Towards Soil Geostatistics.

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Abstract

In a brief survey of some issues in the application of geostatistics in soil science it is shown how the recasting of classical geostatistical methods in the linear mixed model (LMM) framework has allowed the more effective integration of soil knowledge (classifications, covariates) with statistical spatial prediction of soil properties. The LMM framework has also allowed the development of models in which the spatial covariance need not be assumed to be stationary. Such models are generally more plausible than stationary ones from a pedological perspective, and when applied to soil data they have been found to give prediction error variances that better describe the uncertainty of predictions at validation sites. Finally consideration is given to how scientific understanding of variable processes in the soil might be used to infer the likely statistical form of the observed soil variation.

1 Introduction

Some years ago I was privileged to join a discussion between the late Professor Peter Burrough and Dr Philip Beckett on geostatistics and its place in soil survey. At one point Burrough said, 'Of course, that variogram [for soil clay content] might equally describe the pattern on this carpet.' Ever since then I have been interested in the question of how our understanding of the soil and its variation can be made integral to our practice of geostatistics in soil science. Can we develop a soil geostatistics that is appreciably different to the geostatistics of patterns on the carpet?

In an influential paper Webster [1] suggested a conceptual framework for the application of geostatistics in soil science. The properties of the soil arise from deterministic processes, which we understand. However, we are rarely, if ever, able to deploy that understanding directly to answer the land manager or regional planner who needs predictions of soil properties at unsampled sites. This is because of the complexity and multiplicity of the processes involved, and our ignorance of contingent facts in the history and development of the terrain at sites of interest. Just as the outcome from a fair die can be treated as a

random variable, although it is the outcome of processes governed by Newton's laws, so we can treat soil properties as realizations of spatially correlated random functions, regardless of our understanding of the pedogenetic processes that give rise to them.

I believe that this framework is valid, but also that it needs some modification in the light of how we now do geostatistics in environmental science. The emergence of the linear mixed model framework for geostatistics, encouraged by the books of Stein [2] and Diggle and Ribeiro [3], offers ways to integrate understanding of soil processes with stochastic modelling. Furthermore, it allows us to relax, to some extent, the assumptions of stationarity in the variance that make the classical geostatistical model particularly implausible in the eyes of pedologists. Finally, we might start to investigate how understanding of soil processes could influence not just the fixed effects of the linear mixed model but how we constrain the stochastic element of the model.

The reader who has followed me so far might object that the goal of geostatistics in soil science is to compute reliable prediction distributions of soil properties, this might be improved through refinements of the statistical theory and improved computation, but why through attention to pedology? In reply I would suggest that the refinement of the framework of Webster [1] entails making space in the quantitative model of soil variation for understanding of the soil, and expanding that proportion of the soil's variation that is accounted for by what we understand rather than consign to the stochastic component of the model. Doing this successfully is a sign of real scientific progress. Furthermore, it should allow us to make more efficient use of costly field observations and laboratory analyses. Finally, if we can relate aspects of our statistical model of the soil to our understanding of soil processes then we may end up with a sound basis for proposing prior probabilities for model parameters with genuinely informative priors.

My own preoccupation is with the soil. I am aware that there are other fields of environmental science which are more advanced in the development of a geostatistical framework that explicitly includes process understanding. It has been shown, for example, how the spatial covariance function of gravimetric or magnetometric fields can be represented by a generalized Cauchy function with direct physical meaning [4]. I refer to some related examples in section 4 below. In defence of the soil geostatistician it must be said that these variables are rather simpler, in the sense of being more tightly constrained, than a typical soil property: biological, chemical, or morphological. I would suggest that many sciences that use spatial statistics: agronomy, geochemistry, ecology, entomology and archaeology, resemble soil science with respect to the complexity of the variables that they study. As

such, I would hope that this survey may be of interest to workers outside the field of soil geostatistics, which is why I offer it in response to an invitation to air my research interests in the pages of this new journal.

