INFERENCE FOR SPATIAL AUTOCORRELATION FUNCTIONS

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PAUL SWITZER

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ABSTRACT

Some general methods are proposed for generating confidence interval estimates for parameters of a variogram model. Particular attention is paid to scale and shape parameters and to joint estimation procedures for the scale parameter and the replication variance (nugget effect). The connection is made to formal testing of the hypothesis of the absence of spatial autocorrelation at a specified distance scale.

1. INTRODUCTION

This paper describes general and elementary approaches to statistical inference for parameters of a spatial autocorrelation model via the variogram. The first part concerns estimation of a scale parameter primarily intended to describe the linear part of the variogram for short inter-point distances. The second part concerns inferences for a shape parameter, basically describing the variogram for medium and long inter-point distances, and the associated problem of testing for the absence of spatial autocorrelation at specified distance scales. The third part concerns inference for the replication variability at zero distance (nugget effect) and simultaneous inference for the important problem of joint estimation of the nugget effect and the scale parameter of the variogram.

The basic ideas involve linear transformations of the data to uncorrelated quantities of constant variance and the comparisons of certain rank orderings. Fourth moment considerations play no role. Related work on inference for variograms may be found in Matheron [1] and in the time series literature such as Anderson [2]. However, the time series literature depends either on having equally spaced data or on a constructive model for the data or both.

The main application of inference on variograms is to provide confidence intervals for estimation variances which are functionals of the variogram; thereby one obtains more realistic less optimistic interval estimates for interpolated values, block averages, and other quantities which are calculated as linear functions of the data.

2. SCALE PARAMETER ESTIMATION

We consider first the case where the variogram model has been specified completely up to a scaling constant. This would be the case, for example, for the family of linear variograms. For a general stationary spatial process $Z(x)$ let

$$\gamma(h) = \tfrac{1}{2}E[Z(x) - Z(x+h)]^2 = \tau^2 \cdot \tilde{\gamma}(h)$$

where $\tilde{\gamma}(h)$ is completely specified and, for definiteness, $\tilde{\gamma}(h)$ may be taken to have unit slope at the origin. The linear variograms have $\tilde{\gamma}(h) = |h|$. The objective is to make inferences about τ, e.g. a confidence interval of possible τ values which are consistent with the data.

The general plan is to transform the observed random variables $Z(x_i)$, $i=1, \ldots, n$, to a set of uncorrelated random variables with zero mean and a constant variance depending on τ. Then standard procedures are used to obtain confidence intervals for this variance. It is straightforward to first obtain zero-mean linear combinations of the observations which are called "contrasts." For example, in the stationary case every difference $Z(x) - Z(x')$ is a contrast. Suppose we define m linearly independent contrasts $D_1, D_2, \ldots, D_m$. (The discussion of the choice of m and the choice of the D_i is deferred.) The vector of these contrasts may be represented as

$$D = A \cdot Z$$

where A is an $m \times n$ matrix with row sums equal to zero, and Z is the vector of observable data $Z(x_1), \ldots, Z(x_n)$.

The covariance matrix of the vector of contrasts, D, may be expressed as

$$\mathrm{cov}(A \cdot Z) = -(\tau^2)\ A\Gamma A' \equiv \tau^2 \cdot \Sigma$$

where

$$\Gamma_{ij} = \tilde{\gamma}(x_i - x_j) \ .$$

Then Σ is a completely determined $m \times m$ covariance matrix. There now exist known linear transformations of the vector D which will produce a new vector of m uncorrelated contrasts Δ with constant variance, and Δ like D will have zero-mean vector, i.e.,

$$\Delta = T \cdot D \ ;$$

$$\mathrm{cov}(\Delta) = \tau^2 \cdot I_{m \times m} \ ;$$

$$E(\Delta_i) = 0,\ E(\Delta_i^2) = \tau^2, \text{ for } i=1, \ldots, m \ .$$

The $m \times m$ matrix T is not unique. A reasonable choice for T could be the matrix of eigenvectors of Σ, rescaled to give unit variances.

