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Spatial prediction of soil properties using EBLUP with the Matérn covariance function

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Abstract

Spatial prediction with the presence of spatially dense ancillary variables has attracted research in pedometrics. While soil survey and analysis of soil properties are still expensive and time consuming, the secondary data can be made available on a dense grid for the whole area of interest. The main aim of using the ancillary data is to enhance prediction of soil properties by making use of the ancillary variables as covariates. Methods that can be used for this purpose are kriging with external drift, cokriging, regression kriging, and REML-EBLUP (Residual Maximum Likelihood-Empirical Best Linear Unbiased Predictor). Regression kriging is a sub-optimal method that has been utilised extensively because it is easy to use and has been shown empirically to perform as well as other methods. A statically sound method is REML-EBLUP. This paper examines the use of REML-EBLUP in combination with the Matérn covariance function for spatial prediction of soil properties. Methods for estimating parameters of the Matérn variogram using REML, and prediction with EBLUP are described. The prediction capability of REML-EBLUP, regression kriging, and ordinary kriging is compared for four datasets. Results show that although REML-EBLUP generally improves the prediction, the improvement is small compared with regression kriging. Thus, for practical applications regression kriging appears to be a robust method. REML-EBLUP is useful when the trend is strong, and the number of observations is small (<200). We concluded that improvement in the prediction of soil properties does not rely on more sophisticated statistical methods, but rather on gathering more useful and higher quality data.

Keywords: Best Linear Unbiased Predictor; Kriging; Semivariogram; Geostatistics; REML; Digital soil mapping

1. Introduction

Spatial prediction of soil properties has become a common topic in soil science research. This is enhanced by the advancement of technology that enabled collection of on-the-go proximal sensors and also remotely-sensed imagery for use in precision agriculture and digital soil mapping. While soil survey and analysis of soil properties are still expensive and time consuming, the ancillary or secondary data can be made available on a dense grid for the whole area of interest. These data can be from proximal or remote sensing, and digital elevation models. Goovaerts (1997) called this exhaustive secondary data. Spatial prediction with the presence of spatially-dense ancillary variables has attracted research in pedometrics. The aims of using the ancillary data are to remove the trend to achieve spatial stationarity, and more importantly to enhance prediction of soil properties by making use of the ancillary variables as covariates.

The trend in spatial data can be modelled either by a regional geographic trend (internal drift), or ancillary information (external drift). Modelling the trend also allows us to gain knowledge on the processes that gave rise to the spatial variation and improve predictions. The model for prediction of variable z at location x can be written as:

$$z(\mathbf{x}) = f(\mathbf{x}) + \varepsilon(\mathbf{x}) \quad (1)$$

where $\mathbf{x}$ is the vector of spatial coordinates, observation z, $f(.)$ is the trend function, and ε is the residuals with a mean of zero and covariance structure $\mathbf{K}$. The trend function $f(.)$ is usually modelled as linear function of ancillary variables. Most research in pedometrics attempts to use the ancillary information as covariates, these covariates can be related to soil forming or the *scorpan* factors (McBratney et al., 2003).

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Methods for spatial prediction in the presence of exhaustive ancillary information include:

(a) universal kriging or kriging with internal drift, UK (Burgess and Webster, 1980),
(b) kriging with external drift, KED (Goovaerts, 1997),
(c) regression kriging, RK (Odeh et al., 1994, 1995; Hengl et al., 2004),
(d) collocated cokriging, CC (Chilès and Delfiner, 1999).

Universal kriging applied to a special situation where the exhaustive information is provided solely by spatial position. Kriging with external drift is referred to the drift provided from external sources, e.g. ancillary or secondary information. Both UK and KED have the same formulation, the trend and residuals are modelled in a system.

Regression kriging (RK) was first coined by Odeh et al. (1994) referring to methods that combined regression using ancillary variables and kriging. It involves performing regression between the target variable and ancillary variables, calculating residuals of the regression, and combining them with kriging. Odeh et al. (1994, 1995) defined three types of RK:

– RK type A (Odeh et al., 1994), called "kriging combined with regression" by Knotters et al. (1995), where regression is performed, and followed by kriging of regressed values.
– RK type B (Odeh et al., 1994), called "kriging with a guess field" by Ahmed and De Marsily (1987), which involves regression, and calculating the residuals. This is followed by kriging of the regression predicted values and the residuals separately, and summing both values together to obtain the final prediction.
– RK type C (Odeh et al., 1995), similar to type B, but only kriging of the residuals, and summing predicted values from regression and residuals from kriging to obtain the final prediction.

Hengl et al. (2004) defined RK as a generalised least squares model. In this paper we refer regression kriging (RK) as type C of Odeh et al. (1995), where the trend function is modelled using ordinary least squares (OLS), and ordinary kriging is performed on the residuals of the trend function. This is a 'short cut' sub-optimal version, which is also called kriging after detrending. The assumption is that where the trend function and its residuals are uncorrelated, and they can be modelled independently (Odeh et al., 1994).

McBratney et al. (2000) extended the form of $f(.)$ in Eq. (1) not only to linear models but various nonlinear mathematical models such as generalised additive models, regression tree and neural networks. McBratney and Walvoort (2001) proposed Generalised Linear Model Kriging, where the trend can be defined as a generalised linear model.

Rivoirard (2002) discussed the use of kriging with external drift and cokriging. Universal kriging, KED, and kriging of the residuals are optimal when the residuals are orthogonal or uncorrelated to the ancillary variables, otherwise coregionalisation cokriging is theoretically better. However the formulation of cokriging in the presence of exhaustive ancillary variables may be awkward, and requires lots of parameters and heavy computation. Further, Rivoirard (2002) suggested that KED or UK should be used when the trend form is known but the parameters are unknown, and kriging of the residuals is used when the form and parameters of the trend is known. This is the core of the matter, the estimation of the parameters of the model and the covariance structure of the residuals. There is an impasse: the residuals can only be obtained after the trend is determined, and parameters of the trend depend on the residuals.

Regression kriging appears to be the most popular method used by pedometricians because it is easy to use (e.g. Carré and Girard, 2002; Finke et al., 2004; Baxter and Oliver, 2005; Herbst et al., 2006; Simbahan et al., 2006). Furthermore, many papers (Odeh et al., 1995; Herbst et al., 2005; Simbahan et al., 2005) have reported good prediction, outperforming regression, ordinary kriging, and cokriging. However Cressie (1993) and Lark et al. (2006) pointed out that estimating the variogram of the residuals with RK is theoretically biased. Lark et al. (2006) demonstrated with simulations that when variogram of the residuals were estimated using RK there is a bias at long lags. This has consequences that the overall variability is underestimated and the spatial structure cannot be estimated correctly. Thus Lark et al. (2006) advocated pedometricians to use a statistically sound method called REML-EBLUP. Residual maximum likelihood method (REML) estimates parameters of the covariance function and trend model directly from the data. Subsequently the estimated parameters are used for spatial prediction called EBLUP, E refers to empirical or estimated, and BLUP is the best linear unbiased predictor.