2 Linear Mixed Models: soil knowledge in the fixed effects

Ordinary kriging (OK) remains the workhorse of much applied geostatistics, in soil science and elsewhere. We know that it is robust provided that we can assume a constant, but unknown, local mean. In ordinary kriging we proceed on the assumption of intrinsic stationarity requiring that

$$\mathrm{E}\left[Z(\mathbf{s}) - Z(\mathbf{s}+\mathbf{h})\right] \;=\; 0, \quad \forall\, \mathbf{s}, \tag{1}$$

where $Z(\mathrm{s})$ is our random variable at location s, and $\mathbf{h}$ is a lag vector. This assumption is not plausible when our data exhibit a strong trend. Universal kriging (UK) offers a solution [5], but this requires that we can somehow model the covariance of the residual process disentangling the unknown trend. The situation where we need a trend model is a particular case of the more general situation where some exhaustive covariate, e.g. a remote sensor image, is a potential predictor of $Z(\mathbf{x})$ through some linear model. Once again, the problem is to model the covariance of the residual process. A pragmatic approach, commonly applied in soil science, is called regression kriging (RK). The linear model in the proposed covariate is fitted by ordinary least squares, and then a variogram is estimated for the residuals by a method-of-moments estimator. The residuals are kriged and the estimates added to the prediction from the ordinary least squares model at target sites [6]. The problem with this approach is that the resulting variogram estimates are biased estimators of the variogram of the residual process, furthermore in the case of a trend model the bias is lag dependent [7]. Given a covariance model for the residual process, UK, or kriging with an external drift (KED) (as UK generalized from a trend model to a linear model with some other independent variable is called) is equivalent to regression kriging. This proliferation of kriging methodologies, without an adequate method to estimate the covariance model, was far from satisfactory. However, help came from the world of mathematical statistics where it was pointed out [2] that the kriging zoo, simple kriging, OK, UK, KED, RK, are all forms of the empirical best linear unbiased predictor (E-BLUP) based on the linear mixed model:

$$\mathbf{Z} \;=\; \mathbf{X}\boldsymbol{\tau} \;+\mathbf{u} \;+\boldsymbol{\varepsilon}\,, \tag{2}$$

where $\mathbf{Z}$ is a random vector corresponding to our variable at n sites, $\mathbf{X}$ is an $n \times p$ design matrix, containing the values of any predictor variables, $\boldsymbol{\tau}$ are the corresponding fixed effects coefficients, $\mathbf{u}$ is a spatially correlated random variable, and ε is an independently and identically distributed random variable. The random components have the joint distribution:

$$\begin{bmatrix} \mathbf{u}(\mathbf{s}) \\ \varepsilon(\mathbf{s}) \end{bmatrix} \sim \mathcal{N}\left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \sigma^2 \begin{bmatrix} \xi\mathbf{R} & 0 \\ 0 & \mathbf{I} \end{bmatrix} \right\}, \tag{3}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{R}$ is a correlation matrix for the spatially dependent random component, the values of which will depend on the locations of the n sites considered and the parameters, $\boldsymbol{\theta}$, of some model of spatial autocorrelation. The term σ^2 is the variance of ε , equivalent to the nugget variance of classical geostatistics in the current formulation, and ξ is a scaling factor, the ratio of the variance of $\mathbf{u}$ to that of ε . The great advantage of this formulation is that it is possible to propose likelihood based estimators for the parameters of the random effects: $\boldsymbol{\theta}$, σ^2 and ξ. Specifically the residual maximum likelihood (REML) estimator is appropriate, minimizing the bias in the estimates due to uncertainty in the estimated fixed effects coefficients, $\boldsymbol{\tau}$. Lark et al. [8] reviewed and illustrated this approach in a paper for the soil science community, who have taken up the approach widely. See, for example, work in soil hydrology [9], soil pollution [10] and in soil biology [11]. The solution to the technical problem of estimating the fixed effects and random effects coefficients that bedevilled classical geostatistics is important because it immediately opens up the possibility of using the fixed effects component of the model as a vehicle to incorporate soil knowledge.

