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Further results on prediction of soil properties from terrain attributes: heterotopic cokriging and regression-kriging

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Abstract

Several methods involving spatial prediction of soil properties from landform attributes are compared using carefully designed validation procedures. The methods, tested against ordinary kriging and universal kriging of the target variables, include multi-linear regression, isotopic cokriging, heterotopic cokriging and regression-kriging models A, B and C. Prediction performance by ordinary kriging and universal kriging was comparatively poor as the methods do not use covariation of the predictor variable with terrain attributes. Heterotopic cokriging outperformed isotopic cokriging because the former utilised more of the local information from the covariables. The combined regression-kriging methods generally performed well. Both the regression-kriging model C and heterotopic cokriging performed well when soil variables were predicted into a relatively finer gridded digital elevation model (DEM) and when all the local information was utilised. Regression-kriging model C generally performed best and is, perhaps, more flexible than heterotopic cokriging. Potential for further research and developments rests in improving the regression part of model C.

1. Introduction

Developments within the past few decades have made it possible to quantitatively determine land features from remote locations above the earth surface. Digital elevation models (DEMs) (Burrough, 1986) are some of the products of these developments. The DEMs provide a cheap and reliable way of predicting land properties which have strong correlations with attributes derived from elevation data. With lateral resolution ranging from 5 m to 50

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m, the DEMs offers a fairly rational target grid for interpolation of soil attributes. It will seldom be necessary, except for some continuous soil husbandry operations, to interpolate onto a grid finer than defined by the DEM of a region. In a previous study Odeh et al. (1994) compared several methods involving prediction of soil properties from landform attributes. The methods, tested against ordinary kriging and universal kriging of the soil variables, include multi-linear regression, generalised isotopic cokriging (Wackernagel, 1994) and regression-kriging models A and B.

Isotopic cokriging involved fully sampled situations in which all the variables determined at all locations were used for cokriging. This apparently under-utilised the available information by restricting use of landform data to locations where only soil variables were determined, thus giving an inordinate advantage to multi-linear regression that utilised all the local landform data. Heterotopic cokriging (Wackernagel, 1994), which uses more of the available local information, needs to be tested against the methods mentioned above, particularly multi-linear regression. In heterotopic cokriging one or more variables are not sampled at all locations. The aim is to improve the prediction performance of the target variables by using the correlation with the other more fully sampled variables, in this case, the landform attributes.

In the case of regression-kriging models, the regression residuals represent uncertainty which needs to be incorporated into kriging systems. Model A involved, as a first step, regression of a target variable with the landform attributes. Kriging is further pursued with introduction of regression errors into the kriging system as prediction uncertainty. The importance of this is that kriging after regression may improve (with the introduction of the uncertainty due to regression errors into kriging equations) prediction performance in comparison to when regression or kriging are done separately. In model B, the regression part is similar to the first step of model A based on the multi-linear regression model fitted to points where both the target variable and the covariables (the landform variables) were determined. The residuals of the target variable at the same locations are calculated, followed by ordinary kriging of both the residuals and the regressed values to a finer grid. This is based on the assumption that the regression residuals retain some spatial structure inherent to the target soil variable. Both the regressed values and kriged residuals were added together at unsampled locations as the predicted values. We need to modify model B by kriging of the residuals into the same locations at nodes of the fine DEM used to generate landform attributes (i.e., locations where the target (soil) variable was not determined). The residuals are then added to the values of the target variables obtained by regression models at the same locations to give the new predictand. We termed this method as regression-kriging model C.

The major aim of this follow-up paper to that of Odeh et al. (1994) is to further compare the prediction performance of these two additional methods, heterotopic cokriging and regression-kriging model C, with the previously used methods (Odeh et al., 1994). Considering the fact that these methods assume different structures in the data and in this sense are not equivalent, we adopted, as in the previous study (Odeh et al., 1994) suitably designed (and unbiased) testing procedures in which the comparison is based on the same examples and the values at selected locations not utilised for prediction were used to validate the methods.