From the observable data vector Z one now computes the observed vector $\Delta = (T \cdot A) \cdot Z$ and the squared values Δ_i^2, $i=1, \ldots, m$, whose expectations are all equal to the unknown τ^2. If we act as though the uncorrelated Δ_i were statistically independent then we may construct approximate confidence intervals based on the central limit theorem. Specifically, let

$$\hat{\tau}^2 = \Sigma \Delta_i^2 / m, \quad S^2(\hat{\tau}^2) = \Sigma (\Delta_i^2 - \hat{\tau}^2)^2 / m^2 \ .$$

If z_α is the upper α point of a standard Gaussian distribution, then an approximate confidence interval for the scaling constant τ^2 of a family of variograms is given by

$$\hat{\tau}^2 - z_{\alpha/2} \cdot S(\hat{\tau}^2) \leq \tau^2 \leq \hat{\tau}^2 + z_{\alpha/2}\ S(\hat{\tau}^2)$$

with coverage probability $1-\alpha$, approximately.

As an illustration suppose we are interested in estimating the scaling constant of the variogram for short inter-point distances, and are willing to act as though this variogram were linear for short distances and flat at long distances. We may operate on disjoint contrasts of the form $D_i = Z(x_i) - Z(x_i')$ for selected data pairs. For simplicity of the illustration suppose that the separation between data pairs is sufficiently large that the contrasts are uncorrelated with each other. The transformation matrix T can be taken to be the diagonal matrix with

$$T_{ii} = [2|x_i - x_i'|]^{-\frac{1}{2}} .$$

Then $\Delta_i^2 = \frac{1}{2}[Z(x_i) - Z(x_i')]^2/|x_i - x_i'|$.

3. SHAPE PARAMETER ESTIMATION

We now consider a richer parametric family of variogram models of the form

$$\gamma(h) = \tfrac{1}{2}\cdot E[Z(x) - Z(x+h)]^2 = \tau^2\cdot\tilde{\gamma}(h;\theta) ,$$

where θ is a shape parameter, $\tilde{\gamma}$ is a fixed variogram for each θ, and, as before, τ^2 is a pure scaling constant. It is convenient, but not necessary, to parametrize the variogram family so that θ is proportional to the slope of the variogram at $h=0$, i.e.

$$\frac{\partial}{\partial h}\tilde{\gamma}(h;\theta)\bigg|_{h=0} = k\theta, \quad k \text{ fixed and known} .$$

Common examples are the isotropic spherical and exponential families given respectively by

Spherical: $\tilde{\gamma}(h;\theta) = \frac{3}{2}(\theta h) - \frac{1}{2}(\theta h)^3$ for $0 \leq (\theta h) \leq 1$

$= 1$ for $(\theta h) \geq 1$

Exponential: $\tilde{\gamma}(h,\theta) = 1-e^{-(\theta h)}$ for all $h \geq 0;\ \theta > 0$.

Here, the increment h is treated as a scalar.

The correlation between two linear contrasts, as defined earlier, will still be free of the scaling τ^2 but will depend on θ. For a given vector of m linear contrasts $A \cdot Z = D = (D_1, \ldots, D_m)$, their $m \times m$ covariance matrix is

$$\text{cov}(D) = -\tau^2 \cdot A\Gamma(\theta)A' \equiv \tau^2 \Sigma(\theta)$$

where

$$\Gamma_{ij}(\theta) = \tilde{\gamma}(x_i - x_j;\ \theta) \ .$$

The transformation of D to a vector of m uncorrelated equal variance linear contrasts, Δ, now depends on the correct choice for θ. Let $T(\theta_0)$ be such an $m \times m$ transformation matrix for a particular $\theta = \theta_0$, i.e.,

$$\Delta(\theta_0) = T(\theta_0) \cdot D \ ,$$

$$\text{cov}_{\theta_0}\{\Delta(\theta_0)\} \propto I_{m \times m} \ ,$$

and, in particular,

$$E_{\theta_0}\{\Delta_i^2(\theta_0)\} = \text{constant for all } i=1, \ldots, m \ .$$

However, if the correct value of the shape parameter is $\theta \neq \theta_0$, then the covariance matrix of $\Delta(\theta_0)$ will not be proportional to the identity matrix. In particular, the transformed linear contrasts which are the components of

$\Delta(\theta_0)$ will typically not have equal variances, although means of these contrasts must necessarily remain zero, i.e.

$$E_\theta\{\Delta_i^2(\theta_0)\} \neq E_\theta\{\Delta_j^2(\theta_0)\} \quad \text{for} \quad \theta\neq\theta_0 \quad \text{and} \quad i\neq j \ .$$

Let $r_i(\theta_0;\theta)$ be the rank order (fixed) of $E_\theta\{\Delta_i^2(\theta_0)\}$ among the set of m such values for $i=1, \ldots, m$. Similarly, let $R_i(\theta_0)$ be the rank order (stochastic) of the observed value of $\Delta_i^2(\theta)$ among the set of m such values for $i-1, \ldots, m$. Then both rank vectors $r(\theta_0,\theta) = [r_1(\theta_0,\theta), \ldots, r_m(\theta_0,\theta)]$ and $R(\theta_0) = [R_1(\theta_0), \ldots, R_m(\theta_0)]$, are permutations of the integers $1, \ldots, m$. The two permutations will appear to be correlated if the correct parameter value is $\theta\neq\theta_0$.

