rho(\mathbf{s}_i, \mathbf{s}_j) = f(\mathbf{s}_i - \mathbf{s}_j)$, $\forall\ \mathbf{s}_i, \mathbf{s}_j \in \mathbf{S}$. Note, $\|\mathbf{h}\|$ without the subscript is taken to represent the Euclidean norm and for $\alpha < 1$, $\|\mathbf{h}\|_\alpha$ no longer satisfies the conditions of a metric. The concept of isometric embedding is now defined.

Definition Let $\rho_{ij} = \rho(\mathbf{s}_i, \mathbf{s}_j)$ represent distance between points $\mathbf{s}_i$ and $\mathbf{s}_j$ of some metric space represented by $(\mathbf{S}, \rho)$. The metric space $(\mathbf{S}, \rho)$ is said to be *isometrically embedded* in a Euclidean space of dimension N^* if there exists points $\mathbf{s}_i^*$ and $\mathbf{s}_j^*$ and a function ϕ such that

$$\rho_{ij} = \rho(\mathbf{s}_i, \mathbf{s}_j) = \|\mathbf{s}_i^* - \mathbf{s}_j^*\|,$$

for all $\mathbf{s}_i, \mathbf{s}_j \in \mathbf{S}$ and where $\phi(\mathbf{s}) = \mathbf{s}^*$.

Isometric embedding in a Euclidean space (hereafter referred to as embedding), thus defines the situation when a metric distance function is equivalent to a Euclidean norm. The ramifications for the topic at hand is readily apparent. If a non-Euclidean distance function (meaning non-Euclidean in the dimension the process is observed) is embeddable, then the distance function used with existing covariogram and variogram functions will retain the positive and conditionally negative definite properties provided these function are valid in the embedding dimension. Although it is necessary that a distance function ρ satisfy the conditions of a metric for embedding, it is clearly not sufficient as was previously demonstrated. The following theorem, due originally to Schoenberg (1937), see also Young and Householder (1938), provides a necessary and sufficient condition for the embedding of a finite metric space.

Theorem (Schoenberg 1937). The finite metric space $(\mathbf{S}, \rho)$, where $\mathbf{S} = \{\mathbf{s}_0, \mathbf{s}_1, \ldots, \mathbf{s}_n\}$

$n > 2$, is embeddable in $\Re^n$ if and only if

$$(1/2)\sum_{i=1}^{n}\sum_{j=1}^{n}\left\{\rho(\mathbf{s}_0,\mathbf{s}_i)^2+\rho(\mathbf{s}_0,\mathbf{s}_j)^2-\rho(\mathbf{s}_i,\mathbf{s}_j)^2\right\}\xi_i\xi_j \geq 0 \quad (1)$$

for all choices of real numbers $\xi_0, \xi_1, \ldots, \xi_n$.

As pointed out in (Wells and Williams 1970), condition (1) arbitrarily chooses the point $\mathbf{s}_0$ as the origin, which acts solely as a point of reference. Therefore, we are free to set ξ_0 to, say, $\xi_0 = -\sum_1^n \xi_i$. Then by summing over each term in (1) and regrouping, the equivalence of (1) with

$$\sum_{i=0}^{n}\sum_{j=0}^{n}\rho(\mathbf{s}_i,\mathbf{s}_j)^2\xi_i\xi_j \leq 0, \quad (2)$$

for all choices of real numbers $\xi_0, \xi_1, \ldots, \xi_n$ such that $\sum_0^n \xi_i = 0$, can be established. This is precisely the conditionally negative definite property used to characterize variograms (Cressie 1991). Therefore, a distance function ρ is embeddable if and only if ρ^2 is conditionally negative definite. Put another way, for a given distance function ρ, $\rho^{1/2}$ is embeddable, and hence preserves the positive and conditionally negative definite properties of covariogram and variogram functions that are valid in all dimensions, if and only if ρ is conditionally negative definite. This explains another less well known fact that the square root of the variogram is equivalent to a Euclidean norm.

