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I Introduction

In the previous report on geographical information science (GIS) I chose to concentrate on a single theme: uncertainty and geostatistics (Atkinson, 1999). In this report, I also focus on a single theme: nonstationary geostatistics. I have chosen to present this theme within the context of GeoComputation, which I describe first.

There has been a recent surge of interest in GeoComputation in geographical and related circles (for example, Longley *et al*., 1998; Atkinson and Martin, 2000a; Openshaw and Abrahart, 2000). The term 'GeoComputation' was introduced to the wider geographical analysis community in 1996 when Abrahart organized and ran the first International Conference on GeoComputation at the University of Leeds (Openshaw and Abrahart, 1996). The conference was a resounding success and has been repeated every year since: at the University of Otago, New Zealand, in 1997, the University of Bristol in 1998 and Mary Washington College, Frederiksberg, Virginia, USA, in 1999. The 2000 conference was hosted once again by Abrahart at the University of Greenwich. This year's conference will be held in Brisbane, Australia.

The conference series has had a large impact on the geographical analysis and GIS communities. For example, the GeoComputation conferences have resulted in several journal special issues (Table 1). The proliferation of literature resulting from and related to the series, and the promotion of GeoComputation by its various supporters, has meant that GeoComputation is now much more than a conference series. However, there remains much uncertainty about and speculation on what GeoComputation really is.

The GeoComputation conference series has a homepage (http://www.ashville.demon.co.uk/geocomp/) which provides a definition of GeoComputation, as well as the aims of the conference series, information about previous and forthcoming

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conferences, details of the GeoComputation email list and the make-up of the International Steering Committee. The definition of GeoComputation given on the homepage is a version of Gahegan's (1999) guest editorial of *Transactions in GIS* (Table 1). This editorial emphasizes the enabling technology and defines four significant advances in computer science that have enabled GeoComputation:

1) Computer architecture and design (i.e., parallel processing).
2) Search, classification, prediction and modelling (e.g., artificial neural networks).
3) Knowledge discovery (i.e., data mining tools).
4) Visualization (e.g., replacement of statistical summaries with graphics).

This view of GeoComputation as enabled by technology is similar to the view of astronomy enabled by the telescope (MacMillan, 1998).

Longley (1998) describes GeoComputation, emphasizing data mining and data visualization, but particularly dynamic spatial modelling as described by Burrough (1998) in the same book and by Burrough and McDonnell (1998). Dynamic spatial modelling is also known as distributed spatial process modelling, and encompasses cellular automata and numerical approaches. Within physical geography, cellular approaches have been applied for some time, typically in hydrology (e.g., Kirkby *et al.*, 1987). More recently, Aitkenhead *et al*. (1999) modelled the dynamics of water within the soil using cellular automata. Bates *et al.* (1998) coupled a cellular model of flood dynamics with remotely sensed imagery; a concept that has enormous potential (Curran *et al*., 1999). Coulthard *et al.* (1998) investigated the importance of spatial resolution on the cellular approach. Numerical approaches to spatial dynamic modelling typically involve some system for the solution of partial differential equations. The most popular examples of this type of model are the finite element and finite difference schemes. Hardy *et al.* (2000) modelled suspended sediment deposition using a 2-D finite element scheme, while Lane *et al.* (1999) compared 2-D and 3-D computational fluid dynamics approaches to modelling river channel dynamics. Hardy *et al.* (1999) considered the importance of spatial resolution for hydraulic models of floodplain environments.