However, if θ_0 is the correct value then the random variables $\Delta_i(\theta_0)$ have constant variance for all i and are uncorrelated. If we strengthen the assumptions by regarding the $\Delta_i(\theta_0)$ as exchangeable random variables when θ_0 is the correct shape parameter then the stochastic rank vector $R(\theta_0)$ will be a completely random permutation of $1, \ldots, m$ and therefore uncorrelated with the fixed rank vector $r(\theta_0,\theta)$. Hence, a test of θ_0 versus θ can be constructed using a measure of the correlation between the two sets of ranks, and all such tests will be distribution-free.

The inconvenient aspect of the above described test of the shape parameter is that it depends both on the parameter value being tested, θ_0, and an arbitrary "alternative" value, θ, through the fixed rank vector $r(\theta_0;\theta)$. To overcome, in part, the lack of uniformity of the test over θ, we consider only the "local" alternatives near the tested value θ_0, i.e. $\theta=\theta_0+\varepsilon$ for sufficiently small $|\varepsilon|$. Then we are led to define the fixed rank vector $r(\theta_0)$ as follows:

$r_i(\theta_0)$ is the rank order of $\frac{\partial}{\partial\theta} E_\theta\{\Delta_i^2(\theta_0)\}\Big|_{\theta=\theta_0}$

among the set of m such values for $i=1, \ldots, m$.

The test for θ_0 is then based on the correlation of the fixed rank vector $r(\theta_0)$, just defined, with the random rank vector $R(\theta_0)$ defined above.

A common test of the independence of two rank vectors of length m is based on the rank statistic (Spearman's coefficient) as described in Kendall [3]:

$$K(\theta_0) = 1-6 \sum_1^m (R_i - r_i)^2/(m^3-m) .$$

If the rank vectors are independent then the upper $\alpha/2$ point of the random sampling distribution of K is given approximately by

$$K_{\alpha/2} = z_{\alpha/2} \cdot \sqrt{m} .$$

Therefore, a value of the shape parameter θ_0 would be rejected at level α if $|K(\theta_0)| > K_{\alpha/2}$. The set of θ_0 values which are not rejected comprise a confidence set for θ at level $1-\alpha$.

As an example, suppose our linear contrasts are chosen to be differences of data pairs, i.e.,

$$D_i = Z(x_i) - Z(x_i') \quad \text{for} \quad i-1, \ldots, m .$$

Further, suppose that the data pairs are disjoint and well separated from one another so that, for any reasonable value of θ, the data pairs are uncorrelated. For testing that $\theta=\theta_0$, a transformation to uncorrelated equal variance linear contrasts is given by

$$\Delta_i(\theta_0) = [Z(x_i) - Z(x_i')]/[\tilde{\gamma}(x_i - x_i';\ \theta_0]^{\frac{1}{2}} \quad \text{for} \quad i=1,\ \ldots,\ m\ .$$

The rank vector, $R(\theta_0)$, is given by the ranks of the $\Delta_i^2(\theta_0)$ computed using the observed Z data. The fixed rank vector, $r(\theta_0)$, does not depend on the data and is given by the ranks of

$$\frac{\partial}{\partial\theta} E_\theta\{\Delta_i^2(\theta_0)\}\Big|_{\theta=\theta_0} = \frac{\frac{\partial}{\partial\theta}\tilde{\gamma}(x_i - x_i';\ \theta)\Big|_{\theta=\theta_0}}{\tilde{\gamma}(x_i - x_i';\ \theta_0)}\ .$$

In the case of the exponential and spherical variograms and many other parametric models a substantial further simplification is possible. For every possible value of the shape parameter θ_0 it can be shown that the above ranking criterion is a monotone function of the inter-point distances $|x_i - x_i'|$ provided all such distances are less than the range of the variogram. Hence, the fixed rank vector $r(\theta_0)$ would be the same for every θ_0 and corresponds to the ranking of the inter-point distances of the m data pairs.