There is still no formal comparison between REML-EBLUP and other methods for predicting soil properties. In this paper we explore the use of REML-EBLUP in combination with the Matérn covariance function, which was suggested by Minasny and McBratney (2005). The aims of this paper are to examine the use of EBLUP, and to answer the question whether using a more statistically sound method can improve the prediction of soil properties. We examine the prediction power of EBLUP by comparing it with ordinary kriging and regression kriging using four different examples.

2. Theory

2.1. BLUP

Best Linear Unbiased Prediction (BLUP) arises from a statistical theory (Robinson, 1991), a full discussion on the theoretical aspects is given in Lark et al. (2006). Following the main equations are introduced. The general linear spatial model for a random field z is:

$$z(\mathbf{x}) = \mathbf{m}(\mathbf{x})^T\boldsymbol{\beta} + \varepsilon(\mathbf{x}) \quad (2)$$

where $\mathbf{x}$ is the vector of spatial coordinates, $\mathbf{m}(\mathbf{x})$ is the design matrix of the trend function $[m_1,m_2,..m_p]$, $\boldsymbol{\beta}$ is the parameter vector (size $p\times 1$) for the trend, and ε is the residuals with a

mean of zero and covariance structure $\mathbf{K}$. We observe soil properties z at location $\mathbf{x}$ whose n observations form $\mathbf{z}=[z(x_1), \ldots, z(x_n)]^T$ and we wish to predict z at unsampled location $\mathbf{x}_0$, if $\boldsymbol{\beta}$ is known then the solution is:

$$z(\mathbf{x}_0) = \mathbf{m}(\mathbf{x}_0)^T\boldsymbol{\beta} + k^T\mathbf{K}^{-1}(\mathbf{z} - \mathbf{M}\boldsymbol{\beta}) \quad (3)$$

where $\mathbf{M}$ is the $(n \times p)$ design matrix $\mathbf{M}=[\mathbf{m}(x_1)\ldots\mathbf{m}(x_n)]^T$, $\mathbf{K}=\mathrm{cov}(\mathbf{z},\mathbf{z}^T)$, and $\mathbf{k}=\mathrm{cov}\{\mathbf{z},\mathbf{z}(\mathbf{x}_0)\}$. If the covariance function forming $\mathbf{K}$ is known, then vector $\boldsymbol{\beta}$ can be estimated using generalised least squares:

$$\hat{\boldsymbol{\beta}} = (\mathbf{M}^T\mathbf{K}^{-1}\mathbf{M})^{-1}\mathbf{M}^T\mathbf{K}^{-1}z, \quad (4)$$

and $\hat{\boldsymbol{\beta}}$ can replace $\boldsymbol{\beta}$ in Eq. (3):

$$z(\mathbf{x}_0) = \mathbf{m}(\mathbf{x}_0)^T\hat{\boldsymbol{\beta}} + \mathbf{k}^T\mathbf{K}^{-1}(\mathbf{z} - \mathbf{M}\hat{\boldsymbol{\beta}}). \quad (5)$$

The variance of the prediction is:

$$\sigma_z^2 = k_0 - \mathbf{k}^T\mathbf{K}^{-1}\mathbf{c} + \mathbf{d}^T(\mathbf{M}^T\mathbf{K}^{-1}\mathbf{M})^{-1}\mathbf{d} \quad (6)$$

where $k_0=\mathbf{K}(x_0,x_0)$ and $\mathbf{d}=\mathbf{m}(\mathbf{x}_0) - \mathbf{M}^T\mathbf{K}^{-1}\mathbf{k}$.

Stein (1999) showed that Eq. (5) is exactly the same as the formulation of universal kriging (Burgess and Webster, 1980):

$$\begin{bmatrix} \mathbf{K} & \mathbf{M} \\ \mathbf{M}^T & \mathbf{O} \end{bmatrix}\begin{bmatrix} \boldsymbol{\lambda} \\ \psi \end{bmatrix} = \begin{bmatrix} \mathbf{k} \\ \mathbf{m}(\mathbf{x}_0) \end{bmatrix} \quad (7)$$

where $\mathbf{O}$ is a zero matrix, and the predictor is:

$$Z(\mathbf{x}_0) = \boldsymbol{\lambda}^T\mathbf{Z} \quad (8)$$

When $\mathbf{m}(\mathbf{x})=1$, Eq. (7) refers to ordinary kriging, and when $\mathbf{M}$ contains the trend model, it is universal kriging or kriging with external drift.

The formulation of (5) as an alternative to the standard kriging form (7) was also proposed by Davis and Grivet (1984). This form takes advantage of the explicit use of the symmetric positive definite form of $\mathbf{K}$. The inverse of $\mathbf{K}$ can be achieved in a more efficient and stable computation using Cholesky factorisation. Since $\mathbf{K}$ is positive definite, it can be factorized into:

$$\mathbf{K} = \mathbf{L}\mathbf{L}^T. \quad (9)$$

with $\mathbf{L}$ a lower triangular matrix with positive diagonal entries. The inverse of $\mathbf{K}$ can be found by:

$$\mathbf{K}^{-1} = \mathbf{L}^{-1}(\mathbf{L}^{-1})^T \quad (10)$$

In the case where matrix $\mathbf{K}$ is not positive definite (as sometimes found in a smooth spatial process with no nugget effect, e.g. the Gaussian variogram model) the modified Cholesky factorisation algorithm of Gill et al. (1981) can be applied. This involves adding a diagonal term $\mathbf{E}$ to $\mathbf{K}$ to enforce positive-definiteness:

$$\mathbf{K} + \mathbf{E} = \mathbf{L}^T\mathbf{L}. \quad (11)$$

This approach attempts to minimise $\mathbf{E}$, thus disturbing $\mathbf{K}$ as little as possible. The modified Cholesky factorisation is widely used in optimisation algorithms (Gill et al., 1981).

Usually the covariance structure $\mathbf{K}$ is represented as a covariance function with parameter vector θ. The problem for the parameter estimation is that the covariance structure $\mathbf{K}$ is usually unknown a priori, and $\mathbf{K}$ refers to residuals, which can only be obtained after fitting the trend; however from Eq. (4) we see that $\mathbf{K}$ is required to fit the trend. Hence the impasse mentioned above. Thus we need a method that can predict the parameters accurately and unbiasedly.

Methods for estimating θ and β include:

(1) The crude, sub-optimal approach — regression kriging (RK).