Couclelis (1998), also in Longley *et al.* (1998), provides a thought-provoking discussion of GeoComputation in the context of its geographical and, in particular, GIS

Table 1 GeoComputation conferences and related publications

Conference	Year	Publication	Guest editor
Leeds, UK	1996	*Computers and Geosciences* (1998) 24 (4) *Transactions in GIS* (1999) 3 (3)	D. Unwin M. Gahegan
Otago, NZ	1997	*CEUS* (1998) 22 (1)	W. Macmillan
Bristol, UK	1998	*CEUS* (1998) 22 (2) *Hydrological Processes* (2000), in press *Geocomputation: a primer* (1998)	P. Longley P. Longley *et al.*
Frederiksberg, USA	1999	*CEUS* (2000) 24 (5) *Computers and Geosciences* (2001), in press	D. Caldwell

Note: CEUS – Computers, Environment and Urban Systems.

antecedents. Couclelis covers a broad range of subject matter, but most relevant to the present discussion is the view of GeoComputation as separate from mathematical and statistical approaches and, in particular, from quantitative geography. While certain aspects of GeoComputation such as visualization are less amenable to mathematical description, this is not generally the case. Moreover, any computational solution has its roots in mathematics and can be described by mathematical means. I would argue that a large part of GeoComputation is the successful implementation of appropriate (i.e., geographical) mathematics to geographical problems.

A slightly different view is provided by Openshaw (1998). Openshaw has done most to initiate, develop and promote GeoComputation. In my view, Openshaw's argument is essentially a reaction against classical statistical methods that are clearly not applicable to spatial data where the assumption of data independence (lack of statistical correlation) is invalid. The message could be interpreted as follows (after Atkinson and Martin, 2000b). Do not:

1) apply classical statistics to geographical data as though they were statistically independent;
2) 'generalize out' the geography with stationary models (e.g., spatially constant mean or variogram); and
3) rely on model-based statistics for inference when the power of the computer can let spatial data speak for themselves.

These are compelling arguments for geographers, whose very discipline is concerned with variation across space. Why, as geographers, would we want to throw away the geography? However, it is important to realize that this 'call to geographers' to be more geographical does not imply that there is no place for (e.g., statistical) models in geography. The geographically weighted regression (GWR) developed by Brunsdon *et al.* (1996) is a good example of a statistical approach (linear regression) being adapted to emphasize the geography. Similarly, in the field of dynamic spatial modelling, analytical and stochastic approaches very much fit in with Openshaw's view.

There are many strands of GeoComputation, such as visualization of spatial data (see Kraak and MacEachren, 1999; Fuhrmann *et al.*, 2000), spatial data mining and dynamic spatial models (see, for example, the titles of keynote lectures given at recent GeoComputation conferences – Tables 2 and 3). All these subjects have one important common thread: they involve the application of *geographical* tools to *geographical* problems. The essence of GeoComputation is, thus, that geographical tools are applied in place of inappropriate aspatial tools (for example, borrowed from other disciplines).

In the end, GeoComputation will be defined by what GeoComputation researchers do. This 'bottom-up' view is also taken by Ehlen and co-workers in their keynote address at GeoComputation 2000 (Table 3). Ehlen and co-workers used computer algorithms to deconstruct the language used in the papers of past GeoComputation conferences to describe and define GeoComputation. For the purposes of this article, I have chosen to concentrate on one theme that fits well within the framework of GeoComputation: nonstationary modelling. Following my own interests, I have chosen to review nonstationary approaches from a geostatistical perspective.

Table 2 Keynote speakers at GeoComputation 1999

Speaker	Title
G. Kucera	Pluralism in spatial information systems
D. Landgrebe	Information extraction principles for hyperspectral data
A. MacEachren	Exploring geo-data spaces – the search for meaning
M. Oliver	Investigating the spatial variation of radon in soil geostatistically
I. Turton	Geographical data mining: key design issues
R. White	High resolution integrated modelling of the spatial dynamics of urban and regional systems

Table 3 Keynote speakers at GeoComputation 2000

First author	Title
F. Rohlf	Geometric morphometrics and visualizations of statistical analyses of shape
M. Batty	Visualization in GeoComputation
M. Gahegan	Geovista Studio: a geocomputational workbench
G. Tucker	The pitter-pat of tiny raindrops: applications of dynamic landscape modelling in geomorphology, flood hydrology, and archaeology
J. Ehlen	The semantics of geocomputation

II Nonstationary geostatistics

A central decision made in traditional geostatistics is to model the spatial structure in the variable of interest with a *stationary* covariance function or variogram. Stationary in this context means that the covariance function, defined as a parameter of the random function model, is invariant with location **x**. Importantly, the term 'stationary' refers only to the *model* and not to the *data*. There is no such thing as a stationary data set (Myers, 1989). Moreover, we cannot test for stationarity (Journel, 1996).