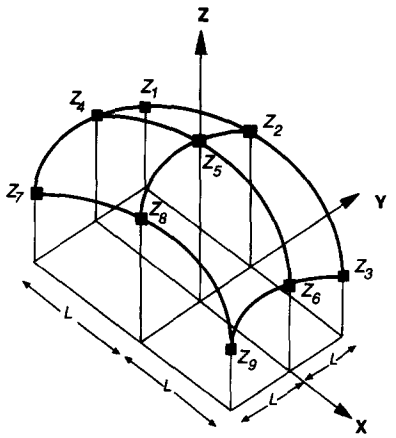

Fig. 1. A 3 × 3 submatrix of elevations, illustrating surface configuration and grid dimensions as used for derivation of landform attributes.

2. Materials and methods

2.1. The soil and landscape data

The area is located in a subcatchment near Forreston in the Mt. Lofty Ranges, about 60 km north-east of Adelaide in South Australia. Geodetically, the subcatchment is at approximately 34°48′N and 138°54′E (Fig. 1) which is equivalent to the Australian National Grid Reference of 6148800mN, 308500mE and 6147800mN, 310100mE. Geologically, the subcatchment is underlain by the Woolshed Flat Formation (Odeh et al., 1994) which is composed of shales, laminated siltstone, phyllite and minor quartzite. The main landform features are gently rolling hills bounded on both sides by relatively high ridges of the Stonyfell Quartzite to the east and the smooth rounded ridges of the Algate Sandstone to the west. The terrain within the subcatchment itself consists of predominantly rounded hills and spurs with slopes ranging from less than 1% on the lower slopes to just over 20% on the middle to upper slopes. The highest point at the south-eastern tip of the subcatchment is a spot height of 478 m above sea level. Relief is about 60 m. There is no conspicuous rock outcrop.

Terrain analysis

An elevation matrix at a grid mesh of 10 m covering the study area was obtained from controlled pairs of aerial photographs using a Zeiss Planicomp Analytical Stereo Plotter (South Australian Department of Lands). The terrain attributes of slope angle, aspect, plan curvature and profile curvature were derived in accordance with the procedure of Zevenbergen and Thorne (1987). The attributes were calculated for every point of the elevation matrix, except the peripheral points, by derivation from the partial quartic equation:

$$Z = Ax^2y^2 + Bx^2y + Cxy^2 + Dx^2 + Ey^2 + Fxy + Gx + Hy + I$$

where Z is the elevation at the centre of the submatrix; A, B,... and I are the nine parameters calculated from a 3 × 3 submatrix of elevations around the central point (Fig. 1); x and y

are the spatial co-ordinates and given that L represents grid length of the submatrix. Upslope area and upslope distance were estimated on the assumption that each point of the altitude matrix represents one grid square area or upslope grid length, respectively. A point receives upslope area (L squared) or upslope distance (L) from any of its eight adjacent points if their slopes face the central point. For more detailed information on terrain analysis, see Zevenbergen and Thorne (1987), Odeh et al. (1991).

Soil sampling

All of the total 232 soil cores (50 mm diameter) were taken at locations that coincided with some of the elevation points in the fine DEM. To ensure an accurate geodetic reference with respect to elevation points, a laser theodolite was used to locate the sampling points with an accuracy of <0.3 m with reference to established spot heights.

The soil cores were taken to the laboratory and key physical, chemical and morphological properties determined. Among the properties are the depth of solum, depth to bedrock, topsoil gravel and subsoil clay, which are used for this study.

2.2. Prediction methods

Multi-linear regression

This involved the use of the classical multiple regression procedure in which the regression models were generated by relating the target variable to the predictor (landform) variables. The regression models are then used to predict the target variables to locations where the landform attributes have been determined. Thus the prediction sites coincides with the fine grid nodes of the DEM where the target variables were not determined.