4. TESTING RANDOMNESS

Consider the problem of testing for the absence of spatial autocorrelation (randomness) at inter-point distances exceeding some specified distance h_0. We may take a subset of the data points whose inter-point distances all exceed h_0. The hypothesis of randomness may be embedded in a parametric family of variogram functions. Since the convention is to parametrize variograms so that the parameter θ is proportional to the slope of the variogram at the origin it follows that the value $\theta=0$ will correspond to randomness.

Hence we may follow the prescription of Section 3 for testing the hypothesis that $\theta=0$ in some parametric family, i.e., if the value $\theta=0$ is not included in the level $1-\alpha$ confidence set for θ then the hypothesis of randomness is rejected at level α. In general, the test of randomness will depend on the choice of parametric family of variogram.

As in Section 3, the test of $\theta=0$ involves the correlation between a stochastic rank vector $R(0)$ and a fixed rank vector $r(0)$. The vector $R(0)$ does not depend on the particular family of variograms insofar as all calculations involve null correlations. However, the vector $r(0)$ will, in general, depend on the particular variogram family so there is clearly no unique test of randomness in this context.

In the particularly convenient case where the contrasts are differences of disjoint data pairs then, as seen in Section 3, the rank vector $r(0)$ typically corresponds to the ranking of interpoint distances within data pairs. In this case also the stochastic rank vector corresponds to the ranking of the squared differences of the data values within pairs. Therefore, the test for randomness here is based on the rank correlation between $|Z(x_i) - Z(x_i')|$ and $|x_i - x_i'|$ for $i=1, \ldots, m$.

Once again we note that the cutoff K_α is derived under the assumption that the data differences $Z(x_i) - Z(x_i')$ are exchangeable random variables which is not quite the same as saying that they are uncorrelated with the same means and variances.

5. REPLICATION VARIANCE ESTIMATION

In many applications there is implicit replication variability which is not negligible relative to spatial variability and which is part of every observation. This variability, called the nugget effect in mining applications, is commonly modelled as additive white noise lacking spatial correlation. It is best estimated directly from replicated observations in standard ways. However, sometimes replicated observations are not available or are very few in number. It is then necessary to estimate replication variance by extrapolation of the spatial variogram to the origin, i.e. to very short inter-point distances. The presence of non-negligible replication variance will also affect the method for estimating other parameters of the variogram model.

The generalized variogram model is of the form

$$\gamma(h) = \tfrac{1}{2}E\{Z(x) - Z(x+h)\}^2 = \tau^2[\eta + \tilde{\gamma}(h;\theta)]$$

where $\tau^2\eta$ is the replication variance and, as before, τ^2 is a scale parameter, θ is a shape parameter, and $\tilde{\gamma}(0;\theta) = 0$ for all θ. In the following development the shape parameter θ is regarded as fixed and the notational dependence on θ is dropped.

Again we consider a vector of m zero-mean linear contrasts $D - A \cdot Z$, where

$$\mathrm{cov}(D) = \tau^2 \cdot \Sigma(\eta)$$

where

$$\Sigma(\eta) = A \cdot [\eta \cdot I - \Gamma] \cdot A'$$

and

$$\Gamma_{ij} = \tilde{\gamma}(x_i - x_j) \ .$$

Now, for a specified η, the linear contrasts, D, may be transformed to another set of linear contrasts, Δ, using the rescaled eigenvectors of $\Sigma(\eta)$, i.e.,

$$\Delta(\eta) = T(\eta)\cdot D$$

with

$$\mathrm{cov}_\eta(\Delta(\eta)) = \tau^2\cdot I_{m\times m} .$$

When $\tau^2\eta$, the replication variance, cannot be estimated directly from replicated data one should estimate this variance <u>jointly</u> with the scale parameter τ^2 of the variogram using the most closely spaced data points. The estimation proceeds in two stages. First, a confidence interval for η is generated (which does not depend on τ^2) at level $1 - \frac{1}{2}\alpha$. Second, a confidence interval for τ^2 is generated for <u>each</u> η, at level $1 - \frac{1}{2}\alpha$. The resulting joint confidence set for τ^2 and η will have coverage probability greater than $1-\alpha$ by the Bonferroni inequality. This joint confidence set may then be transformed to a joint confidence set for τ^2 and $\tau^2\eta$, the actual replication variance.