Geostatistics has, to my mind, always been eminently suitable for application in physical geography. It allows *local* optimal interpolation and simulation of spatial variables – tasks that are found frequently in physical geography. However, geographers have been slow to adopt geostatistical approaches, and one possible reason for this is the dependence on a stationary covariance function. Recent geostatistical applications in which *nonstationary* models have been applied should, thus, be of interest to proponents of GeoComputation. I first introduce the random function model and basic geostatistical concepts to facilitate interpretation of the nonstationary modelling that follows.

1 The random function model

The most important distinction to make in geostatistics is that between model and data. A first step in most geostatistical analyses consists of estimating some function such as the covariance function or, more commonly, the variogram (hereafter I refer to the variogram) to describe the spatial variation in a region of interest. This variogram must be obtained from sample data (referred to as an experimental variogram). To use the experimental variogram to *infer* further information about the region of interest (e.g., to predict spatially some unobserved value), generally, we need to adopt some formal model of the spatial variation. Most commonly, the random function (RF) model is used. The variogram is then defined as a *parameter* of this RF model and may, itself, comprise several parameters. To estimate the variogram function (defined as a parameter) from the experimental variogram it is necessary to fit some continuous mathematical function to the experimental values. Then, the fitted function *estimates* the RF model parameter.

Let us define a continuous random variable (RV) $Z(\mathbf{x}_0)$ at location $\mathbf{x}_0$ as fully characterized by the cumulative distribution function (cdf) which gives the probability that $Z(\mathbf{x}_0)$ is no greater than a given threshold z:

$$F(\mathbf{x}_0; z) = \text{Prob}\{Z(\mathbf{x}_0) \leq z\} \qquad \forall z \tag{1}$$

An RF is then a set of RVs arranged spatially such that their interdependence may be expressed as a function of separating distance. The $\alpha = 1, 2, \ldots n$ RVs $Z(\mathbf{x}_\alpha)$ may be fully characterized by the n-variate or n-point cdf:

$$F(\mathbf{x}_1, \ldots, \mathbf{x}_n; z_1, \ldots, z_n) = \text{Prob}\{Z(\mathbf{x}_1) \leq z_1, \ldots, Z(\mathbf{x}_n) \leq z_n\} \qquad \forall z \tag{2}$$

Equation 2, defined for any choice of n and any location $\mathbf{x}_\alpha$, is known as the spatial law of the RF $Z(\mathbf{x}_\alpha)$. For most geostatistical applications we do not need the entire spatial law, and can restrict our analysis to the one- and two-point cdfs, the covariance function, autocorrelation function and variogram.

For continuous variables, the experimental semivariance is defined as half the average squared difference between values separated by a given lag $\mathbf{h}$, where $\mathbf{h}$ is a vector in both distance and direction. Thus, the experimental variogram $\gamma(\mathbf{h})$ may be obtained from =1, 2, . . . , $P(\mathbf{h})$ pairs of observations $\{z(\mathbf{x}), z(\mathbf{x} + \mathbf{h})\}$ at locations $\{\mathbf{x}, \mathbf{x} + \mathbf{h}\}$ separated by a fixed lag $\mathbf{h}$:

$$\gamma(\mathbf{h}) = \frac{1}{2P(\mathbf{h})} \sum_{\alpha=1}^{P(\mathbf{h})} [z(\mathbf{x}_\alpha) - z(\mathbf{x}_\alpha + \mathbf{h})]^2 \tag{3}$$

Where the RVs which constitute the RF $Z(\mathbf{x})$ are not independent it should be possible to predict spatially one value, say $Z(\mathbf{x}_0)$, from neighbouring data using techniques such as kriging.