Ordinary kriging

Let us suppose that an intrinsic random function denoted by $Z(s_i)$, s_i being the locations for all $i=1, ..., n$, at which we have sampled and determined the random variable, the ordinary kriging predictor for an unsampled location, $z(s_0)$, is defined by:

$$z^*(s_0) = \sum_{i=1}^{n} \lambda_i z(s_i)$$

where λ_i are the weights associated with the sampling points. The weights sum to unity, a condition which assures unbiased estimation. Minimisation of kriging variance can be achieved when:

$$\sum_{j=1}^{n} \lambda_i \lambda_j \gamma(s_i, s_j) + \mu(s_i, s_0) \quad i=1, ..., n$$

The weights, λ, are calculated from the matrix equation:

$$\boldsymbol{c} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{1}$$

where:

$$A = \begin{bmatrix} \gamma(s_1, s_1) & \gamma(s_2, s_1) & \cdot & \cdot & \cdot & \gamma(s_n, s_1) & 1 \\ \gamma(s_1, s_2) & \gamma(s_2, s_2) & \cdot & \cdot & \cdot & \gamma(s_n, s_2) & 1 \\ \cdot & \cdot & \cdot & & & \cdot & \\ \cdot & \cdot & & \cdot & & \cdot & \\ \cdot & \cdot & & & \cdot & \cdot & \\ \gamma(s_1, s_n) & \gamma(s_2, s_n) & \cdot & \cdot & \cdot & \gamma(s_n, s_n) & 1 \\ 1 & 1 & & & & 1 & 0 \end{bmatrix}$$

$$b = \begin{bmatrix} \gamma(s_1, s_0) \\ \gamma(s_2, s_0) \\ \cdot \\ \cdot \\ \cdot \\ \gamma(s_n, s_0) \\ 1 \end{bmatrix} \quad \text{and} \quad c = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda_n \\ \varphi \end{bmatrix}$$

A is a matrix of semivariances between the data points; b is a vector of estimated semivariances between the data points and the points at which we wish to predict the variable z; and c is the resulting weights and the Lagrange multipliers φ.

Global universal kriging using restricted maximum likelihood

A method that has been used for a non-stationary stochastic model is termed universal kriging. This is achieved by superimposition of a stationary stochastic model on a global low-order polynomial trend surface (Laslett and McBratney, 1990). However, there are difficulties with using universal kriging as it is problematic to simultaneously estimate the parameters of the trend surface and the variogram of the stochastic component. These could be overcome by the use of a statistical procedure termed "restricted maximum likelihood" (REML). Thus the coefficients of pseudo-covariance functions defining the trend surface can be estimated by REML. An advantage of RELM, unlike maximum likelihood estimator, is that REML converges easily to the correct value even with increasing sample size. Detailed description of this method can be found in the work by Kitanidis (1983) and Laslett and McBratney (1990). The method, as adopted here, involved the use of all the data points for model fitting and kriging calculations, hence the term global.

Generalised cokriging

Cokriging is an extension of kriging in which random variables are simultaneously predicted by utilising their interrelationships and their spatial co-dependence (Myers, 1982, McBratney and Webster, 1983). In defining generalised cokriging we suppose that $Z_1(s)$, ..., $Z_m(s)$ denote random functions where s is the location in 1, ..., n space, m being the number of random variables; the linear predictor for the random variables $Z(s)$ based on the assumption of intrinsic random functions, is in the form of matrix equations (Myers, 1982):

$$\boldsymbol{Z}^*(s_0) \sum_{j=1}^{n} \boldsymbol{\Lambda}_j \boldsymbol{z}(s_j)$$

$$\sum_{j=1}^{n} \boldsymbol{\Gamma}(s_i, s_j)\boldsymbol{\Lambda}_j + \boldsymbol{\Psi} = \boldsymbol{\Gamma}(s_i, s_0) \quad i = 1, ..., n$$

$$\sum_{j=1}^{n} \boldsymbol{\Lambda}_j = \boldsymbol{I}$$

where $\boldsymbol{z}(s_j)$ is the vector $z_1(s_j)...z_m(s_j)$, $\boldsymbol{\Gamma}(s_i, s_j)$ and $\boldsymbol{\Gamma}(s_i, s_0)$ are the cross-variograms, $\boldsymbol{\Lambda}_j$ are the weights associated with prediction, $\boldsymbol{\Psi}$ are the Lagrange multipliers and $\boldsymbol{I}$ is an identity matrix. Cokriging can be isotopic whereby all the variables are measured at the same locations, or heterotopic where the target variable is undersampled (Wackernagel, 1994). Both types are considered in more detail later.