The embedding and conditionally negative definite property are linked to positive definiteness by the following result (e.g. Wells and Williams 1970),

$$\exp(-a\rho(\cdot)) \text{ is positive definite } \forall a > 0 \text{ iff } \rho(\cdot) \text{ is conditionally negative definite} \quad (3)$$

Note, the multiplication and addition by positively restricted parameters (τ^2, σ^2), for example $\tau^2 + \sigma^2 \exp(-a\rho(\cdot))$ do not change the result.

In practice spatial processes are usually assumed stationary. Letting $\mathbf{h} = \mathbf{s}_i - \mathbf{s}_j, \forall\, \mathbf{s}_i, \mathbf{s}_j \in D$, second-order stationarity is defined for $Z(\mathbf{s})$ by a constant mean and covariance a function of $\mathbf{h}$, denoted by the covariogram function $C(\mathbf{h})$. Intrinsic stationarity is defined as a constant mean and variance of the increments $Z(\mathbf{s}_i) - Z(\mathbf{s}_j)$ to be a function of $\mathbf{h}$, denoted by the variogram $2\gamma(\mathbf{h})$, $\gamma(\mathbf{h})$ the semivariogram. Isotropy further assumes covariograms and variograms to only be a function of distance with $\|\mathbf{h}\|$ as the measure of distance. Geometric anisotropy refers to the linear transformation of coordinates to achieve isotropy, denoted by $\|\mathbf{A}\mathbf{h}\|$, with matrix $\mathbf{A}$ representing in geostatistical terminology the rotation and stretching transformation of coordinates $\mathbf{h}$ (Cressie 1991).

As reviewed in the literature, the positive definite property fully characterizes the class of valid covariograms. Hence, the eigenvalue approach used in Section 2 provides a simple way to exclude candidate models. Valid variograms are necessarily conditionally negative definite as in (2) and also must grow more slowly than $\|\mathbf{h}\|^2$ (Matheron 1973, Christakos 1984). Since the square root of a conditionally negative definite function must represent a Euclidean norm, the multidimensional scaling technique of Mardia et al. (1995, Theorem 14.2.1, p. 397) can be used for verification. This theorem provides a straight forward computational method for determining if a given distance matrix can be represented as a Euclidean norm. This approach was applied to the motivating example in Section 2 to establish that the Gaussian and other referenced corresponding variograms (excluding the exponential) are no longer conditionally negative definite when used with the city block metric.

4 Norm Dependent Isotropic Functions

There are certain covariogram and variogram functions that retain their positive definite and conditionally negative definite properties when used with distance norms other than the Euclidean norm. Although not new, much of these results have yet to appear in mainstream geostatistical literature or application. Rigorous mathematical development of these and related concepts can be found in Gneiting (1998, 1999b, 2000) and references within. The demonstration here hinges on results from Richards (1985) who provides the following sufficient conditions for which certain power transforms of α-norms are conditionally negative definite.

Proposition Richards (1985).

(a) *On* $\Re^2$, $\|\mathbf{h}\|_\alpha^\beta$ *is conditionally negative definite if*

  (i) $0 < \beta \leq 1,\ 1 \leq \alpha \leq \infty$, or

  (ii) $0 < \beta \leq \alpha \leq 2$.

(b) *On* $\Re^N$, $N \geq 3$, $\|\mathbf{h}\|_\alpha^\beta$ *is conditionally negative definite if*

  (i) $0 < \beta \leq \alpha \leq 2$, *and if*

  (ii) $\alpha > 2$ *it is not conditionally negative definite for* $\beta > 1$.

These results in combination with Schoenberg's Theorem and (3) can now be used to demonstrate the class of Euclidean isotropic covariogram and variogram functions by allowing for non-Euclidean norm dependent measures of distance. Greater flexibility is gained with processes restricted to $\Re^2$, and since most applications involve analyzing data in $\Re^2$ these extensions are stated separately.