2 Spatially nonstationary mean

For most traditional geostatistical applications, for example, mining and petroleum geology, data are expensive. Thus, the number of data available to estimate the variogram and predict spatially is often limited to about 100 (mining) or less (petroleum geology), depending on the application. Where data are sufficient (e.g., around 100), it may be possible to model a locally varying mean with a nonstationary model of the mean, termed a trend (or drift). Much early geostatistical research was devoted to developing methods for modelling a locally varying mean using trends, and these are discussed below.

All kriging algorithms are variants of the least squares regression predictor (Goovaerts, 1997):

$$\hat{Z}(\mathbf{V}) - m(\mathbf{V}) = \sum_{\alpha=1}^{n(\mathbf{V})} \lambda_\alpha(\mathbf{V})[Z(\mathbf{x}_\alpha) - m(\mathbf{x}_\alpha)] \tag{4}$$

where λ_α are the weights applied to data $z(\mathbf{x}_\alpha)$ interpreted as realizations of the RV $Z(\mathbf{x}_\alpha)$, and $m(\mathbf{V})$ and $m(\mathbf{x}_\alpha)$ are the means of the RVs $Z(\mathbf{V})$ and $Z(\mathbf{x}_\alpha)$. In practice, prediction is achieved using *only* the $n(\mathbf{V})$ point or quasi-point data $z(\mathbf{x}_\alpha)$ at locations $\mathbf{x}_\alpha$ within a *local neighbourhood* $W(\mathbf{V})$.

The actual type of kriging predictor adopted varies depending on the model adopted for the RF. In general, the RF can be decomposed into two components as follows:

$$Z(\mathbf{V}) = R(\mathbf{V}) + m(\mathbf{V}) \tag{5}$$

where $R(\mathbf{V})$ is modelled as having zero mean or expectation and its variation is modelled using the variogram. The component $m(\mathbf{V})$ is the mean of the RF $Z(\mathbf{V})$ and this can be modelled in various ways depending on the type of kriging predictor adopted.

In simple kriging (SK), the mean is modelled as known and *stationary* across space. Ordinary kriging (OK) is an extension of SK to the case of an unknown mean. The local mean within a moving window around each location $\mathbf{x}_0$ to be predicted is used to estimate the unknown locally stationary mean within that window (Journel and Huijbregts, 1978). Thus, for OK the mean is neither known nor stationary across the region of interest. Kriging with a trend model (KT) (also known as universal kriging) was developed to model a local mean that is not stationary, even within a local neighbourhood (Matheron, 1969; Armstrong, 1984; Goovaerts, 1997). In KT the trend is fitted to the data using some least squares algorithm and kriging is performed on the residuals (Kitanidis, 1997). An important distinction occurs between global KT in which the trend is fitted once and local KT in which the trend is fitted locally to data neighbouring each $\mathbf{x}_0$. For global KT, kriging is applied to the residuals from the trend using the detrended variogram. However, for local KT the locally detrended variogram is unknown, presenting problems for successful application. This problem is important because local KT often provides sizeable increases in prediction accuracy over OK. An alternative model for a locally varying mean is provided by the so-called intrinsic random functions of order-k (IRF-k) (Delfiner, 1976; Chiles and Delfiner,

1999). In the IRF-*k* model the trend is modelled as a series of monomials that are just sufficient to filter the trend from the data leaving residuals with a stationary covariance function.

3 Spatially nonstationary variogram

Where the number of data is limited (as with mining and petroleum geology), the investigator has little choice but to decide to use a stationary model of the variogram. That is, the variogram is modelled as being spatially invariant within the region of interest. However, for environmental applications, the number of data available is often much greater than 100. For example, for remote sensing and other spatial properties that are inexpensive to measure, such as elevation, the number of observations can be in excess of 1 000 000. Such sources of data allow for the possibility of nonstationary *variogram* models.