Regression-kriging model A

This model, introduced to soil science by Knotters et al. (1992, 1995), is based on normal regression followed by ordinary kriging of the regressed values. The ordinary kriging system is modified by replacing the variances in the diagonal of the $\boldsymbol{A}$ matrix with error terms that represent uncertainty. The method is equivalent to "kriging with uncertain data" (Ahmed and DeMarsily, 1987), in which a realisation of an intrinsic random function $Z(s)$ is uncertain. The uncertainty gives rise to:

$$Z(s) = z(s_i) + \epsilon(s_i) \quad i = 1, ..., n$$

where $z(s_i)$ is the true value and $\epsilon(s_i)$ represent the uncertainty or errors whose variance is δ_i^2. The uncertainty may be due to measurement errors or, as in this case, regression errors. The errors are assumed to be unsystematic ($\mathrm{E}[\epsilon(s_i)] = 0$), uncorrelated among themselves ($\mathrm{Cov}[e(s_i), \epsilon(s_i)] = 0$) and uncorrelated with the variables ($\mathrm{Cov}[\epsilon(s_i)\, z(s_i)] = 0$), $i = 1, ..., n$). The kriging equation is modified accordingly:

$$\sum_{j=1}^{n} \lambda_i \lambda_j \gamma(s_i, s_j) - \lambda_i \epsilon_i + \mu = \gamma(s_i, s_0) \quad i = 1, ..., n$$

To be didactic, the matrix $\boldsymbol{A}$ of Eq. (1) is modified such that the general variance in the diagonal is replaced by the uncertainty, and in this case, the regression errors, $e(s_i)$, $i = 1, ..., n$:

$$\begin{bmatrix} \epsilon(s_1)^2 & \gamma(s_2, s_1) & \cdot & \cdot & \cdot & \gamma(s_n, s_1) & 1 \\ \gamma(s_1, s_2) & \epsilon(s_2)^2 & \cdot & \cdot & \cdot & \gamma(s_n, s_2) & 1 \\ \cdot & \cdot & \cdot & & & \cdot & \\ \cdot & \cdot & & \cdot & & \cdot & \\ \cdot & \cdot & & & \cdot & \cdot & \\ \gamma(s_1, s_n) & \gamma(s_2, s_n) & \cdot & \cdot & \cdot & \epsilon(s_n)^2 & 1 \\ 1 & 1 & & & & 1 & 0 \end{bmatrix}$$

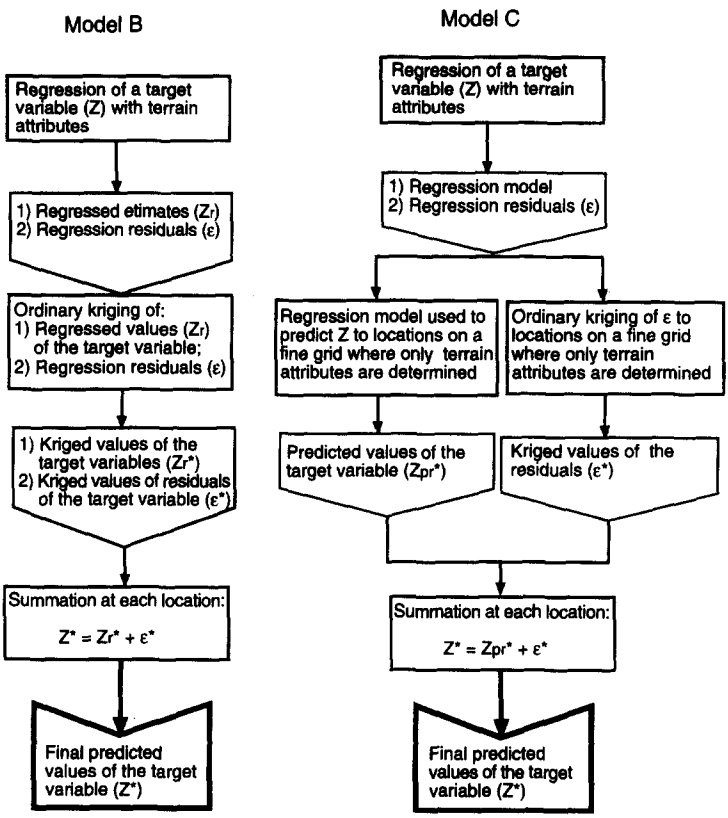

Fig. 2. Flow chart showing steps of regression-kriging models B and C.

