Landmark Papers: No. 8

Burgess, T.M. & Webster, R. 1980. Optimal interpolation and isarithmic mapping of soil properties. I. The semi-variogram and punctual kriging. *Journal of Soil Science*, 31, 315–331.

Commentary on the impact of Burgess & Webster (1980a) by R.M. Lark, G.B.M. Heuvelink and T.F.A. Bishop

Introduction.

This landmark paper by Burgess & Webster (1980a) signalled a new era in the spatial mapping of the soil. The emergence of pedometrics as a distinct subdiscipline of soil science was a gradual process, and had its roots in earlier studies than this one, but if one publication is to mark the start of pedometrics, then this is it.

The publication of this paper, and the successors in the series that it initiated, showed that statistics could do more than just assist the soil surveyor in quantitative prediction from maps based on a legend of discrete units. It showed soil scientists that there was a very different way of mapping the soil, namely through geostatistical interpolation.

The impact of the paper on practice has been substantial. Soil scientists have used geostatistical prediction to map the distribution of nutrients or pests at within-field scale for precision agriculture, to delineate contaminated land, to map changes in soil properties over time at the regional scale to map the risk of problems such as salinity and even for forensic inference.

The value of geostatistics was soon recognized in soil science. This is, in part, because when one considers the state of the art at the time of its publication it is clear that it fulfilled a need for new methods. At the same time, its impact was not simply due to the method it introduced to soil science, ordinary kriging, but to the interest it stimulated among soil scientists and applied statisticians who went on to develop and improve the methodology in several critical ways.

The paper and its background.

In the 1960s and 1970s soil scientists in various centres started to consider how the process of soil mapping and prediction of properties from soil maps could be made more quantitative. In particular they asked how the quality of a soil map for prediction might be measured. The Soil Science Laboratory at Oxford was one such centre, and it was there that Richard Webster undertook work on the prediction of soil properties from interpretation of air photographs. The principle was that physiographic units delineated in such an interpretation should be more internally uniform with respect to soil properties than the landscape as a whole. That being so, the mean value of the soil property for a unit, estimated from an appropriate sample, could be treated as a prediction of that property at any unsampled site in the unit. The difference between units might be examined by an analysis of variance (ANOVA), the outputs of which would indicate both the extent to which the interpretation had been successful in accounting for soil variation, and allow the errors of resulting predictions to be quantified (Webster & Beckett, 1968).

We may consider a conventional soil map, with delineated map units corresponding to a legend based on some soil classification, as a predictive model of the soil. As such it has two drawbacks. First, it implies discontinuous spatial variation of the soil, and the predicted value of any soil property is a constant within any map unit. Furthermore, there is no basis to treat the variation within the map unit as anything other than uncorrelated white noise, that is to say the variance within any small sub-region of the map unit is the same as the variance within the map unit as a whole.

Both these features of the conventional soil map are clearly unrealistic as representations of the spatial variation of soil. The soil varies over multiple spatial scales, and so, even where a set of boundaries within a landscape constitutes a meaningful, if somewhat artificial, model of soil variation, we expect the variation within the boundaries to have a complex and spatially-dependent structure.

This was the state of affairs when soil scientists came upon geostatistical methodology. This did not happen in a sudden revelation. Analysis of the variation of the soil as a spatially-dependent process had been undertaken by Youden & Mehlich (1937) using spatially nested sampling. Some forty years later than this Philip Beckett and Stein Bie analysed data from soil samples they collected on a journey from Alice Springs to Darwin in Australia's Northern Territory. They computed the mean variances of their observations within intervals of increasing length and plotted the result for each interval against its length. In a closing remark they noted that these graphs are related to Matheron's variogram (Beckett & Bie, 1976). In fact these graphs are also related to the correlograms computed by Webster & Cuanalo (1975) from soil properties measured at regular intervals on a transect in the north of Oxfordshire. This work on spatial variation was presented in terms of the description of spatially-dependent variation in the soil and was not connected to prediction, but together with the perceived deficiencies of prediction by map-unit means, it served as a *praeparatio evangelica* for the dissemination of geostatistical ideas in soil science.

As expressed in the title, this landmark paper focused on spatial prediction of soil properties as an isarithmic map. On such a map soil variation is visualized by isarithms or contours, where one isarithm joins locations where the property takes a common value. Isarithms can be drawn once the variable of interest has been interpolated at the nodes of a fine grid. Burgess & Webster (1980a) noted that various methods exist to do this interpolation (e.g. triangulation with linear interpolation) but that these are essentially arbitrary methods. They are not based on a statistical model of spatial variation of soil. As a result there is no guarantee that they are unbiased, they provide no measure of the uncertainty in the prediction and still less do they minimize that uncertainty. Kriging is advantageous over these other methods in all three respects.