Nonstationary models of the variogram have generally tended to fall into three groups: 1) those based on prior segmentation; 2) locally adaptive approaches; and 3) deformation approaches. Deformation approaches, as decribed by Sampson and Guttorp (1992), are beyond the scope of this report. The segmentation approach is based on the assumption that the region of interest can be divided into separate subregions within which the variogram can reasonably be modelled as stationary. There are two ways of achieving the segmentation: 1) prior knowledge (e.g., physical units such as soil types); or 2) automatic division of the space based on some property of the variogram. Segmentation based on prior knowledge has been implemented for many years. For example, Berberoglu *et al.* (2000) segmented a remotely sensed image based on vector polygon data and used variograms estimated within segments to aid per-field classification. Data on some prior 'statification' are generally incorporated into the kriging process via stratified kriging which is nothing more than kriging applied to the strata independently (e.g., Goovaerts, 1997).

Automatic segmentation can be achieved using either a classification algorithm or a segmentation algorithm (in which spatial proximity of like classes is promoted). Generally, segmentation is preferred over classification because the resulting division of space tends to involve fewer and more compact subregions. However, Allard (1998) and co-workers (Allard and Monestiez, 1999; Allard and Guillot, 2000) have implemented classification-based approaches within a geostatistical framework. Further, the geostatistical classification of Oliver and Webster (1989) is a useful way of incorporating a spatial weighting into an unsupervised classification algorithm.

Ideally, where the objective is to identify populations with different variograms, automatic segmentation should be based on some property of the variogram such as the fitted variogram model range. It is well known that change in the sill variance of the fitted variogram model does not affect the kriged predictions (Isaaks and Srivastava, 1989). Rather, change in the range coefficient, change in the nugget variance relative to the sill variance and change in the form of the variogram model have most effect. Ramstein and Raffy (1989) allowed automatic fitting of an exponential model to local variograms estimated for remotely sensed imagery and subsequently segmented on the basis of the range coefficient. St-Onge and Cavayas (1997) employed a similar approach while Lloyd and Atkinson (2001) chose to segment on the basis of the local fractal

dimension because this reduced effectively the information in the local variogram to a single variable.

The locally adaptive kriging (LAK) approach has been applied in a limited number of cases. For example, Haas (1990a; 1990b) was the first to implement a LAK approach (called moving window kriging) applied to atmospheric data. Pieters *et al*. (2001) applied moving window kriging to soil pollution data while Lloyd and Atkinson (2000) used LAK to map digital elevation data. The variogram was estimated and modelled locally and the model coefficients were used in OK locally.

The major problem with LAK (and methods of segmentation based on variogram model coefficients) is that the variogram estimated locally must be fitted with a mathematical model automatically. In some cases, the local experimental variogram has the same general shape for all **x**. For example, for a photogrammetrically derived DEM, Lloyd and Atkinson (2000) found that the Gaussian model provided a reasonable fit in almost all cases because of the inherent smoothness in the data. If the general shape of the experimental variogram varies with **x** then automatic fitting can be difficult. For these reasons, such 'blind' automatic fitting of variogram models without check is discouraged in geostatistical practice. Clearly, what is needed is some alternative method of utilizing the local information on spatial structure without the need for inappropriate 'blind' model fitting.

4 Spatially nonstationary relations: lessons from human geography

One of the most important developments made in recent years in quantitative human geography has been the application of spatial nonstationary models to geographical applications. In particular, the Geographical Analysis Machine (GAM) and Geographical Explanation Machine (GEM) (Openshaw *et al.*, 1987; Openshaw, 1998) represented something of a breakthrough in geographical analysis. While conceptually simple, the GAM represents one of the first attempts to address, in a geographical manner, a clearly geographical problem. The specific problem addressed by Openshaw was to detect clusters of leukaemia in spatial data. The solution involved counting the number of people with and without leukaemia within a circle of given diameter and repeating for all positions on a grid. The exercise was then repeated for various circle diameters. The results were superimposed to provide a scale-independent map of clusters of high incidence (and, by inference, high risk). The Geographical Explanations Machine (GEM) extended this basic approach to the relations between variables rather than cluster detection. The important themes in the GAM were 'local analysis' and 'independence from a statistical model'.

