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A tutorial guide to geostatistics: Computing and modelling variograms and kriging

M.A. Oliver [a], R. Webster [b,*]

[a] Soil Research Centre, Department of Geography and Environmental Science, University of Reading, Reading RG6 6DW, Great Britain, United Kingdom
[b] Rothamsted Research, Harpenden AL5 2JQ, Great Britain, United Kingdom

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ABSTRACT

Many environmental scientists are analysing spatial data by geostatistical methods and interpolating from sparse sample data by kriging to make maps. They recognize its merits in providing unbiased estimates with minimum variance. Several statistical packages now have the facilities they require, as do some geographic information systems. In the latter kriging is an option for interpolation that can be done at the press of a few buttons. Unfortunately, the ease conferred by this allows one to krige without understanding and to produce unreliable and even misleading results. Crucial for sound kriging is a plausible function for the spatial covariances or, more widely, of the variogram. The variogram must be estimated reliably and then modelled with valid mathematical functions. This requires an understanding of the assumptions in the underlying theory of random processes on which geostatistics is based. Here we guide readers through computing the sample variogram and modelling it by weighted least-squares fitting. We explain how to choose the most suitable functions by a combination of graphics and statistical diagnostics. Ordinary kriging follows straightforwardly from the model, but small changes in the model function and its parameters can affect the kriging error variances. When kriging is automated these effects remain unknown. We explain the choices to be made when kriging, i.e. whether the support is at points or over blocks, and whether the predictions are global or within moving windows.

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* Corresponding author at: Rothamsted Research, Harpenden, Hertfordshire AL5 2JQ, Great Britain, United Kingdom. Tel.: +44 1582 763133.
E-mail address: richard.webster@rothamsted.ac.uk (R. Webster).

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1. Introduction

Daniel Krige, the doyen of geostatistics, died earlier this year at the grand age of 93. Early in his career he developed empirically statistical methods to predict ore grades from spatially correlated sample data in the gold mines of South Africa (Krige, 1951, 1966). In the 1960s his approach was formalized by Matheron (1963, 1965), and the term 'kriging' was coined in his honour. In the two decades that followed environmental scientists – pedologists, hydrologists, geologists, and atmospheric scientists, to name a few – saw the merit of this technology in their own fields (e.g. Burgess and Webster, 1980; de Marsily and Ahmed, 1987; Gajem et al., 1981; McBratney et al., 1982; Vauclin et al., 1983; Russo, 1984; Oliver and Webster, 1987). Now kriging is applied widely and with increasing sophistication in petroleum engineering, mining and geology, meteorology, hydrology, soil science, precision agriculture, pollution control, public health, fishery, plant and animal ecology, and remote sensing. Kriging has become a generic term for several closely related least-squares methods that provide best linear unbiased predictions (BLUP) and also some non-linear types of prediction. It is a major advance over the mathematical methods of interpolation common in the first half of the 20th century.

Environmental surveys are almost always based on samples, but in general the measurements represent a continuum in space from which the sample has been drawn. Most analysts and their clients want to know what values are likely at intervening places. Kriging enables them to predict those values optimally, i.e. without bias and with minimum variance; hence its popularity.

Initially practitioners had to write their own code for geostatistical analysis; they had to have understanding of numerical analysis to program the methods. In the last 20 years the situation has changed dramatically with powerful software that has become widely and cheaply available in the public domain, such as GSLIB (Deutsch and Journel, 1998), gstat (Pebesma, 2004; Pebesma and Wesseling, 1998) and GenStat (Payne, 2013). Gstat in particular is now accessible through R free of charge (see http://cran.r-project.org/web/packages/gstat/index.html). Several geographic information system (GIS) packages also have facilities for geostatistical analysis, and kriging has become one of the favoured interpolation routines, if not *the* favoured one. The 'Spatial Analyst' component of ArcGIS (3D-Analyst and Geostatistical Analyst Tool, ArcGIS version 9.2) is especially congenial with attractive graphics. It has encouraged many environmental scientists to use geostatistics, and specifically ordinary kriging (see Section 4), for interpolation and mapping. With kriging in its various forms, environmental scientists can make spatial predictions at any location between their observation points without bias and take proper account of the errors, which are minimized and also estimated together with the predicted values. Unfortunately, the ease with which modern software can be used means that anyone can produce maps by kriging without understanding what happens between the data and the resulting maps. At the press of a few buttons on a computer one can interpolate from scattered data and display the result as a map. The software becomes a 'black box' in which, somehow, a variogram is computed and values from it are inserted into kriging equations without any intervention or assessment by the user.

There are several textbooks on geostatistics (e.g. Chilès and Delfiner, 2012; Goovaerts, 1997; Olea, 1999), including our own (Webster and Oliver, 2007). Judging from the numerous scripts we are asked to read for this journal and others, however, we have the strong impression that these books do not provide the succinct guidance that authors seek to practice geostatistics wisely. Most authors seem to cull their knowledge from journal articles, many of which are sketchy or misleading and some that are actually wrong.

Our purpose here is deliberately educational; it is to guide investigators, in particular those intent on publishing records of their research in *Catena*, to use the basic geostatistical tools correctly and with understanding, and to avoid the pitfalls that lead to worthless results and misleading claims and to scientific papers that require major revision based on fresh analysis and often more data.

Many environmental scientists who use geostatistical packages have maps as their ultimate goals. But kriging for interpolation is only the penultimate step in a chain that begins with sampling and proceeds through the exploration and screening of data, perhaps transformation, crucially the estimation and modelling of one or more variograms, and ends with graphic display. Here we look at each of these steps and the assumptions required to implement them. We also tell intending authors what they should report so that readers know and could repeat what they have done. We introduce some algebraic notation for brevity, but we have placed most of the essential equations in Appendix A so as not to break the flow of the narrative. You can find them all with explanations in the textbooks cited above.

We are soil scientists, and we set the scene and illustrate the procedures with examples in soil survey. There are close analogies in other branches of land research, and scientists in those fields should find our guide equally apt.

2. Random processes

Features of the environment, such as soil, are the product of many interacting physical, chemical and biological processes. These processes are physically determined, but their interactions are so complex that the variation appears to be random. This complexity and incomplete understanding of the processes means that a deterministic or mathematical solution to quantify the variation is out of reach at present. The logical solution required a leap of imagination by Matheron (1965) in his seminal thesis to treat the variation as though it were random. Let us first translate this idea of a random property into a mathematical one, which we call a random process. We can formalize it in the notation that has become conventional as follows.

1. The value of a property, say z, at any place $\mathbf{x}$, equivalent to x_1,x_2 in two dimensions, and denoted by $z(\mathbf{x})$ is one of an infinity of values of a random variable $Z(\mathbf{x})$ at that place. We call it a 'realization' of the process.
2. The set of random values at all such places, again infinite in number, in a region is a random process, and also denoted $Z(\mathbf{x})$.
3. The random variable is spatially correlated at some scale.

Variables, such as the heights of water tables, the concentrations of elements in soil, air temperatures and rainfall, for example, are regarded as spatial random variables. For each, however, we have only a single realization. Consequently, we cannot compute statistics for the realization or draw inferences from it. Inference requires many realizations, and so