To illustrate, the above results in combination with (3) leads to the following class of norm dependent isotropic powered exponential covariograms. For $\mathbf{h} \in \Re^2$, the functions

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \exp(-\|\mathbf{h}\|_\alpha^\beta/\phi), \quad 0 < \beta \leq 1,\ 1 \leq \alpha \leq \infty \quad \text{or} \quad 0 < \beta \leq \alpha \leq 2$$

and for $\mathbf{h} \in \Re^N,\ N \geq 3,$ the functions

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \exp(-\|\mathbf{h}\|_\alpha^\beta/\phi), \qquad 0 < \beta \leq \alpha \leq 2,$$

are positive definite and hence valid covariograms for $\tau^2, \sigma^2 > 0$. The Euclidean isotropic exponential and Gaussian covariogram functions can be obtained by setting (α, β) to (2,1) and (2,2) respectively. Fixing $\alpha = 2$ provides the current definition of the powered exponential covariogram function (Stein 1999, p. 32-33). Setting $\alpha = \beta = 1$ demonstrates the city block metric with the exponential covariogram, whereas $\alpha = 1$ and $\beta = 2$ (city block metric with the Gaussian covariogram) is not admissible, as was demonstrated previously with the motivating example. For $\mathbf{h} \in \Re^2$, all norms are admissible provided $0 < \beta \leq 1$.

Combining the results from Richards (1985) and Schoenberg's Theorem provides conditions for which $\|\mathbf{h}\|_\alpha^{\beta/2}$ is embeddable and thus can be used with existing isotropic covariogram and variogram functions that are valid in all dimensions. This approach is applied to the Matern class of Euclidean isotropic covariogram functions (Cressie 1991), which is now shown for

$\mathbf{h} \in \Re^2$, to include the functions

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \left\{ (2^{\kappa-1}\Gamma(\kappa))^{-1} \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi \right)^\kappa K_\kappa \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi \right) \right\}, \quad \begin{array}{c} 0 < \beta \leq 1,\ 1 \leq \alpha \leq \infty \\ \text{or} \\ 0 < \beta \leq \alpha \leq 2 \end{array}$$

and for $\mathbf{h} \in \Re^N,\ N \geq 3,$ to include the functions

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \left\{ (2^{\kappa-1}\Gamma(\kappa))^{-1} \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi \right)^\kappa K_\kappa \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi \right) \right\}, \qquad 0 < \beta \leq \alpha \leq 2,$$

for $\tau^2, \sigma^2 > 0$, where $K_\kappa(\cdot)$ represents the modified Bessel function of the third kind of order κ. Setting $\alpha = \beta = 2$ provides the class of Euclidean isotropic Matern covariogram functions and for $\kappa = 0.5, \infty$ in this case the Matern covariogram reduces to the exponential and Gaussian covariogram respectively. Again, for $\mathbf{h} \in \Re^2$, all norms are admissible provided $0 < \beta \leq 1$. However, unlike for the powered norm dependent exponential covariogram above, the exact form of the Matern covariogram is not retained due the exponent $\beta/2$ which equals 1 only when $\alpha = \beta = 2$.

Forms of other existing covariogram functions can be used to demonstrate other classes of norm dependent isotropic covariograms in a similar fashion. Assuming second-order stationarity, relation $\gamma(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h})$ demonstrates corresponding classes of norm dependent isotropic (semi)variogram functions.