This approach assumes that the deterministic (trend) part and the random error can be modelled independently. First a trend function is formulated:

$$\mathbf{z} = \mathbf{M}\boldsymbol{\beta} + \mathbf{r}, \quad (12)$$

where $\mathbf{r}$ is $(n \times 1)$ column vector of residuals. Parameter vector $\boldsymbol{\beta}$ is estimated using ordinary least-squares:

$$\hat{\boldsymbol{\beta}} = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T\mathbf{z}. \quad (13)$$

Replacing $\boldsymbol{\beta}$ with $\hat{\boldsymbol{\beta}}$ in Eq. (12) gives us the prediction for $\mathbf{z}$

$$\hat{\mathbf{z}} = \mathbf{M}\hat{\boldsymbol{\beta}}, \quad (14)$$

the prediction variance is given by (Agterberg, 1974):

$$\sigma_0^2 = \mathbf{m}(x_0)^T(\mathbf{M}^T\mathbf{M})^{-1}\mathbf{m}(\mathbf{x}_0)\sigma_E^2 \quad (15)$$

where σ_E^2 is the residuals variance, estimated as SSR/(n-p-1) with SSR = sum of squared of the residuals. The second step in RK is calculating the semivariance of the residuals using the method of moments and θ is estimated by fitting a variogram function to the empirical variogram. The residuals are then predicted for the whole area using ordinary kriging. The final prediction is obtained by adding the OLS predicted value with kriging interpolated residuals:

$$\hat{z}(\mathbf{x}) = \mathbf{m}(\mathbf{x})^T\hat{\boldsymbol{\beta}} + r(\mathbf{x}) \quad (16)$$

The prediction variance is simply the sum of variance of the prediction according to OLS (σ_o^2) and prediction variance of the residuals by kriging (σ_r^2):

$$\sigma^2 = \sigma_o^2 + \sigma_r^2 \quad (17)$$

(2) Maximum likelihood (ML) (Mardia and Marshall, 1984; Hengl et al., 2004).

In the context of generalised least squares, an initial β is estimated by ordinary least-squares (Eq. (13)), then θ is estimated by maximising the log-likelihood:

$$\ell(\boldsymbol{\theta},\boldsymbol{\beta}) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\mathbf{K}| - \frac{1}{2}(\mathbf{z}-\mathbf{M}\boldsymbol{\beta})^T\mathbf{K}^{-1}(\mathbf{z}-\mathbf{M}\boldsymbol{\beta}) \quad (18)$$

$\boldsymbol{\beta}$ is then re-estimated using (4), and this process is then repeated to get a stable solution.

(3) Restricted maximum likelihood (REML) (Kitanidis, 1983; Stein, 1999).

This is a more robust method to estimate θ and it does not depend on correct estimates of β. REML is due to Patterson and Thompson (1971) and Kitanidis (1983) was the first to use it for estimating spatial covariance functions. First, it transforms the data **z** into stationary data increments, **y**:

$$\mathbf{y} = \mathbf{Tz} \tag{19}$$

The transformation matrix **T** is selected so that the trends defined in **M** can be filtered out:

$$\mathbf{T} = \mathbf{I} - \mathbf{M}(\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T \tag{20}$$

where **I** is the identity matrix. θ is then estimated by maximizing the log-likelihood function:

$$L(\theta, \mathbf{y}) = -\frac{n-p}{2}\log(2\pi) - \frac{1}{2}\log|\mathbf{K}| - \frac{1}{2}\log|\mathbf{W}| - \frac{1}{2}\mathbf{y}^T\mathbf{K}^{-1}\mathbf{Q}\mathbf{y} \tag{21}$$

where $\mathbf{W}=\mathbf{M}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{M}$ and $\mathbf{Q}=\mathbf{I}-\mathbf{M}\mathbf{W}^{-1}\mathbf{M}^{\mathrm{T}}\mathbf{K}^{-1}$.

REML appears to be the most statistically sound method, and recently has gained much attention in pedometrics (Lark and Cullis, 2004) and also has been used for analysis of spatial crop yield data (Hong et al., 2005).

The use of REML for estimating parameters of a spatial covariance function is not new; it was first proposed by Kitanidis (1983), and Kitanidis and Lane (1985). In pedometrics, Laslett and McBratney (1990) used REML to estimate the variogram of soil pH. Knotters et al. (1995) used REML to estimate parameters of the covariance function for kriging with external drift.

The steps for prediction using BLUP are summarised as:

- define the trend function and design matrix **M**.
- estimate θ with REML by maximizing the log-likelihood function (Eq. (21))
- estimate β using Eq. (4) with $\hat{\theta}$.
- apply spatial prediction to unknown sites using Eq. (5).

This is called REML-EBLUP (Stein, 1999). The "E" refers to empirical or estimated because $\hat{\theta}$ is estimator of θ.

2.2. REML estimation of the variogram

Minasny and McBratney (2005) suggested the Matérn function as a general soil variation model for **K**:

$$K_{ij} = c_0\delta_{ij} + c_1\left[\frac{1}{2^{v-1}\Gamma(v)}\left(\frac{h}{r}\right)^v K_v\left(\frac{h}{r}\right)\right] \tag{22}$$

with parameter vector $\theta=[c_0, c_1, r, v]$. δ_{ij} is the Kronecker delta, c_0 is the nugget variance, and c_0+c_1 is the sill variance, h is the separation distance, K_v is a modified Bessel function of the second kind of order v, Γ is the gamma function, r is the distance or 'range' parameter and v is the 'smoothness' parameter which allows great flexibility for modelling the local spatial covariance. When v is small ($v\to 0$) it implies that the spatial process is rough (rapid changes in variation at small lags), and when it is large ($v\to\infty$) that the process is smooth (smooth changes in variation at small lags). Minasny and McBratney (2005) showed that the Matérn function can describe the spatial structure of various soil properties.

Because the model (Eq. (22)) has 4 parameters, optimisation algorithms can easily get stuck in local minima. Thus we used the profile likelihood method for the REML estimation of θ (McCullagh and Clifford, 2006). The procedure is as follows:

- Choose a set of values for v and r.
- For each combination of v and r, maximise the log-likelihood by estimating $[c_0, c_1]$ using an optimisation algorithm.
- Plot the log-likelihood L, values as a function of v and r, and find a combination of v and r that has largest L.

3. Methods

3.1. Datasets

An application of REML-EBLUP for spatial prediction of soil properties using the Matérn covariance function is given.