This modification of the kriging system does not alter the condition for optimal prediction as $E[\epsilon(s_i)] = 0$ and λ_i sum to unity for $i = 1, ..., n$.

Regression-kriging models B and C

These models involved the normal regression followed by ordinary kriging of the regressed values (model B) or kriging of both the regressed values of the target variable and the regression residuals (models C). A succinct step by step description of the two methods is presented in Fig. 2.

2.3. Test of prediction performance

Prediction of the four soil variables, topsoil gravel content (affects tillage operations); subsoil clay, depth of solum, and depth to bedrock (affect drainage condition of the soil), was performed using all the prediction methods.

As in the previous study (Odeh et al., 1994), we utilised the same combinations of attributes to predict a given soil variable. In comparing the performance of the methods, we adopted suitably designed (and unbiased) testing procedures the comparison of which is based on separate controlled data set (90 profiles) at different locations used to validate the

Table 1
Prediction root mean square error

Soil variable	Prediction method							
	Multi-linear regression	Ordinary kriging	Universal kriging	Isotopic cokriging	Heterotopic cokriging	Regression-kriging model A	Regression-kriging model B	Regression-kriging model C
Depth of solum (cm)	11.92	15.76	13.89	15.70	21.74	8.45	11.20	10.01
Depth to bedrock (cm)	21.04	26.71	26.43	24.86	22.45	20.22	19.89	16.51
Topsoil gravel (%)	4.97	12.82	10.31	8.98	3.72	9.65	4.54	5.01
Subsoil clay (%)	10.22	15.20	14.63	10.24	5.89	9.11	9.26	8.04

methods by computing the root mean square error (RMSE) of prediction. RMSE is a measure of accuracy of prediction, defined as the mean square root of sum of squared prediction error. Further comparison was based on computed mean ranks and standard deviation of ranks (Laslett et al., 1987; Odeh et al., 1994) of the methods in predicting the target variables at each of the validation points. A method that performs well should have low mean rank as well as low standard deviation of ranks.

3. Results and discussion

Table 1 shows the RMSEs of prediction for all the methods in predicting the soil variables. Unlike the previous paper (Odeh et al., 1994) which indicated superiority of multi-linear regression over isotopic cokriging, there is considerable improvement in prediction performance by heterotopic cokriging over multi-linear regression with the exception of depth of solum. This is not surprising because the heterotopic cokriging used the correlation with attributes determined at more of the local finer grid points where soil variables were not determined and also due to the fact that the method utilised the spatial dependency of all the variables. It is clearly shown by best performance of heterotopic cokriging of topsoil gravel the variation of which is most accounted for by the landform attributes used for prediction (coefficient of determination was 75% in comparison with around 50% for other soil variables as reported by Odeh et al. (1994)). Comparison of isotopic cokriging with heterotopic cokriging shows similar results because heterotopic cokriging systems of computation use more of local information from the covariables than isotopic systems (Fig. 3).

As shown in Fig. 3a, isotopic cokriging at each prediction site was carried out using 15 sample points where both the target (soil) variable and the landform attributes were determined. This is within a radius of approximately 60 m. In Fig. 3b, heterotopic cokriging at the same prediction site using sample points within the same radius encompasses 94 sample