Assuming only intrinsic stationarity, the embedding approach can also be used to demonstrate classes of norm dependent conditionally negative definite functions. For example, consider the power variogram function currently defined for $\mathbf{h} \in \Re^N,\ N \geq 1$, to be

$$2\gamma(\mathbf{h}) = \tau^2 + \phi\|\mathbf{h}\|^\delta, \quad 0 < \delta < 2,$$

for $\tau^2, \phi > 0$. Substituting the embeddable norms $\|\mathbf{h}\|_\alpha^{\beta/2}$ for the Euclidean norm $\|\mathbf{h}\|$ in above yields the following class of norm dependent isotropic conditionally negative definite functions. To ensure identifiability, the functions are parameterized with a single exponent parameter $\lambda = \beta\delta/2$. For $\mathbf{h} \in \Re^2$, the functions

$$2\gamma(\mathbf{h}) = \tau^2 + \phi\|\mathbf{h}\|_\alpha^\lambda, \quad 0 \le \lambda \le 1,\ 1 \le \alpha \le \infty, \quad \text{or} \quad 0 < \lambda < 2,\ \lambda \le \alpha \le 2,$$

and for $\mathbf{h} \in \Re^N,\ N \ge 3,$ the functions

$$2\gamma(\mathbf{h}) = \tau^2 + \phi\|\mathbf{h}\|_\alpha^\lambda, \quad 0 < \lambda < 2,\ \lambda \le \alpha \le 2,$$

for $\tau^2, \phi > 0$, are conditionally negative definite. Setting $\alpha = 2$ provides the Euclidean isotropic family of power variogram models. For $\mathbf{h} \in \Re^2$, all norms yield a conditionally negative definite function provided $0 \le \lambda \le 1$.

Note, for intrinsic stationarity care was taken not to refer to the class of norm dependent conditionally negative definite functions as valid variograms. As stated previously there is a growth condition variograms must satisfy (Matheron 1973) that in the Euclidean norm case is tied directly to the isotropic measure of distance. Resolving this issue for the more general norm dependent class of conditionally negative definite functions would need to be addressed. Pragmatically speaking though, the greater mathematical flexibility achieved by assuming intrinsic stationarity over second-order stationarity is not often realized in applications (author's opinion).

5 Applications

Two examples are provided to demonstrate the process of characterizing isotropic spatial dependence by allowing the data to potentially choose a non-Euclidean inter-point distance measure. The exposition is kept simple only to highlight the general concept, with more application specific details provided in possible future work. All computing was performed in R (R Development Core Team 2005) with necessary modifications applied to functions from the geoR (Ribeiro and Diggle 2001) contributed package.

5.1 Simulated Data

Data were simulated on a 20 × 20 regular grid (n=400) with unit spacing. The norm dependent exponential covariogram function

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \exp(-\|\mathbf{h}\|_\alpha/\phi) \quad 1 \leq \alpha \leq \infty$$

$\tau^2, \sigma^2, \phi > 0$, obtained by fixing the exponent parameter $\beta = 1$, was used to characterize spatial structure. Covariance parameters τ^2, σ^2, and ϕ were set at 0, 10, and 3 respectively. Four data sets were simulated based on setting the distance norm parameter α =1, 2, 3, and 4. For each data set, parameters were estimated via restricted maximum likelihood considering (a) the distance norm parameter α to be fixed at 2 representing Euclidean isotropy and (b) allowing the α parameter to vary $1 \leq \alpha \leq \infty$ representing possible non-Euclidean norm dependent isotropy. Results are listed in Table 1.

For the non-Euclidean isotropic cases $\alpha = 1, 3, 4$, the approach based on allowing the data to estimate the distance norm resulted in smaller minimized negative log restricted likelihoods (NegLogRLike) than the approach based on assuming Euclidean isotropy with $\alpha = 2$ fixed. When α was kept as a parameter it was also estimated in the neighborhood of its true value. For the simulated data set based on Euclidean isotropy $\alpha = 2$, both methods produced similar results. Clearly though with such a well behaved design and one simulation run, the intention here is only as a demonstration.