This has generally been done by including fixed effects that represent generalized soil information (e.g. maps of parent material), that are assumed to reflect factors of soil formation (e.g. information on land use, rainfall or variables derived from a digital elevation model). This is what McBratney et al. [12] call the SCORPAN approach to spatial prediction of soil properties, using covariates (categorical or continuous) as predictors. Incorporating the SCORPAN predictors as fixed effects in a linear mixed model allows the remaining variation in the target soil properties to be modelled as spatially dependent random effects. The final prediction by the associated E-BLUP combines information from the covariates and a kriging-type prediction of the variation that the covariates do not explain. Examples of this approach in the soils literature are provided by Wang et al. [13] who found that rainfall, land use and soil class were useful covariates to predict the thickness of the dry layer forming in soils of China's loess plateau. Rawlins et al. [14] used elevation and measured passive gamma ray emission as covariates to model the variation of soil organic carbon across Northern Ireland. The SCORPAN approach depends on finding appropriate linear relation-

ships between available predictors and the soil properties of interest. By contrast, Stacey et al [15] used a model from the soil science literature to predict the rate of nitrous oxide emission from available soil data. By treating the model prediction as a fixed effect they were able to form better predictions of emission rate by the E-BLUP than was possible either by the model alone or by kriging alone. Using model predictions as fixed effects in a linear mixed model is a potentially fruitful mechanism for assimilating process models with data. Note that soil scientists have previously been able to incorporate soil knowledge into predictive statistical models through a state-space approach when the model describes the evolution of a variable over time [16].

The E-BLUP as presented above is a 'plug-in' approach to spatial prediction in that it assumes that the spatial covariance model, estimated by REML, is correct. Marchant and Lark [17] developed an expression to show how uncertainty in the covariance model parameters propagates to uncertainty in the final predictions. This allows us to optimize sampling schemes for spatial prediction, accounting for both the uncertainty in the final predictions due to spatial variability of the variable in question (which can be reduced by reducing the interval of the final sampling grid) and effects of uncertainty in the covariance parameters. A similar approach was proposed by Zhu and Stein [18].

A more comprehensive account of how uncertainty in the underlying statistical model of a variable propagates to predictions is possible in a Bayesian framework. Orton et al. [19] demonstrated this in a case study for spatial prediction of selenium concentration in the soil, showing how the Markov Chain Monte Carlo (MCMC) approach allows the posterior distribution of a complex model to be approximated efficiently. There is a growing interest in this approach in soil science [20]. Orton et al [21] also showed how the Bayesian approach allows expert opinion on the mathematical modelling of processes in soil to be incorporated into the assimilation of alternative models with data.

In summary, the linear mixed model framework provides a fruitful way to incorporate soil knowledge into geostatistical prediction, whether that knowledge be a simple understanding that a particular covariate represents a factor of soil formation, or more complex process models. It has also allowed the development of more sophisticated methods to design efficient sampling schemes for geostatistical prediction. Through the Bayesian framework there is scope for a comprehensive account of the sources of uncertainty in spatial prediction of the soil.

3 Linear Mixed Models: non-stationarity in the variance

Equation (1) above is a component of the intrinsic hypothesis of stationarity that is proposed in a conventional geostatistical analysis. The second component of this assumption is that we can define a variogram function, $\gamma(\mathbf{h})$, with the lag interval $\mathbf{h}$ its sole argument:

$$\gamma(\mathbf{h}) \; = \; \frac{1}{2}\mathrm{E}\left[\{Z(\mathbf{s}) - Z(\mathbf{s}+\mathbf{h})\}^2\right] \quad \forall\, \mathbf{s}. \tag{4}$$

Without some such assumption a geostatistical model cannot be estimated, since this is a model for a proposed random function of which our data are a single realization. Since we cannot observe multiple realizations of $Z(\mathbf{s}_i)$ and $Z(\mathbf{s}_j)$, some generalization is needed, and under stationarity assumptions such as the intrinsic hypothesis it is assumed that the covariance or variogram depends only on the increment, $\mathbf{s}_i - \mathbf{s}_j$, and so all pairs of observations, separated by some interval $\mathbf{h}$ provide information from which to estimate the covariance or variogram. However, the soil scientist might wonder about the plausibility of this assumption, particularly when it is made for a complex region. Is it plausible that the covariance over $\mathbf{h}$ is the same on a floodplain, on residual terrace gravels and on a loess-covered plateau, which could all plausibly be components of a single study area?