3.1.1. (1) Zn concentration along the Meuse River

This famous example comes from Burrough and McDonnell (1998) where topsoil zinc concentration along the river Meuse, the Netherlands was observed. This dataset shows a strong trend and it is expected to be a good application for BLUP. The data are obtained from the internet at Dr. David Rossiter's website: http://www.itc.nl/personal/rossiter/teach/lecnotes.html#l6. 155 observations were taken from the top 0–20 cm of alluvial soils in a 5 km × 2 km part of the floodplain of the River Meuse, near the village of Stein in the south of the Netherlands. The average distance between sampling points is around 100 m where each 'point' datum refers to a support of 10 m × 10 m, the area in which bulked samples were collected. The data shows a strong trend of zinc concentration decreasing with increasing distance from the river. Pebesma and Heuvelink (1999) suggested a linear relation between the log of zinc concentration and the square root of distance to the river d:

$$\log(z(x)) = \beta_0 + \beta_1\sqrt{d(x)} + \varepsilon(x). \tag{23}$$

3.1.2. (2) Soil pH data

Top soil pH from a survey in the Pokolbin area of the lower Hunter Valley, New South Wales, where 399 samples of soil were taken at a depth of 0–10 cm by Latin hypercube sampling of the ancillary data (Minasny and McBratney, 2006). The average separation distance between samples is 200 m (Fig. 1). Soil pH were measured using $CaCl_2$ in a 1:5 soil to water ratio. The purpose is to map the topsoil pH over the area. The data is randomly split into 250 observations as a training or prediction set and 149 observations as a validation set. Land-use in the area is classified using the available Landsat TM satellite images. Analysis of variance shows that areas with viticulture are statistically significant 0.5 pH unit larger. Further analysis of the data shows that there is a decreasing trend from west to east. Thus, the trend model is:

$$z(x) = \beta_0 + \beta_1\ \text{Easting} + \beta_2\ \text{Viticulture} + \varepsilon(x) \tag{24}$$

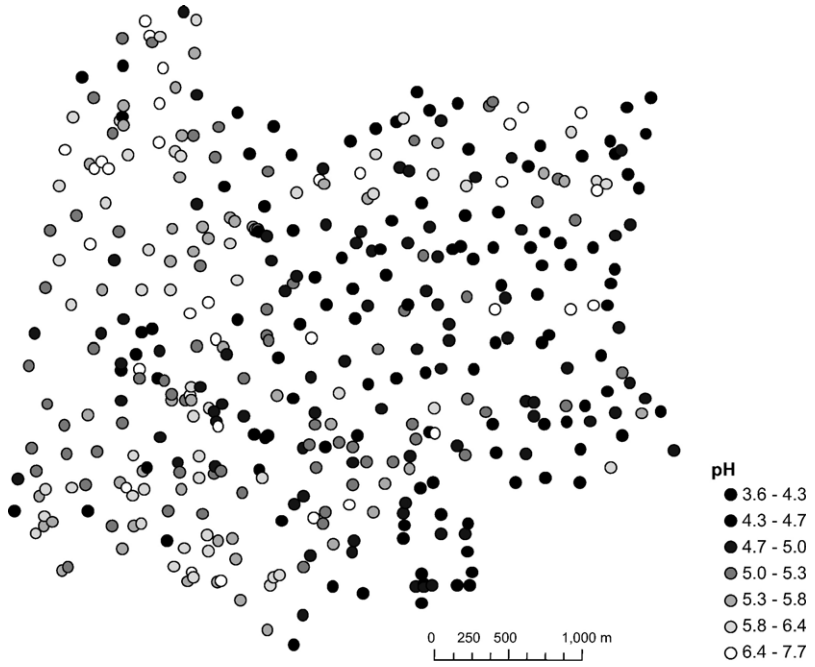

Fig. 1. Topsoil pH data in the Hunter Valley.

Where Easting refers to the Easting coordinates (in m) and Viticulture is an index of 1 and 0 indicating whether the land-use is viticulture or some other.

3.1.3. (3) Top soil clay content in the Edgeroi

These are data on top soil (0–10 cm) clay content from the Edgeroi area, NSW, Australia. The soil dataset consists of 341 soil observations, of which 210 are arranged on a systematic, equilateral triangular grid with approximately 2.8 km spacing between sites, and 131 are distributed more irregularly or on transects. Details of this area can be found in Minasny et al. (2006). The purpose is the creation of a digital soil map using soil environmental variables (McBratney et al., 2003):

$$z(x) = f(s, o, r) + \varepsilon(x) \tag{25}$$

where s refers to soil properties, o refers to organisms and r refers to relief.

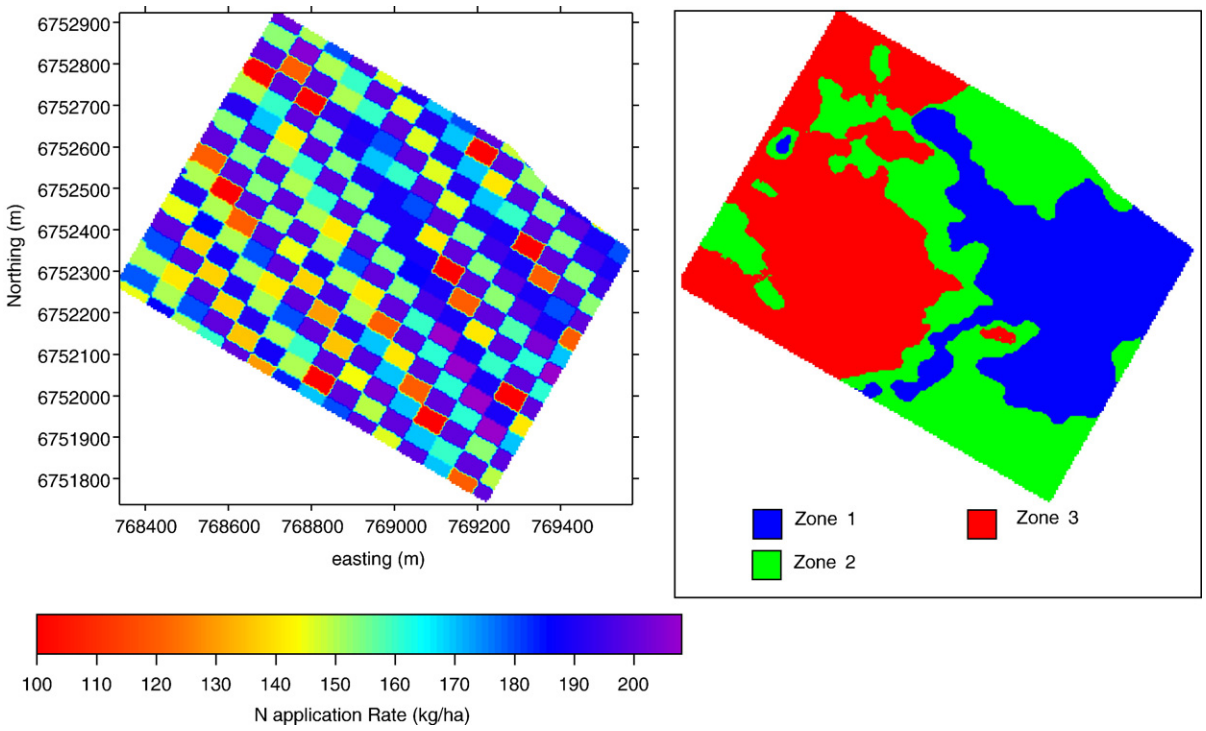

Fig. 2. Map of nitrogen fertilizer application rate (left) and the three management zones (right). After Stewart (2003).