The estimation of the replication parameter, η, proceeds as though it were a shape parameter of the variogram. For each putative value η_0, a rank vector $R(\eta_0)$ is obtained from the calculated values of $\Delta_i^2(\eta_0)$. This rank vector is matched with the fixed rank vector, $r(\eta_0)$, based on the values of

$$\frac{\partial}{\partial\eta} E_\eta\{\Delta_i^2(\eta_0)\}\Big|_{\eta=\eta_0} .$$

If the two rank vectors are uncorrelated at level $\alpha/2$ then η_0 is part of the confidence set for η. It is important to note that the scale parameter τ^2 plays no role so far.

Now, if η_0 belongs to the confidence interval for η then we construct a confidence interval for the scale parameter τ^2, according to the method of Section 2, using the m calculated values $\Delta_1^2(\eta_0), \ldots, \Delta_m^2(\eta_0)$. In this way the joint confidence region for η and τ^2 is constructed. The illustration of the next section demonstrates these procedures.

The same paradigm for constructing joint confidence sets for τ^2 and η may also be used to construct joint confidence sets for τ^2 and θ, the scale and shape parameters of the variogram. Sometimes it may also be useful to have joint confidence sets for all three parameters but this will require extension of the methods described here and will be reported later.

6. ILLUSTRATION

When estimating the variogram for small arguments it is reasonable to use contrasts of closely spaced data points such as close spaced differences of data pairs. If the data pairs are sufficiently well separated from one another to be regarded as uncorrelated then it may be sensible to treat the variogram as linear for short distances and flat for long distances. Then the shape parameter θ is explicitly absent in the construction of the joint confidence region for τ^2 and θ, the scale and replication variance parameters.

For example, consider contrasts which are differences of such data pairs. Then the covariance matrix $\Sigma(\eta)$ is the diagonal matrix with

$$\Sigma_{ii}(\eta) = 2\eta + 2|x_i - x_i'| \quad \text{for} \quad i=1, \ldots, m .$$

Then

$$\Delta_i^2(\eta) = \tfrac{1}{2}[Z(x_i) - Z(x_i')]^2/[\eta + |x_i - x_i'|] ,$$

and the ranking criterion for the fixed rank vector $r(\eta)$ is a monotone function of the inter-point distances within pairs.

The table below gives hypothetical values of $[Z(x_i) - Z(x_i')]^2/2$ for 25 such data pairs at indicated distances. These "data" were used to calculate $\Delta_i^2(\eta)$, i=1, ..., 25, for values of η at intervals of 0.1. For each η, a ranking of the $\Delta_i^2(\eta)$ is correlated with the ranks of the inter-point distances using the statistic K of Section 3. It was found that this rank correlation was too large negative for $\eta < 0.3$ and too large positive for $\eta > 2.8$ at the $\alpha = 10\%$ significance level. Hence the 90% confidence interval for η is approximately

$$0.3 \leq \eta \leq 2.8 \; .$$

Hypothetical Numbers Used to Generate a Joint Confidence Region for Parameters of a Variogram

(1,1)	(2.1)	(3,2)	(4,2)	(5,2)
(1,1)	(2,2)	(3,2)	(4,3)	(5,4)
(1,1)	(2,2)	(3,3)	(4,3)	(5,4)
(1,2)	(2,2)	(3,3)	(4,3)	(5,4)
(1,2)	(2,3)	(3,4)	(4,4)	(5,5)

First coordinate: Inter-point distance $|x_i - x_i'|$

Second coordinate: $\frac{1}{2}[Z(x_i) - Z(x_i')]^2$

For each of the accepted η values above, a 90% confidence interval for τ^2 was calculated from the already computed values of $\Delta_i^2(\eta)$ by the standard method described in Section 2. The collection of these τ^2 confidence intervals comprises the joint confidence region for η and τ^2 with coverage probability 80% (by the Bonferroni inequality). Examples of these confidence intervals are:

$$0.75 \leq \tau^2 \leq 0.95 \quad \text{for} \quad \eta = 0.3$$

$$0.60 \leq \tau^2 \leq 0.75 \quad \text{for} \quad \eta = 1.0$$

$$0.40 \leq \tau^2 \leq 0.50 \quad \text{for} \quad \eta = 2.8 \; .$$

It is straightforward to convert the joint confidence region for η and τ^2 to a region for $\tau^2\eta$ and τ^2, i.e., the replication variance and scale parameter. This 80% confidence region is shown in Figure 1. The requirement of a higher confidence probability would have given a larger region.