The paper gave the reader a clear introduction to ordinary kriging, with three case studies. The first was on the sodium content of a field at the Welsh Plant Breeding Station, Plas Gogerddan. A linear isotropic variogram model was fitted. The authors note the effect of the relatively large nugget variance in the somewhat 'spotty' appearance of the resulting map which arises because of discontinuities of the kriged surface at sample locations. In a second case study, they kriged the depth of cover loam at Hole Farm in Norfolk, this time with the bounded spherical variogram model.

Finally, the authors returned to Plas Gogerddan and kriged the stone content of the soil, using a suitable variogram model to represent this variable's marked anisotropy.

This first paper used punctual (point) kriging. The second paper in the series (Burgess & Webster, 1980b) introduced block kriging, in which rather than predicting at a point location one predicts the mean value of the soil property across a block.

The third paper (Webster & Burgess, 1980) introduced universal kriging, to be used when the assumption of stationarity of the mean of the target variable appeared implausible. Alex McBratney joined the authors in the next paper, on the use of the variogram to select a spacing for a sample grid (Burgess *et al.,* 1981), and the fifth extended the analysis to the multivariate case for co-kriging (McBratney & Webster, 1983). A few years later Webster & Oliver (1989) completed the series with a paper on non-linear geostatistics, specifically disjunctive kriging.

In this series of papers, initiated by the Landmark paper we are considering, Burgess, Webster and colleagues set out the stall of what one might call 'mining geostatistics', the geostatistical methodology that Matheron derived from the pioneering work of Danie Krige. We take this name from the title of the influential textbook by Journel & Huijbregts (1978) to which Burgess & Webster (1980a) referred their readers for more detail on geostatistical methods. Putting these tools into the hands of soil scientists had a substantial impact on how they thought about the spatial prediction of the soil, particularly as computer programs to undertake the calculations became more widely available.

What happened next.

As with all papers that are true landmarks, the article by Burgess & Webster (1980a) marked the beginning of methodological development in soil science, rather than the end of the search for a suite of methods for spatial prediction. This work was published in various journals of soil science, earth sciences and environmental science, but here we focus on those published in this journal, and included in the virtual special issue to accompany this Landmark paper. Some of these developments were essentially refinements of the mining geostatistics framework. For example, Webster & McBratney (1989) examined the problem of selecting a variogram model, Laslett & McBratney (1990) combined modelling of measurement error and soil variation and Goovaerts (1992) used factorial kriging to analyse the variation of soil into separate additive components associated with different spatial scales of variation. Bierkens & Burrough (1993) were the first to use indicator kriging for mapping categorical soil data. Geostatistical methodology was also applied to the problem of soil monitoring (Papritz & Webster, 1995; Rawlins *et al.,* 2017). Lark (2000) examined alternative estimators for the empirical variogram, and Van Meirvenne *et al.,* (2008) investigated historical soil contamination using geostatistics.

However, soil scientists were to find themselves pushing mining geostatistics to its limit. One reason for this was the desire to include ancilliary soil information in the prediction process. In some respects geostatistics, at least ordinary kriging, pushed the pedologist out of the business of predicting soil conditions in space. This was undesirable because our knowledge of soil-forming processes, and how they vary across the landscape, is substantial, and should be incorporated into the statistical prediction of soil properties rather than supplanted by it. Leenhardt *et al.* (1994) attempted this in a study on prediction of soil water. However, this is not easy to do in the mining geostatistics framework. One approach, exemplified in this journal by Bourennane *et al.* (1996), was to use the universal kriging method expounded by Webster & Burgess (1980). This approach was first developed to incorporate a model of drift, local trend, into the geostatistical model, by which the mean value of the target property is not a constant but is expressed as a spatial trend. In the method of kriging with external drift the trend model for the mean is replaced by a model which is a function of some environmental variable, in this example the slope gradient. This incorporates knowledge of factors which influence soil variation (and can also include categorical predictors such as soil classes or map units). However, in the mining geostatistics framework the challenge is to estimate correctly the variogram which expresses the variation of the soil after the trend or external drift is accounted for. This process of structural analysis is neither straightforward nor entirely repeatable. In their original exposition Webster & Burgess (1980) observed that it requires 'trial and error combined with good judgement'. This is clearly far from satisfactory.