It is worth noting some numerical comparisons between distance norms to further explore issues related to their involvement in geostatistics. For example,

$$\|\mathbf{h}\|_{\alpha_1} \geq \|\mathbf{h}\|_{\alpha_2} \quad \text{for} \ \ \alpha_1 \geq \alpha_2.$$

A geometric interpretation of which is provided by letting $\mathbf{s}_0$ represent a point of origin and consider other locations $\mathbf{s}_i$ a fixed α-norm distance from $\mathbf{s}_0$, say $\|\mathbf{s}_0 - \mathbf{s}_i\|_\alpha = d$. The diagram below displays the shapes of the distance buffers around $\mathbf{s}_0$ such that for all locations $\mathbf{s}_i$, $\|\mathbf{s}_0 - \mathbf{s}_i\|_\alpha = d$, for $\alpha = 1, 2, \infty$.

[Diagram here]

For $\alpha = 2$ Euclidean norm, all points within a distance d of $\mathbf{s}_0$ fall within a circle of radius d (i.e. radial distance). In contrast, all points within an α-norm distance d of $\mathbf{s}_0$, $\alpha = 1, \infty$, correspond to diamond and square shaped buffers respectively. Shapes for distance buffers based on α norms not shown fit respectively within those displayed.

In terms of the traditional graphical approach towards characterizing spatial dependence Figure 1 displays estimated variograms using the method of moments estimator (Cressie 1991), adjusted to consider $\|\mathbf{h}\|_\alpha$ isotropy. Using the simulated data set above for $\alpha = 2$ Euclidean isotropy, shown are estimated variograms based on $\alpha = 1, 2, 3, 4$. Immediate from Figure 1 is the similarity in estimates, especially for the more important distances near the origin. This is an artifact not only of the sample design but that distance norms themselves not being very different for relatively small distances. Add to this the practice of distance binning, common for real data not sampled on a regular grid, that may further mask any differences when considering different norm isotropies. This of course only applies to the method of moments variogram estimator and similar graphical procedures used to characterize spatial dependence.

5.2 Swiss Rainfall Data

Spatial Interpolation Comparison 1997 (SIC97) was a public domain exercise in spatial data analysis organized under the auspices of the Radioactive Environmental Monitoring (REM) institutional support program of the Environmental Institute at the Joint Research Center in Ispra, Italy (http://www.ai-geostats.org/events/sic97/SIC97_description.htm). The main objective of SIC97 was to provide a general overview and highlight latest developments in spatial statistics by having different individuals analyze the same data set. Results from this endeavor have been published in a special issue of the *Journal of Geographic Information Decision and Analysis* (GIDA 1998, v2, no 1-2). As part of this exercise 100 daily rainfall measurements made in Switzerland on May 8, 1986 were made available to participants. One source for this data can be found in the geoR contributed R package (Ribeiro and Diggle 2001).

Following Christenson et. al (2001), who used the same data to demonstrate a transformation based approach for positive-valued spatial data, we begin with the square root transform of the SIC97 rainfall data. The norm dependent isotropic Matern class of covariograms,

$$C(\mathbf{h}) = \tau^2 + \sigma^2 \left\{ \left(2^{\kappa-1}\Gamma(\kappa)\right)^{-1} \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi\right)^{\kappa} K_\kappa \left(\|\mathbf{h}\|_\alpha^{\beta/2}/\phi\right) \right\}, \quad \begin{array}{c} 0 < \beta \leq 1, \ 1 \leq \alpha \leq \infty \\ \text{or} \\ 0 < \beta \leq \alpha \leq 2, \end{array}$$

with $\tau^2, \sigma^2, \phi > 0$ is selected to characterize spatial structure. To minimize the number of parameters requiring estimation, we fix $\kappa = 0.5, 1, 2$. The parameter β is also fixed at $\beta = 1$ when focus is on the effect of allowing the data to chose among all possible α-norms. Covariance parameters including the distance norm parameter α are estimated via restricted maximum likelihood.