If the data at the five fixed inter-point distances had been averaged, the resulting five points would appear to lie very close to a straight line, perhaps giving the impression that the variogram has been precisely estimated. In fact, we may derive confidence intervals for the variogram function itself at fixed values of its argument from the joint confidence region for its parameters. This is done by projection of the region onto the straight lines $\tau^2\eta + \tau^2 h$ for selected values of h. This is shown in Figure 2. The coverage probability of 80% applies simultaneously at all arguments h so that, at a fixed single argument, the confidence interval is conservative. For example, a conservative 80% confidence interval for $\gamma(1) = \tau^2(\eta+1)$ is given by

$$1.2 \leq \gamma(1) \leq 2.0 .$$

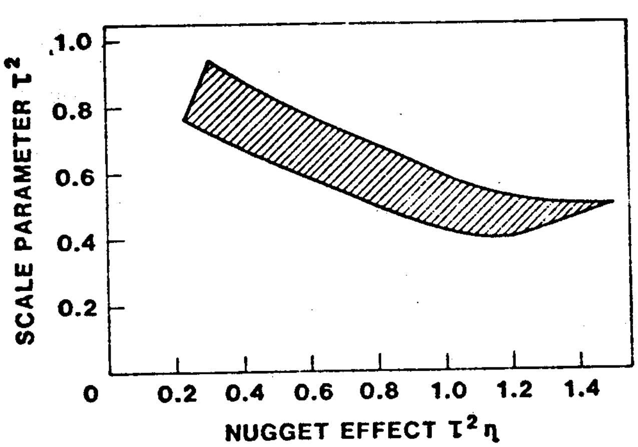

FIG.1 80% JOINT CONFIDENCE SET FOR VARIOGRAM PARAMETER

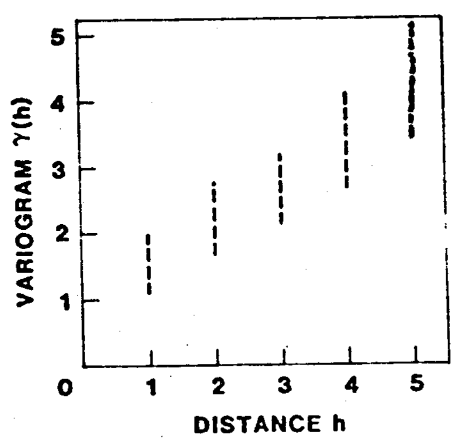

FIG. 2 PROJECTED SIMULTANEOUS CONFIDENCE INTERVALS FOR THE VARIOGRAM AT SELECTED DISTANCES

It must be kept in mind that such confidence intervals are tied to the parametric form adopted for the variogram. If one had a sufficient number of uncorrelated data pairs at a fixed distance h then a confidence interval for $\gamma(h)$ could be computed directly for that h without reference to any parametric model. It would then be interesting to compare it with the conservative intervals derived under parametric modelling.

The method of projecting joint confidence regions for parameters may also be used to obtain simultaneous confidence intervals for variances of interpolatation errors and related quantities, since such variances may be expressed as functions of the parameters of the variogram. Indeed, this may be the most important use of the confidence regions.

7. CONCLUSION

The procedures we have described for inference on the parameters of variogram models are incomplete in many respects and do not lead to any automatic analysis of the second-order properties of spatial data. It will always be important to view the data carefully if only for the purpose of segregating stationary domains and selecting distance scales for modelling variograms. Among the issues not addressed here is the choice of the parametric family of variogram models and the goodness-of-fit issue. In principle, by introducing an extra parameter for model selection, it may be possible to address these issues by the methods here described. Also, we have said nothing about optimization of inference procedures, in particular regarding the choice of linear contrasts which are the basis of the analysis. Presumably, the more such contrasts the sharper is the inference. The illustrations we have used are not meant to exemplify actual practice. Rather they were chosen to exhibit procedures in the least complicated way.

It should be kept in mind that formal inference of the kind described in this paper serves only as a guide to calibration of uncertainty. For example, significance probabilities may be grossly affected by failure to remove nonstationarity or by selective application of inference procedures after prior inspection of the data.

8. REFERENCES

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