The environmental factors representing the *s*, *o*, *r* factors are: gamma radiometrics, Landsat TM images, a digital elevation model and derived terrain attributes. The ratio of the Landsat TM bands which can enhance soil and vegetation attributes were calculated, i.e. the clay index, which is calculated from Landsat TM band 5/ band 7, this ratio aims to separate land and water, since soils exhibit strong absorption in the band 7 (2.08–2.35 μm) and high reflectance in band 5 (1.55–1.75 μm). The data are divided into a prediction set of 200 observations, and a validation set of 141 observations.

3.1.4. (4) Nitrogen fertiliser field experiment

This involves a field-scale fertiliser experiment (Stewart, 2003). A field of 83 hectares in NSW, Australia was divided into 3 management zones based on previous yield maps and electromagnetic induction survey using the k-means clustering algorithm. Nitrogen fertiliser was applied as anhydrous ammonia with a fertiliser application map shown in Fig. 2. The field was divided into blocks of 48 m × 70 m, and at each block N fertiliser at different rates were applied. The rates were determined based on treatments of uniform application, continuous fertilisation based on soil analysis, and management zones. Cotton lint yield was collected using a yield monitor on a cotton harvester, and the average yield for each N level within a block was calculated, which gives 248 observations. Thus each observation represents the yield averaged over an area of 3360 m^2. The data is normally distributed with a mean of 1.6 Mg/ha and variance of 0.11 $(Mg/ha)^2$. The purpose is to obtain the optimal N application rate for each of the management zones. A quadratic response function was fitted to the N application rate, the model is:

$$z(x) = \begin{cases} \text{If Zone} = 1 \rightarrow \alpha_0 + \alpha_1 \text{Rate} + \alpha_2 \text{Rate}^2 \\ \text{If Zone} = 2 \rightarrow \beta_0 + \beta_1 \text{Rate} + \beta_2 \text{Rate}^2 + \varepsilon(x) \\ \text{If Zone} = 3 \rightarrow \chi_0 + \chi_1 \text{Rate} + \chi_2 \text{Rate}^2 \end{cases} \quad (26)$$

where Rate is the applied N fertiliser rate (kg ha^{-1}).

3.2. Methods of comparison

To see the benefit of the computation using more advanced and statistically sound BLUP, we compare it with methods conventionally used in pedometrics:

(1) REML-EBLUP with the Matérn covariance function:
- define the trend function and design matrix **M**,
- estimate θ of the Matern function with REML by profile likelihood method,
- estimate β using Eq. (4) with predicted θ,
- apply spatial prediction at unvisited sites using (5).

(2) Regression kriging (RK), which involves:
- estimate β by fitting a linear trend model to observed data using ordinary least squares (OLS) (Eq. (13)),
- calculating residuals of the trend model,
- computing the experimental variogram of the residuals using method of moments,
- fitting an exponential model to the experimental variogram using weighted nonlinear least squares,
- performing kriging of the residuals at the unvisited site,
- calculating values of the trend from OLS at the unvisited site,
- Final prediction is obtained by summing the OLS prediction and residuals from kriging.

(3) Ordinary kriging (OK), assuming spatial stationarity:
- computing the experimental variogram of the data using method of moments,
- fitting an exponential model to the experimental variogram using weighted nonlinear least squares,
- performing kriging of the data at the unvisited sites.

All of the procedures use global estimates, or using all the data points for prediction at unknown sites. For prediction using regression kriging and kriging we used the exponential function for the variogram, this is because it is stable in nonlinear least-squares fitting and was found to represent most soil properties (Minasny and McBratney, 2005). The procedures are programmed in Matlab (Mathworks, 2004), and the codes are available from the authors' website www.usyd.edu.au/su/agric/acpa/software.

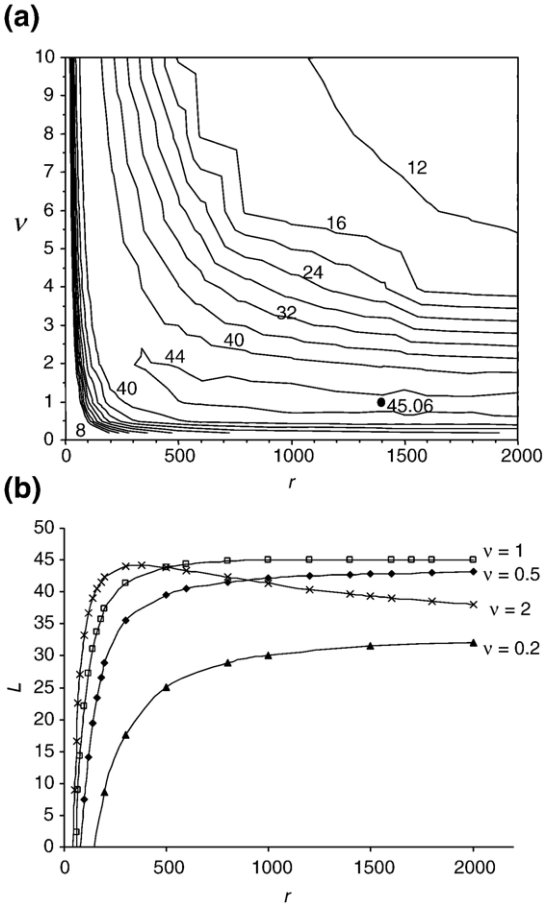

Fig. 3. Profile log-likelihood of the log(Zn) data: (a) contour plot of REML log-likelihood L as a function of distance parameter r and smoothness ν; (b) Log-likelihood L as a function of r at selected values of ν.

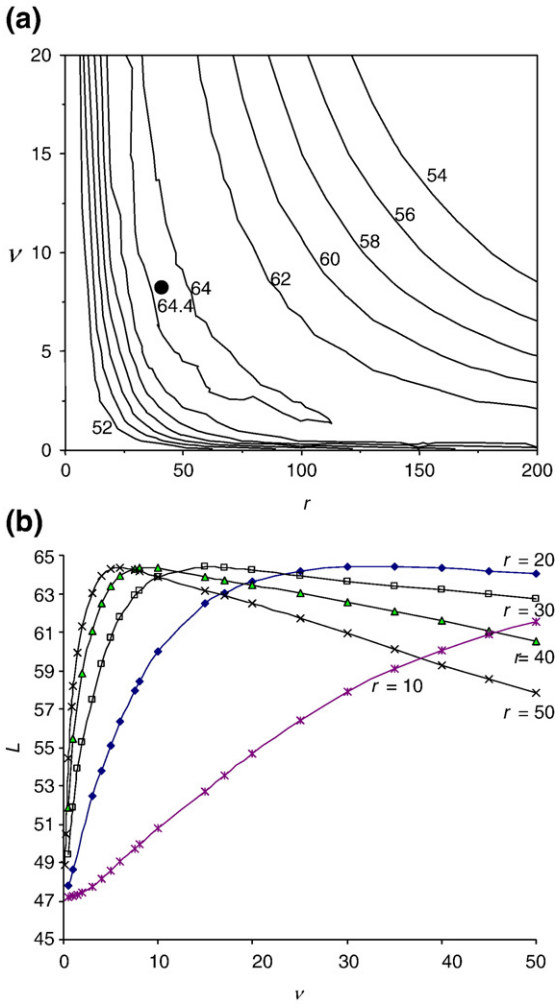

Fig. 4. Profile log-likelihood of the residuals: (a) contour plot of REML log-likelihood L as a function of distance parameter r and smoothness ν; (b) Log-likelihood L as a function of r at selected values of ν.