Table 2 lists the results for various fits of the norm dependent Matern class of covariogram functions. First listed are the models corresponding to Euclidean isotropy (with parameters $\alpha = \beta = 2$ fixed), followed by results allowing the α-norm parameter to vary $1 \leq \alpha \leq \infty$ with $\beta = 1$ fixed. The minimum negative log restricted likelihood is achieved by setting $\kappa = 2.0$, $\beta = 1$ and allowing the data to choose the distance norm which was estimated to be $\widehat{\alpha} = 6.24$. Although as clearly shown, the difference between this and the fixed Euclidean isotropic cases is negligible in terms of this criterion. Support for the claim that spatial dependence be a function of Euclidean distance in the $\Re^2$ dimension in which rainfall was measured is certainly a scientifically plausible interpretation.

6 Discussion

A simple example was used to demonstrate there are no guarantees that the existing pool of isotropic covariogram and variogram functions remain valid when used with a distance measure other than Euclidean. It is therefore essential to establish the validity of these functions when an alternative measure of distance is proposed. By linking the concepts of isometric embedding, conditionally negative definiteness, and positive definiteness, an approach for demonstrating classes of norm dependent isotropic covariogram and variogram functions was provided. An appealing proposition from this is that in practice data can be used to estimate the distance norm, as was shown with the examples in the previous section. These examples though were for demonstration purposes only, with further work required to fully explore such a proposition. Also, covariogram/variogram function identification and estimation is usually an intermediate step towards some form of spatial prediction. Evaluating the practical benefit of a non-Euclidean norm dependent isotropic approach should certainly involve results at this prediction stage.

Define the non-Euclidean distance problem in geostatistical related applications to include issues stemming from the process of using a non-Euclidean distance (at least non-Euclidean in the dimension the process is observed) to characterize isotropic spatial dependence via a covariogram or variogram function. As demonstrated here, existing isotropic functions are likely norm dependent, such as Euclidean distance or the extensions outlined in Section 4. Not considered here are the situations involving a distance measure ρ that is not necessarily a norm function, for example distances traveled through complex waterways or roads as can be computed using geographic information systems. Establishing the validity of $C(\rho)$ or $2\gamma(\rho)$ as functions of isotropic spatial dependence, either for known covariograms and variograms or for newly developed classes of such functions, may be mathematically challenging. Methods for dealing with such situations has not received much attention, possibly due to the lack of convincing evidence for any practical benefits.

One approach for using a general non-Euclidean distance measure ρ for geostatistical applications could be based on multidimensional scaling. Multidimensional scaling (Mardia et al. 1995) is a multivariate statistical technique concerned with the problem of constructing a set of points so that the Euclidean distance between these points matches (exact or most often approximate) a set of given distances that are likely not Euclidean. The concept of isometric embedding relates to the situation when such a configuration can be found for an exact match. For geostatistical applications a matrix of non-Euclidean inter-point distances (such as those traveled through complex waterways) would be approximated by the Euclidean distance between a set of points (often in a much higher dimension) generated by multidimensional scaling. The analysis would proceed using the approximate Euclidean distances hence avoiding issues of covariogram/variogram validity. In a sense transforming the application to the new Euclidean space determined by the multidimensional scaling. Sampson and Guttorp (1992) propose a similar approach to a different problem. For dealing with Non-Euclidean isotropy in geostatistics, such an idea was originally proposed in Curriero (1996) and more recently applied in Loland and Host (2003). A potential drawback of this approach is based on the fact that the multidimensional scaling Euclidean distance approximation does not consider spatial variation, that is it only considers approximating inter-point distances and ignores the outcome data. Further, it is sample design dependent, in the sense that adding and/or deleting a location (and hence an inter-point distance) can change the distance approximation elsewhere.