The solution was to come from statisticians who showed that kriging and the geostatistical model are one case of, respectively, the best linear unbiased predictor (BLUP) based on a linear mixed model in which covariates or spatial trend can be expressed as fixed effects, and a correlated Gaussian random field is included in the random effects. A thorough account of this is given by Stein (1999). In this approach the parameters of the random effects part of the model (equivalent to the variogram parameters in mining geostatistics) are estimated by residual maximum likelihood. The BLUP can be shown to be equivalent to ordinary kriging under the assumption of a locally stationary unknown mean, and to universal kriging with an external drift when the external drift variable is included in the linear mixed model as a fixed effect. This approach was described in the journal by Lark *et al.* (2006) and has been variously applied (e.g. Kempen *et al.,* 2010).

Another important line of development is the adoption of a Bayesian framework for the linear mixed model. In frequentist geostatistics the estimated parameters of the random effects are 'plugged in' to the equations for the BLUP as if they were known without uncertainty. In many circumstances this has little effect, but a Bayesian approach, in which the parameters are treated as random variables and the process of estimation from data entails obtaining posterior distributions for these parameters, can be useful for dealing with the uncertainty in the parameters particularly when data are sparse. An example is provided by Orton *et al.* (2011) who used a Bayesian approach to deal with both the uncertainty arising from the spatial variation of observations, and the uncertainty about the appropriate form of a model to express the relationship between the target variable and a set of covariates.

Finally, we mention a paper in this journal which records, perhaps, the first application of multiple-point geostatistics in soil science (Meerschman *et al.,* 2013). Multiple-point geostatistics aims to deal with some limitations of the Gaussian assumption in the linear mixed model. A

Gaussian model, even after transformation of data, can be very poor for characterizing highly structured variation (such as spatial patterns of soil driven by infilled channels or braided streams in a texturally-contrasting matrix). At present the methodology for multiple-point methods is cumbersome, and very data-demanding, but it could be that this work ultimately leads to radical transformation of spatial statistics in the earth sciences.

The future.

In an era when advanced statistical tools are readily available for open-source platforms, and in which the availability of methods such as kriging can be taken for granted, it is easy to forget how radical a change Burgess & Webster (1980a) made to the provision of soil information. The paper has been transformative, but most particularly through stimulating new ideas. That is surely the most effective way for science to work, and is something worth celebrating here. Burgess & Webster (1980a) marked a critical step in the development of methods for spatial prediction of soil properties, but this step was the beginning of further innovations which have allowed geostatistical prediction to take greater account of soil knowledge, particularly as represented by covariates provided by remote sensors, soil surveyors or geophysical instruments. In doing this, Burgess & Webster (1980a) started the process of methodological development which has led to the current practice of digital soil mapping (McBratney *et al.,* 2001). Lagacherie *et al.* (2012) exemplify this approach within the pages of this journal, and there are many examples elsewhere.

Digital soil mapping owes a great deal to the pioneering work of this Landmark paper. We suggest that the value of republishing it now goes beyond mere historical curiosity. It is important to reflect on the story that we tell above when looking to the future of digital soil mapping and spatial prediction of soil properties more generally.

Digital soil mappers have embraced a range of methods for spatial prediction of soil properties from covariates. In addition to the BLUP, based on a linear mixed model, there has been a good deal of enthusiasm for machine learning methods. In a machine learning approach a predictive relationship between soil properties and covariates is derived by an algorithm rather than a statistical model in the sense of the linear mixed model. This may be the way forward, but we think that caution is needed. We noted above that when kriging was adopted by soil scientists for prediction, other methods of interpolation were available. However, these had no underpinning model. It was therefore not possible to claim that they produced results that were unbiased, or that they represented the best prediction possible from the data in some sense. Furthermore, there was no reliable basis for quantifying their uncertainty. Kriging won on all counts.

Little attention has been paid to these questions in the application of machine learning in digital soil mapping. For example, these methods appear to take no account of the fact that available soil data are rarely collected according to an independent random sampling design but are often selected on grids or transects, or include some intentional clustering. In a geostatistical linear mixed model we do not require any assumptions of independence because the spatial dependence of the observations is explicitly modelled, and so our estimates of variance components or of fixed effects coefficients are reliable if the model is valid. We may check the validity of the model, and identify the need for robust estimation, or non-stationary covariance structure as required (e.g. Marchant *et al.,* 2006). This gives us a basis for treating the model as robust and for quantifying the uncertainty of its predictions with some confidence. It is not clear, at least at present, how this can be matched by the machine learning methods currently in vogue.

The future for reliable, robust digital soil data will depend, not on the uncritical adoption of *ad hoc* algorithms but on careful and statistically sound development which does not let go of the benefits that geostatistics introduced. Perhaps we should be looking for the next Landmark paper to achieve and exemplify this.

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