The following indices were used for comparing the performance of the various spatial prediction methods:

– Root mean squared deviation (RMSD), which measures the accuracy of predictions:

$$\mathrm{RMSD} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left\{z(x_i) - \hat{z}(x_i)\right\}^2} \tag{27}$$

– Standardised squared deviation, which measures the goodness of theoretical estimates:

$$\theta(x) = \frac{\left\{z(x) - \hat{z}(x)\right\}^2}{\sigma_x^2} \tag{28}$$

where $z(x)$ is measured value and $\hat{z}(x)$ is predicted value with variance σ_x^2. A mean of θ (**x**) close to 1 indicates a good estimate (Voltz and Webster, 1990). Lark (2000a) suggested the median of θ (**x**) was a better estimate as it is more robust against outliers. A median value close to 0.455 indicates kriging with a correct variogram. If the median is significantly less than 0.455 it indicates kriging overestimates the variance, and when it is significantly greater than 0.455 it underestimates the variance.

4. Results

4.1. The Zn concentration along the Meuse River

First we determine parameters of the Matérn variogram of the data and residuals using the profile-likelihood method. Fig. 3a shows the log-likelihood contour as a function of r and ν for the data. The plot shows the optimum value of ν is around 1 with r values from 500 to 2000 m. The largest value of log-likelihood L from these ranges is obtained when $\nu = 1$ and $r = 1400$. The plot of the variogram of the data is given in Fig. 5, the symbols represent the empirical variogram, while the smoothed line is the Matérn function fitted using REML. It shows that the variogram calculated using REML is similar to the empirical variogram to distances around 500 m and starts to increase exponentially. This discrepancy of semivariance at large lags has been observed by Cressie (1993) and Lark et al. (2006). But more importantly the variogram from REML showed increasing semivariance with increasing separation distance, suggesting the presence of a trend. The profile log-likelihood for the residuals is shown in Fig. 4, values of r and ν are correlated with the contour line of maximum L that is

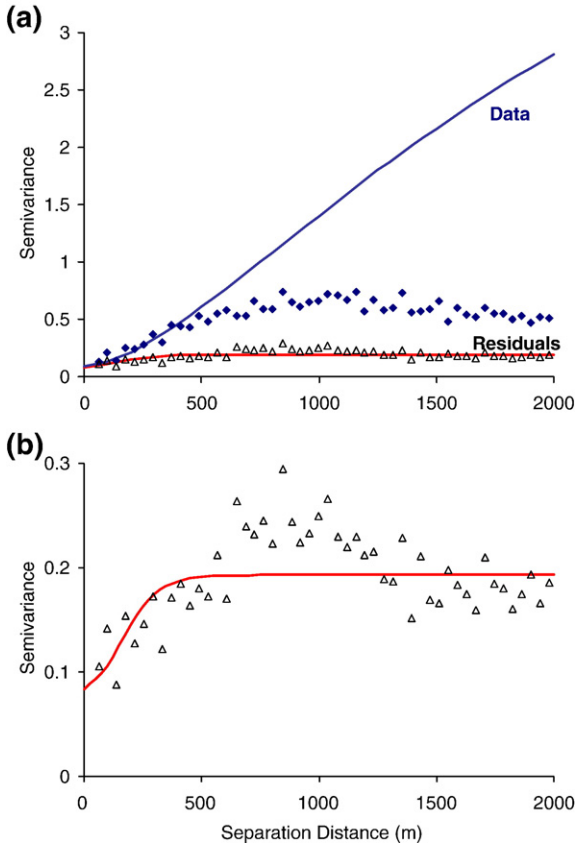

Fig. 5. Variogram for the (a) log(Zn) concentration data, (b) residuals. Dots represent empirical variograms, and smoothed lines represent Matérn function obtained using REML.

Table 1
Root mean squared deviation (RMSD) and standardised squared deviation $\theta(\mathbf{x})$ using leave-one-out cross validation on the Meuse Zn data using different prediction methods

Prediction method	RMSD (log [ppm])	Mean $\theta(\mathbf{x})$	Median $\theta(\mathbf{x})$
REML-EBLUP	0.368	0.996	0.317
Regression Kriging	0.376	1.131	0.347
Kriging	0.424	1.440	0.553

elongated, showing the higher the smoothness parameter the shorter the range r. The plot indicates that values for ν that maximise L is quite high (greater than 5) implying a smooth spatial process. We estimated parameter values for the covariance of the residuals are $c_0=0.084$, $c_1=0.109$, $r=40$, $\nu=8$ (Fig. 5b), although we realise that there are other ν values (which are greater 5) that give similar log-likelihood L values and similar variograms.

Both data and residuals show a smooth spatial process (Fig. 5), which can be explained as the data 'points' are bulk averaged over an area of 100 m^2 (Burrough and McDonnell, 1998). This is an advantage of using REML with the 'universal' variogram model, as we are able to gain insight on the spatial process which sometimes cannot be gained by experimental variograms. In contrast, Pebesma and Heuvelink (1999) calculated the experimental variogram and fitted an exponential variogram (which assumes $\nu=0.5$) to the data.

Parameters of the trend (Eq. (23)) estimated using REML are $\beta_0=6.966$ and $\beta_1=-2.542$ while OLS estimated parameters do not differ much with $\beta_0=6.994$ and $\beta_1=-2.549$. We used the leave-one-out cross-validation procedure to calculate the performance indices: root mean squared deviation (RMSD) and the mean and median of standardised squared deviation θ (**x**) for EBLUP, OK, and RK. Cross validation results on Table 1 show that EBLUP has the lowest RMSD, followed by RK and OK. The mean of θ (**x**) for EBLUP is the closest to 1, followed by RK (1.13) and OK (1.44). The median of θ (**x**) for EBLUP is 0.32 and for RK=0.35 lower than the critical value of 0.455 suggested by Lark (2000a) implying an overestimation of the variance.

Fig. 6 shows maps of the predicted log(Zn) concentration on a regular grid of 40 musing EBLUP, RK and OK. Compared with OK, the maps showed that the prediction variance is higher when using EBLUP. Fig. 6 shows no major difference between maps obtained using EBLUP and RK. However the variance is underestimated for RK as it assumed independent variance contribution from OLS and kriging, and variance obtained from OLS (Eq. (15)) is quite small.