Its worth mentioning a few valid criticism related to the general idea of non-Euclidean isotropy in geostatistics. First, in the norm dependent case when the data are used to guide the distance norm, one to two extra parameters (α for the norm and β for its power) require estimation in addition to the usual range, sill, and nugget parameters. Issues of identifiability and reliable estimation certainly come into play. Although in regards to reliable estimation the same can be said for the two extra rotation and stretching parameters involved with geometric anisotropy. Alternatively, the distance norm parameter α and/or β can be set a priori to represent several possible choices and evaluated. A second issue is the fact that for geostatistical applications characterizing spatial dependence is most crucial for smaller distances near the origin of the covariogram or variogram. It may be such that non-Euclidean inter-point distances are very close to their Euclidean counterparts at these smaller distances, a fact that is certainly true for distance norms.

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Table 1: Restricted maximum likelihood parameter estimates and corresponding minimized negative log restricted likelihood (NegLogRLike) for the four simulated data sets based on the norm dependent exponential covariogram with norm isotropy $\|\mathbf{h}\|_\alpha$, $\alpha = 1, 2, 3, 4$. Values denoted by * indicate corresponding parameter was fixed at that value.

	Parameter Estimates				
Distance Norm	τ^2	σ^2	ϕ	α	NegLogRLike
$\alpha = 1$	0.00	8.18	2.03	2.00^*	844.33
	0.00	9.77	2.91	1.00	756.37
$\alpha = 2$	0.00	9.51	2.65	2.00^*	830.05
	0.00	9.73	2.72	2.15^*	829.79
$\alpha = 3$	0.33	9.28	3.29	2.00^*	815.59
	0.23	10.49	3.50	3.45	805.41
$\alpha = 4$	0.08	9.93	3.20	2.00^*	813.10
	0.00	9.25	2.71	5.16	794.78

Table 2: Restricted maximum likelihood parameter estimates and corresponding minimized negative log restricted likelihood (NegLogRLike) for the Swiss rainfall data using the norm dependent isotropic Matern class of covariogram functions. Values denoted by * indicate corresponding parameter was fixed at that value.

Parameter Estimates						
κ	τ^2	σ^2	ϕ	α	β	NegLogRLike
0.5	0.00	24.54	50.89	2.00*	2.00*	246.28
1.0	0.00	21.14	18.35	2.00*	2.00*	243.50
2.0	0.00	18.70	8.47	2.00*	2.00*	245.45
0.5	0.00	67978.88	36447.43	12.35	1.00*	249.31
1.0	0.00	9172.12	215.49	4.61	1.00*	243.60
2.0	0.00	68.61	5.65	6.24	1.00*	243.19