The geographically weighted regression (GWR) proposed by Brunsdon *et al.* (1996) and described by Fotheringham *et al.* (2000) provides an inherently geographical method of analysing relations in geographical data. The model involves applying regression within a local window or kernel to obtain local regression coefficients in place of the usual global set of coefficients. Thus, the result of GWR is a set of maps of regression coefficients. The underlying philosophy of such an approach is either that 1) there is some change in the nature of the relation over space; 2) there may be some properties with low spatial frequency that have not or cannot be measured; or 3) so many properties affect the dependent variable that the full global model is

cumbersome. While it is unlikely in physical geography that (1) can be supported, (2) and (3) often can be.

5 Spatially nonstationary relations: geostatistics

In geostatistics, researchers have analysed the spatial cross-correlation between variables often represented with the cross-variogram. This represents the spatial cross-correlation as well as the simple correlation. The technique of cokriging has been applied widely to predict spatially a primary variable from a sparse sample of that variable plus generous coverage of a secondary correlated variable. Cokriging makes use of the full spatial cross-correlation and, thus, represents a favourable alternative to regression (which utilizes only the simple correlation). Kelly and Atkinson (1999) reported a standard application of cokriging to predict snow depth in the UK from DEM data under a nonstationary (segmented) model of the cross-correlation structure. This amounted to the application of cokriging in Scotland and regression in the remainder of the UK.

A problem with cokriging is that the linear model of coregionalization (LMC) (essentially the combined variogram and cross-variogram models) must satisfy certain constraints that are time-consuming to verify. Recent developments in geostatistics have circumvented the need to fit the LMC. For example, kriging with an external drift (KED) is a modification of the more usual KT in which the trend is modelled as a function of some secondary variable with which it is linearly related rather than as a function of the co-ordinates (Goovaerts, 1997). Further, simple kriging with locally varying means (SKlm) is an extension of simple kriging (with a known constant mean) to the case of varying local mean expressed as a function of some secondary variable. Both methods avoid the need to fit the LMC. Goovaerts (1999) provides a comparison of these approaches. Recently, Ma and Journel (1999) have introduced Markov models that allow one to apply cokriging treating one variogram as a linear function of the other.

An important development of cokriging has been colocated cokriging in which the spatial cross-correlation structure is ignored and only the simple correlation is used in predicting the primary variable at unknown observations. Clearly, for this to be viable, one must have complete coverage of the secondary variable as with remotely sensed images or digital elevation models. Colocated cokriging has striking similarities to GWR, the main difference being that the variogram model fitted to the primary variable is used for prediction in addition to the regression coefficients. Clearly, colocated cokriging depends on a stationary model of the variogram and correlation. However, where primary data are sufficiently numerous the regression coefficients can be obtained locally (Pereira *et al.*, 2000) amounting to a version of GWR that incorporates *spatial* information in the prediction.

III Conclusion

In simple terms, GeoComputation is the application of *geographical* computation to *geographical* problems. For problems to be truly geographical they should have a spatial

component such that for their solution they require a geographical model or algorithm. It is the spatial or geographical components of models and algorithms that make GeoComputation different from other forms of computation. Geostatistics fits into the GeoComputation paradigm only in that prediction and simulation are explicitly local. The decision of stationarity taken in most geostatistical applications seems inherently aspatial. However, with the availability of large spatial data sets, increasing application of nonstationary geostatistics (involving nonstationary mean, variogram and regression parameters) should help to narrow the gap.

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