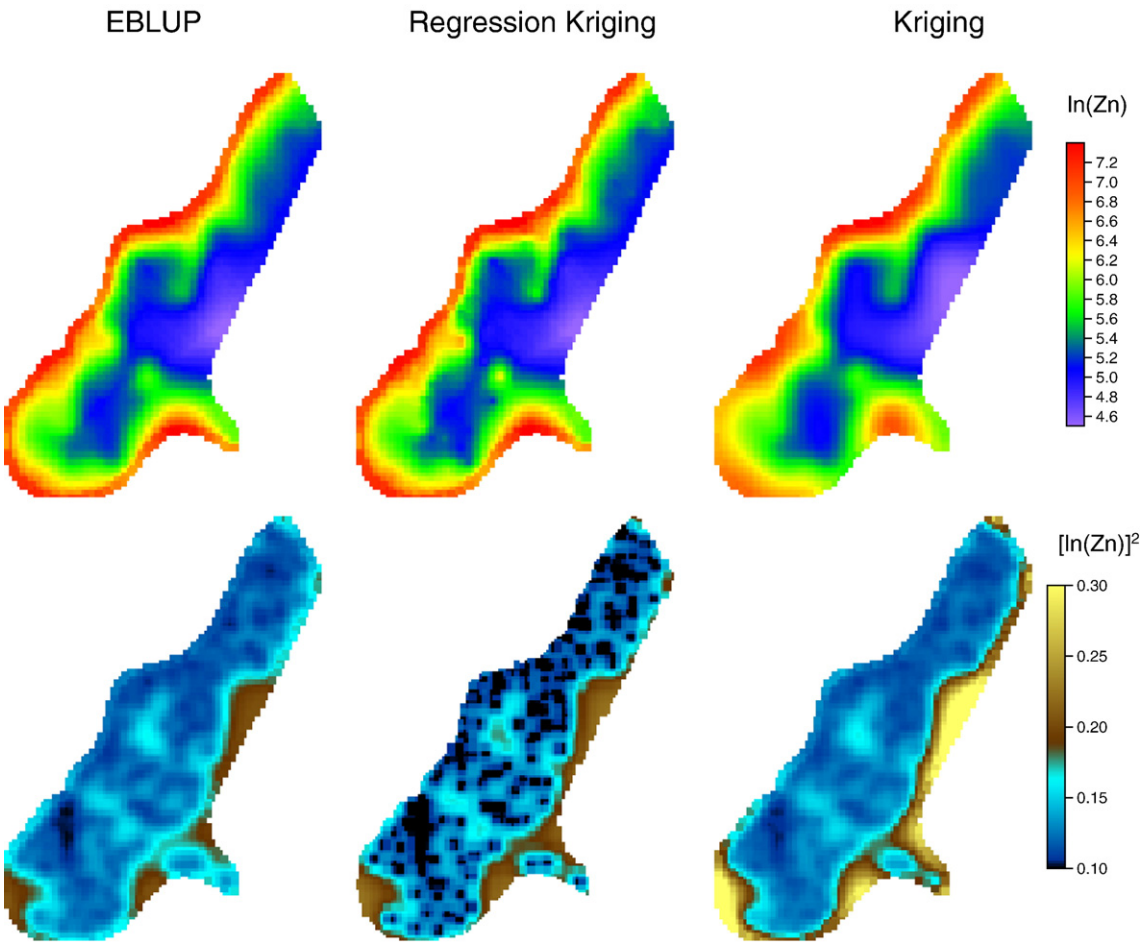

Fig. 6. Maps of predicted log(Zn) concentration (top) and its variance (bottom) using EBLUP, regression kriging and kriging.

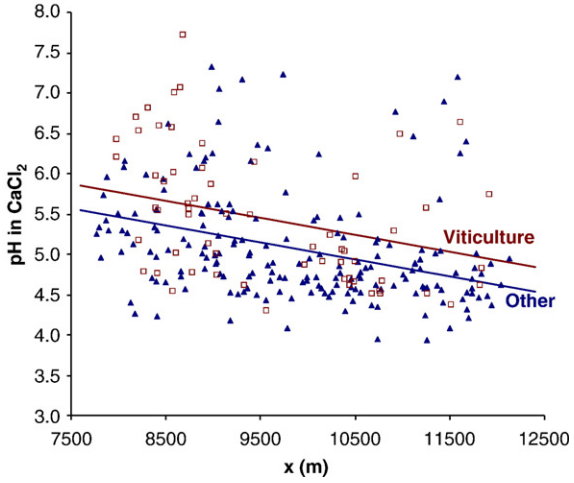

Fig. 7. Trend function for topsoil pH data in the Hunter Valley.

4.2. Soil pH data in the Hunter Valley

Fig. 7 shows the trend model (Eq. (23)) fitted to the soil pH data, using REMLthe parameters are: $\beta_0=7.14$, $\beta_1=-0.0002$, $\beta_2=0.31$ (RMSD=0.67). It illustrates the decrease in soil pH about 1 unit with distance of 4 km from west to east, and the increase pH of 0.3 unit with viticulture land-use due to liming. Fig. 8 shows the variogram of the data and residuals, where the REML estimated variogram and empirical variograms appear to be quite similar. Although the trend is apparent in the data, it does not have a large influence on the variogram.

The dataset is divided into a prediction (training) set (250 observations) and a validation set (149 points). Table 2 shows the prediction power using the 3 methods on the validation set, EBLUP appears to have the lowest RMSD. However according to the $\theta(\mathbf{x})$ statistics, EBLUP performs worst with mean 2.45 (greatest deviation from 1), and median 0.69 (deviates the most from 0.455), which implies EBLUP underestimates the variance.

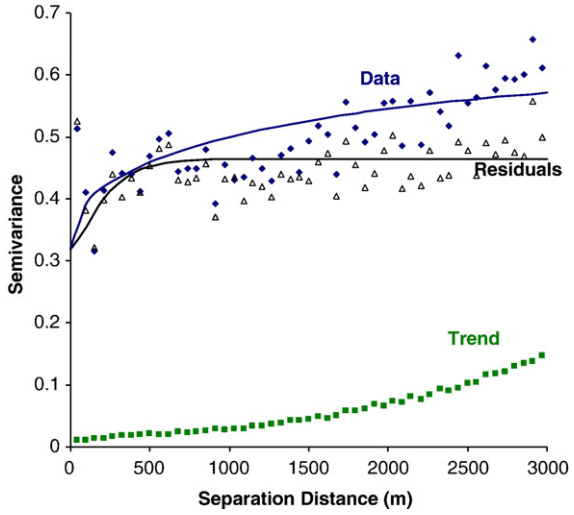

Fig. 8. Variogram of topsoil pH data in the Hunter Valley. Dots (points) represent experimental variogram calculated using method of moments. Smoothed lines are Matern function estimated using REML.

Table 2
Prediction of topsoil pH in the Hunter Valley for the validation set

Prediction method	RMSD	Mean $\theta(\mathbf{x})$	Median $\theta(\mathbf{x})$
REML-EBLUP	0.674	2.45	0.69
Regression Kriging	0.682	1.07	0.32
Kriging	0.690	1.09	0.34

Ordinary kriging and regression kriging perform similarly according to $\theta(\mathbf{x})$ statistics.