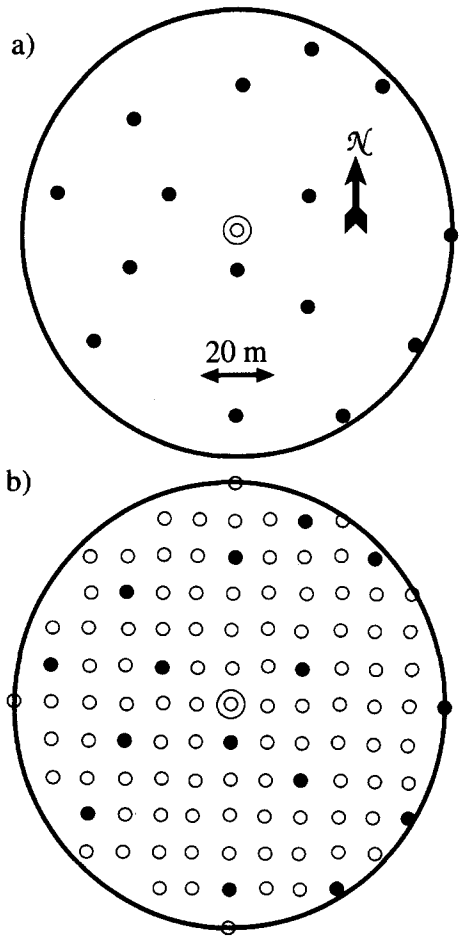

Fig. 3. Spatial layout of sampling points used for (a) isotopic and (b) heterotopic cokriging at a prediction site ◎; the data sites denoted by circles have only values of landform attributes and the sites by dots have values of target (soil) variable and the landform attributes.

points where only the landform attributes were determined, in addition to the 15 sample points where both the target variable and the landform attributes were obtained. Of course in either of the cases, they would be less number of sample sites used for prediction the closer the prediction site is to the edge of the study area. The minimum allowable was 6 sites. Essentially, Fig. 3 illustrates how heterotopic cokriging utilised more of the local information for prediction in comparison with isotopic cokriging, thus leading to heterotopic cokriging being more precise and accurate.

Consideration of performance of regression-kriging model C in comparison with other regression-kriging models, as shown by RMSEs in Table 1, indicates a considerable improvement in prediction of all the soil variables except topsoil gravel. In predicting topsoil gravel, regression-kriging model B (RMSE = 4.54) is only slightly superior to model C (RMSE = 5.01). The generally superior performance of model C is due to its utilisation of more of the local information from the covariables, determined on the nodes of the fine (10

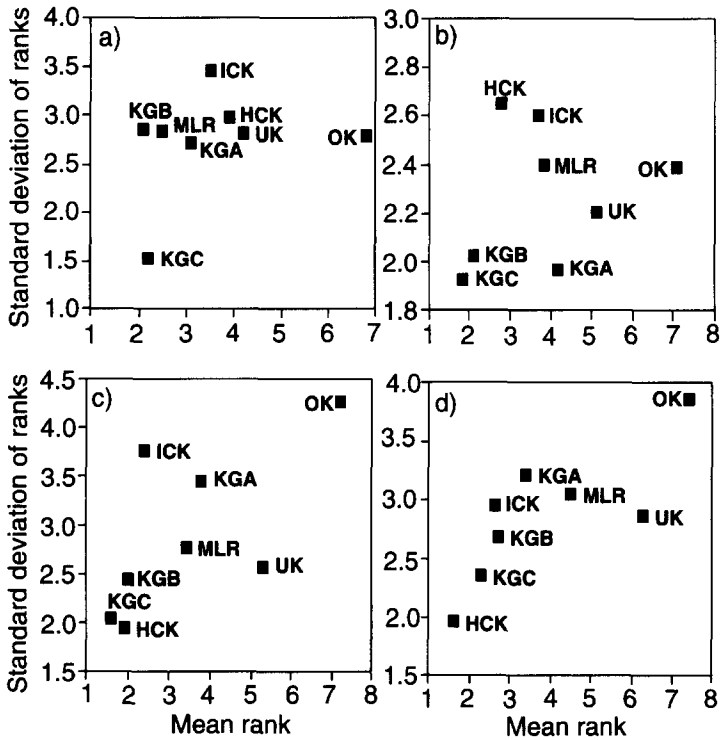

Fig. 4. Mean rank plotted against the standard deviation of ranks resulting from various prediction methods on (a) depth of solum, (b) depth to bedrock, (c) topsoil gravel and (d) subsoil clay. Note: MLR = multi-linear regression; OK = ordinary kriging; UK = universal kriging; ICK = isotopic cokriging; HCK = heterotopic cokriging; KGA = regression-kriging model A; KGB = regression-kriging model B; and KGC = regression-kriging model C.

m) grid, that were first used in the regression model to generate the regressed values of the soil variable. Subsequent summation of the regressed values and the kriged residuals (which are regarded as uncertainties) accounted for the reduced RMSE (see Fig. 2). It is important to note that in regression-kriging model C (and indeed model B) uncertainties were not considered during kriging of residuals.