Soil scientists have turned to the wavelet transform as a method to investigate scale-dependent variation and covariation of soil properties without invoking assumptions of stationarity [22, 23]. The wavelet transform, like the Fourier transform, uses basis functions to compute coefficients that represent components of a data set. In the Fourier transform the basis functions are sinusoids oscillating uniformly from $-\infty$ to ∞ and the coefficients represent the stationary variance and phase of components of particular spatial frequency. By contrast the basis functions in a wavelet analysis are wavelets, oscillating functions that take non-zero values only over a narrow window, the support. A particular wavelet coefficient therefore represents local variation over some interval of spatial frequency. In the discrete wavelet transform we work with a set of wavelet basis functions obtained by dilating (changing the spatial frequency) and translating (changing the location of the support) a mother wavelet function. The resulting set of wavelet functions corresponds to a partition of the space/frequency plane corresponding to our data. It is therefore possible to test null hypotheses that our data on one or more soil variables are realizations of underlying random functions with stationary auto- and cross-covariances, and to identify locations at which the variance of a variable at some scale, or the correlation of two variables, appears to change [24, 25, 26], and this has been applied in soil science [27, 28, 29, 30].

The wavelet analyses described above give insight into the multiscale spatial variation of soil properties, and its complexity, but leave the problem of spatial prediction to one side. In principle, however, the linear mixed modelling framework for geostatistics has greater potential to deal with the issue of non-stationary variance because it is based on parametric variance models fitted to the whole data set, rather than point estimates of the variogram formed from separate pair-comparisons. Stein [31] reviews some approaches that have been taken to this problem. The key challenge is to propose a parameterization of the variance structure that is more flexible than one based on stationarity assumptions, but which is also estimable and ensures a positive definite covariance matrix. The simplest approach is to assume a stationary correlation structure, but to allow the variance of the random effects to change as a function of some covariates. This was demonstrated by Lark [32] for some soil data. It was found to be a practically useful approach in a case study on monitoring the phosphorous content of soils in a water conservation area in Florida by Marchant et al [33] who found that mapped variations in the occurrence of *Typha spp.* across the area was a useful predictor of the variance of soil phosphorous content. Spatial predictions based on this non-stationary model were more sensitive to particular features of the spread of phosphorous enrichment than those obtained by stationary geostatistical methods, and the prediction error variances gave a better account of the uncertainty of predictions at validation sites.

In many cases, however, it will not be sufficient to confine the assumption of stationarity just to the autocorrelation and an appropriate parameterization of the random effects to allow non-stationary correlation is necessary. One interesting approach, spectral tempering, was proposed by Pintore and Holmes [34]. The spectrum of a spatially correlated process is obtained by the Fourier transform of its autocovariance function, and represents the distribution of the total variance between components with different spatial frequency. Any spectrum with all positive values is valid (i.e. it corresponds to positive definite covariance structures). In spectral tempering we propose that the local spectrum of some variable is obtained by raising the local spectrum to some power, $\eta > 0$. If $\eta > 1$ then the effect of tempering is to make the variation smoother, while tempering with a spectrum $\eta < 1$ enhances the variation at fine spatial scales. The approach in [34] is based on a Karhunen-Loève transformation of the data to an empirical spectrum based on a stationary covariance model. Haskard and Lark [35] developed the method, and suggested some amendments [36]. Haskard et al [37] showed how the method could be used to improve the geostatistical modelling and prediction of data on nitrous oxide emissions from soils, using both continuous soil information and

classification of the soil to model the value of the local tempering parameter. The prediction error variances at validation sites obtained by this non-stationary geostatistical method were found to account for the uncertainty of the predictions better than did a conventional stationary geostatistical model.

4 Soil knowledge in the random effects?

So far we have seen how recasting conventional geostatistical modelling and prediction in terms of the linear mixed model and its associated E-BLUP has allowed soil knowledge to be more naturally incorporated into geostatistics, using more realistic (non-stationary) models. Finally, I want to consider how understanding of soil processed might contribute to the development and selection of the basic models of spatial autocorrelation.