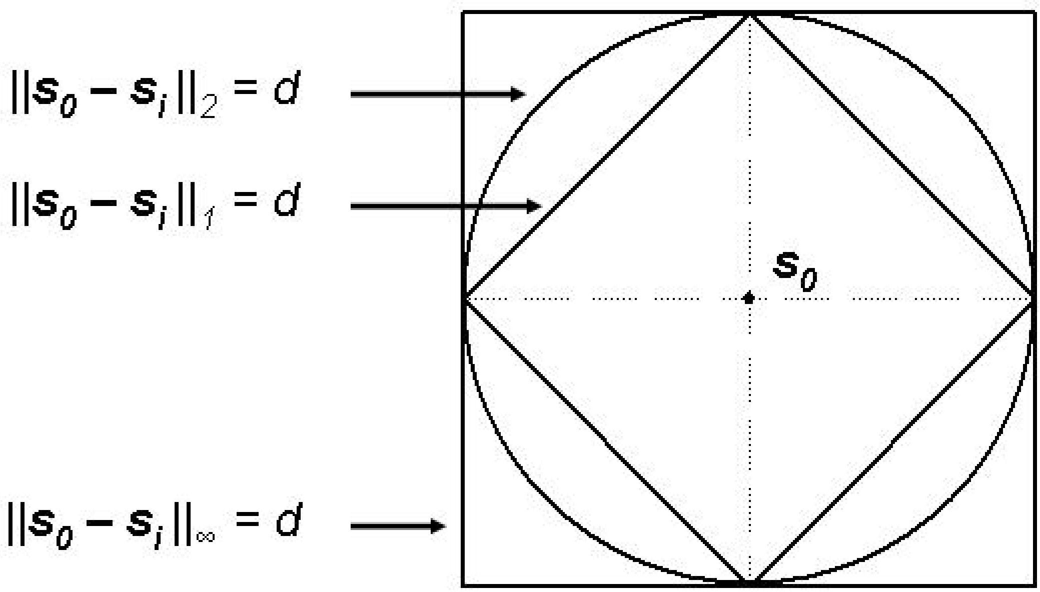

Diagram: α-norm distance buffers, α = 1, 2, ∞.

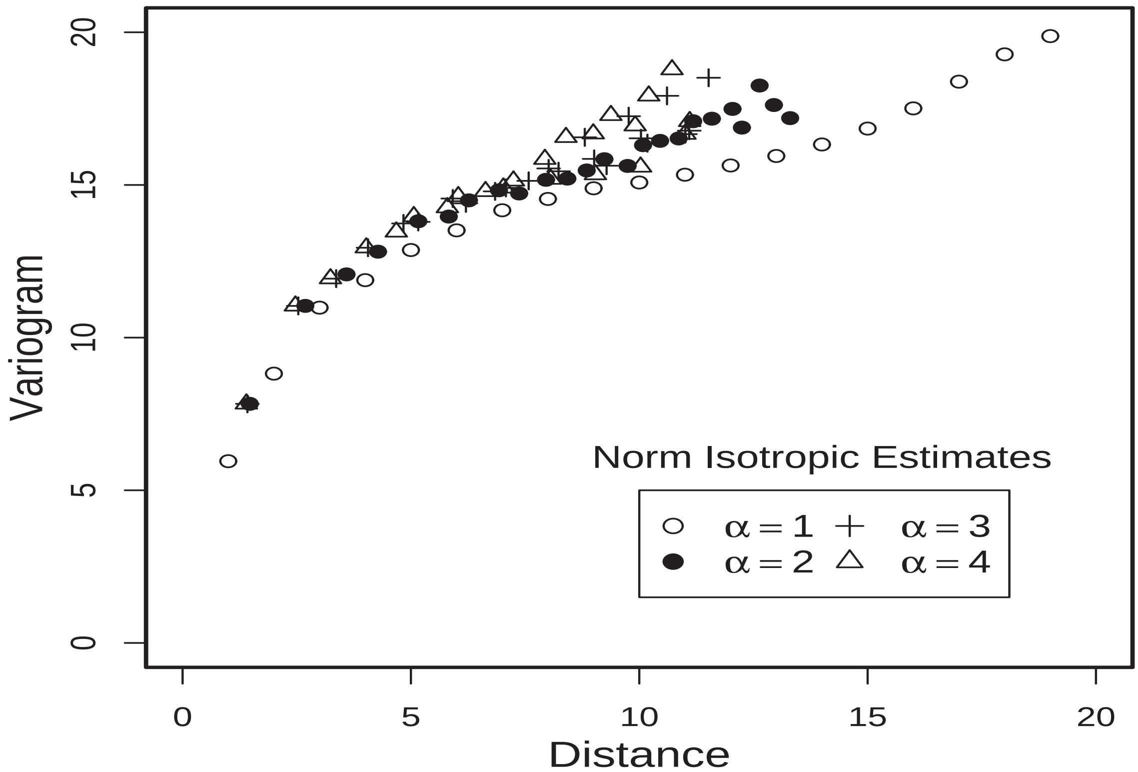

Figure 1: Variogram estimates for the $\alpha = 2$ Euclidean isotropic simulated data set. Shown are the α isotropic method of moments estimator for $\alpha = 1, 2, 3, 4$.