Linear regression models implicitly disregard spatial covariation, in addition to their lack of sensitivity to measurement error. The latter is also true of kriging methods. Kriging methods, in particular, are characterised by overfitting or undersmoothing of the data (Laslett and McBratney, 1990). It is, therefore, not surprising that regression-kriging models, which take uncertainties due to regression and measurement errors into consideration, generally performed better than either multi-linear regression only or kriging methods. This is particularly so for prediction of depth of solum and depth to bedrock (Table 1).

Further comparison of the methods is shown in Fig. 4. The criterion for comparison in Fig. 4 is that a method that performs well should have low mean rank as well as low mean standard deviation of ranks (Laslett et al., 1987; Odeh et al., 1994). Whereas heterotopic cokriging is shown here to have performed better than all the other methods in predicting topsoil gravel (Fig. 4c) and subsoil clay (Fig. 4d), regression-kriging model C is better in predicting depth of solum and depth to bedrock. However, the mean rank of model C is the

lowest, and is slightly lower than that of heterotopic cokriging. Clearly regression-kriging model C is generally superior to other methods by either coming first or second in mean ranking or standard deviation of ranks. This could be explained by summation of the regressed and kriged residual values of the target variable which compensates for relative insensitivity of either regression or kriging (when used separately) to unsystematic variation of the variables. The improvement of regression-kriging model C in comparison with regression-kriging model B is due to the former using more of the local information (covariables).

The erratic performance of heterotopic cokriging in predicting different soil variables (Fig. 4) is probably due to difference in noise-to-signal ratios between the soil variables. This explains the better performance by the method in predicting variables that are relatively more correlated with the landform attributes, i.e., topsoil gravel (Fig. 4c) and subsoil clay (Fig. 4d) which has smaller noise-to-signal ratios than the other variables. These variables vary more systematically across the landscape than either the depth of solum or depth to bedrock. Additionally, heterotopic cokriging does not take into account uncertainties due to measurement (or regression) errors as regression-kriging models, although such a modification could be made. Multi-linear regression is shown to be inferior to heterotopic cokriging in predicting all the soil variables except depth of solum. As explained above, this may be due to heterotopic cokriging utilising, in addition to correlation, spatial covariation of the variables. As reported in the previous paper (Odeh et al., 1994) ordinary kriging is the most inferior of all the methods as it consistently has the highest mean rank for all the soil variables. The large standard deviation of ranks of heterotopic cokriging of depth to bedrock and multi-linear regression of depth to bedrock and depth of solum as compared to their relatively low mean rank (Fig. 2a, b) may be explained by influence of outliers.

Our advance here is to develop quantitative and statistical models that are explicit, consistent and repeatable. Regression-kriging models B and C show potential for incorporating regression with kriging in which the regression part can be replaced by generalised linear models (McCullagh and Nelder, 1989) and therefore can include more ancillary variables that are measured on non-interval nominal or ordinal scales, e.g., parent material, vegetation type, etc. Besides generalised linear models the regression part can be replaced by other types of model. The non-linear features of generalised additive models (Hastie and Tibshirani, 1990), tree-based models all provide a possibility. The complex steps of the regression-kriging models could be built into a neural network (Demuth and Beale, 1993). There is great potential for further research and developments in these exciting advances in the use of ancillary information for spatially predicting soil properties.

4. Conclusions

The results presented here show that heterotopic cokriging and regression-kriging model C perform well when soil attributes are to be predicted into a relatively fine grid DEM and when all local information is utilised. Regression-kriging model C generally performs best and is, perhaps, more flexible than heterotopic cokriging. There is, however, no single best method for all the variables. Each case should be examined carefully before deciding on

the best method. With increasing availability of computing power at low cost, technological constraint, in terms of hardware limitation, is no longer the reason for not searching for the best spatial prediction methods for a specific situation. It is our limited intuition that continues to hinder our efforts to get the best out of limited number of data we are capable of collecting.

The flexibility of regression-kriging model C makes it possible for the regression part of the model to be replaced by generalised linear models which can include more ancillary variables, e.g., parent material, vegetation type, etc. The regression part can also be replaced by the non-linear features of generalised additive models or tree-based models. This augurs well for exciting advances in the use of ancillary information for spatially predicting soil properties.

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