Whittle [38, 39] demonstrated how spatial covariance models could be computed for variables driven by diffusion from random sources in one, two or three dimensions. In this context we can infer the form of the covariance model for a process from understanding of the process's physical basis. There are other cases where physical and statistical properties can be directly linked. Chilès and Delfiner [4] give the example of the gravimetric field of a target comprising parallellpipeds of random size, shape and orientation, and mean depth $d = a/2$. The covariance function for such a random variable is given by a particular form of the Cauchy model:

$$C(\mathbf{h}) \;=\; \sigma^2 \left(1 + \frac{|\mathbf{h}|^2}{a^2}\right)^{-\frac{1}{2}} \tag{5}$$

A clear advantage of using this model, for the case of interest, rather than an alternative that simply happens to fit, is that the key parameter, a, has physical meaning and so we can put reasonable bounds on values that it might take, perhaps formally as a prior distribution for the parameter. For example, in one case where they wanted to krige from very sparse data on hydraulic head, Brochu and Marcotte [40] argued, from analogies between the physics of the gravimetric field and the hydraulic field, that a Cauchy model was appropriate. There has been further statistical work on the properties of random fields that are generated by stochastic differential equations, and this has been fruitfully applied to problems in the earth sciences [41].

Usually soil geostatistics proceeds with a covariance model that is selected because it fits best to the available data. In some respects this is scientifically weaker than, for example, the selection of a physically-based model for gravimetric data. However, it is reasonable for

the soil scientist to argue that the variables we study are often complex, and cannot be accounted for by the relatively simple models that lie behind the gravimetric form of the Cauchy model, or the models proposed by Whittle [38, 39] for diffusion processes. In fact, reflection on the comment by Whittle [39] that the good fit of the diffusion model in three dimensions to the yield data of Fairfield Smith [42] could be explained by the dependence of yield on the concentrations of nutrients that diffuse in the 3-D volume of soil illustrates this. Most soil scientists would not expect diffusion to be a major factor determining their spatial variation at the scales at which we observe variations in crop yield. Diffusion is a key process driving variation between the rhizosphere and the bulk soil, or the surface and centre of soil aggregates, but at plot scale mass flow of water within the soil and at the surface, the patchy distribution of organic inputs to the soil, the effects of cultivations and the broad-scale distribution of the rhizospheres of individual plants are expected to dominate. These are complex factors, and while they are mediated by physical processes, such as the distribution of water under gravity, they are unlikely to be amenable to the sort of direct physical parameterization used to compute the covariance functions for the physical properties of simpler origin.

The quest to link understanding of soil processes to the forms of their statistical distribution is likely to be less precise, but it may still be useful. In an insightful paper on geochemistry, Allègre and Lewin [43] drew links between different processes that influence the mineralization of particular elements, and the statistical distributions that measurements of the concentrations of these elements might be expected to follow. Lark [44] proposed that progress might be made by inference from the nature of the processes that cause soil variation to the form of a particular mathematical operator that might be expected to represent the form of such variation, and so to the resulting distribution. An example of such a process-operator-distribution trio was provided by Brown et al. [45] who proposed what they called ‘blur’ models in which the processes that take place in the dispersion of gaseous pollutants into the atmosphere were linked conceptually to a simple mathematical operator (convolution) and so to the expected form of the spatial covariance function. We might aim to identify such process-operator-distribution trios in soil science, advancing them as testable hypotheses about the form and origin of soil variation. Lark [46] considered the case where the dominant process in soil spatial variation is the division of space into discrete domains (e.g. different parent materials or land uses). It was proposed that an operator corresponding to such a process is Poisson Voronoi tessellation, and the covariance function for this operator was derived and fitted to some exemplar soil data sets. Lark [44] went on to inves-

tigate further the statistical distribution for variables generated by this operator, and showed that the discrete domain–tessellation–distribution trio gave a better account of several soil data sets than an alternative local mixing processes–convolution–multivariate normal trio. In due course this might provide a basis for using stochastic geometric simulations to generate training images from which to form the sets of conditional distributions that constitute a multiple point geostatistical model for soil properties [47].

5 Conclusions

Geostatistics has been an invaluable tool in soil science over the 30 years since the early work by Burgess and Webster [48]. Theoretical developments in geostatistics, most notably through the linear mixed model formulation, has allowed a closer integration of soil knowledge into geostatistical prediction, and the development of models which, by allowing the use of covariance structures that are not necessarily stationary, are more pedologically plausible. Soil scientists deal with complex variables, arising from many processes not all of which are well-understood. For this reason it is unlikely that the covariance models used in soil geostatistics can be as tightly linked to process understanding as has been achieved in areas of geophysics and hydrology, but we may hope for further development of a framework in which soil-forming processes are linked to likely statistical distributions through appropriate mathematical operators.

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