We used a different number of observations (50, 60, 70, 80, 100, 150, 200, 250) for calibrating the model and predicting it on a validation set. This is to test whether prediction can be enhanced using REML-EBLUP when the number of observations is reduced. Lark (2000b) demonstrated that with 60 samples, a variogram estimated using the maximum likelihood is similar to that achieved by the method of moments with 90–120 data which is often regarded as the minimum sample size required.

The prediction set is sampled 10 times for a particular number of observations: 50, 60, 70, 80, 100, 150, and 200. For each replication of a particular sample size the parameters of the Matérn variogram were estimated using REML, and the validation set is predicted using EBLUP. Similarly for regression kriging it involves, fitting a linear model using OLS, calculating the residuals, calculating experimental variogram, fitting an exponential model to the experimental variogram, kriging the residuals to the validation set, applying the trend model to the test set, then summing the linear model and the kriged residuals. The root mean squared deviation on the validation set is calculated each time.

Table 3 shows the average RMSD for prediction on the test set using the prediction set at different number of samples from 50 to 250. For each sample size, we tested REML-EBLUP and regression kriging with and without the trend model. Results in Table 3 indicated that there are some benefits of using REML-EBLUP for sample size <70; however, the improvement is not significant. Cressie (1993) made a remark that the bias of variograms in RK is important when the number of data is small and the lag distance is large. Fig. 9 shows that REML estimates of the residual variograms are quite consistent even just using 50 observations.

Surprisingly regression kriging predicts the same or better in some instances compared with the more complicated calculation of REML-EBLUP. There is also an indication that adding

Table 3
RMSD of prediction for the validation set using different spatial prediction methods and various number of data points

No. of data samples used	With Trend		Without trend	
	EBLUP (Matérn)	RK (Exponential)	EBLUP (Matérn)	Kriging (Exponential)
50	0.718	0.743	0.746	0.761
60	0.697	0.710	0.737	0.747
70	0.705	0.693	0.734	0.757
80	0.701	0.706	0.726	0.712
100	0.692	0.687	0.717	0.706
150	0.688	0.678	0.705	0.698
200	0.679	0.677	0.686	0.692
250	0.666	0.669	0.669	0.688

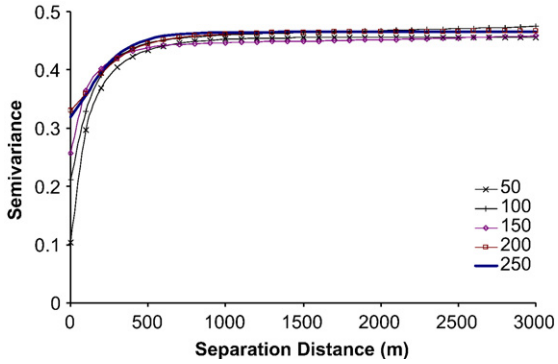

Fig. 9. Variogram of the residuals for topsoil pH data in the Hunter Valley calculated using REML with different number of observations.

the trend component improves the prediction when the number of observations is <200. As we see from Fig. 8 the trend model has a small influence on the variogram. This may explain why EBLUP does not perform much better when the number of observations is greater than 200.

4.3. Topsoil clay content in the Edgeroi area

Using stepwise regression on the prediction set (200 observations), we obtained the following linear regression of top soil clay content as a function of Clay_Index (Landsat TM [Band#5/ Band#7]), Radiometrics K (K), elevation (Elev), and topographic wetness index (qwet):

$$\begin{aligned}\text{Clay} = {} & 0.68 - 0.14\text{Clay\_Index} + 0.11\text{K} - 0.001\text{Elev} \\ & + 0.011\,\text{Slope} + 0.01\text{qwet} \\ & (R^2 = 0.38, \text{RMSD} = 0.14\text{kg kg}^{-1})\end{aligned} \quad (29)$$

Using REML, we obtain the following prediction equation:

$$\begin{aligned}\text{Clay}(x) = {} & 0.95 - 0.07\ \text{Clay\_Index} + 0.04\ \text{K} - 0.002\ \text{Elev} \\ & + 0.019\ \text{Slope} + 0.002\ \text{qwet} + e(x).\end{aligned} \quad (30)$$

Fig. 10 shows the variogram of the data, trend model, and residuals. REML estimated parameters of the variogram as:

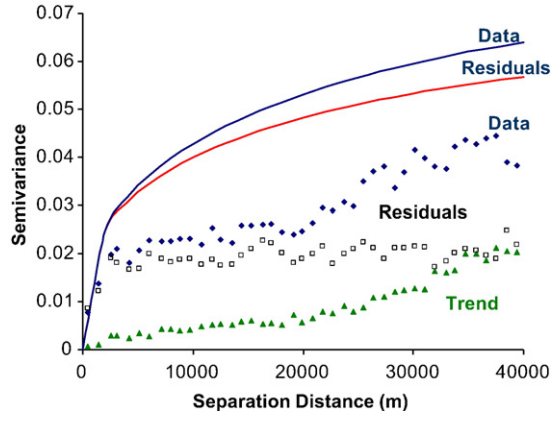

Fig. 10. Variogram of clay content in the Edgeroi area. Dots represent empirical variograms, and smooth lines represent Matérn function estimated using REML.

Table 4
Prediction of clay content in the Edgeroi area for the validation set

Prediction methods	RMSD (kg/kg)	Mean $\theta(\mathbf{x})$	Median $\theta(\mathbf{x})$
REML-EBLUP	0.120	0.58	0.27
Regression Kriging	0.122	1.01	0.45
Kriging	0.126	1.08	0.58
Ordinary LS (Trend only)	0.139		

$c_0 = 0.0$, $c_1 = 0.067$, $r = 50000$ and $v = 0.15$. We fixed the range parameter to the maximum distance of the area as the log-likelihood is increasing with increasing r, suggesting a very long range. Fig. 10 shows the discrepancy between the variogram obtained by REML and method of moments. The variance estimated using REML is much larger. This may be the problem of biased estimation of variograms as observed by Lark et al. (2006). We can see that the trend model only constitutes a small part of the variance.

Table 4 shows the prediction on the validation set (141 observations), as with previous examples using RMSD the performance of EBLUP is just slightly better than the others. According to the $\theta(\mathbf{x})$ statistics, REML-EBLUP performs worst with mean 0.58 and median 0.27 implying overestimation of the variance. The best predictor according to the $\theta(\mathbf{x})$ statistics is regression kriging. Fig. 11 shows prediction on the test set using EBLUP and RK, there are only minor differences between regression kriging and kriging.

4.4. Nitrogen fertiliser field experiment

Fig. 12 shows the profile likelihood estimation of the optimal smoothness parameter v of the Matérn function. The plot points to 1.2 as an optimal value for v, suggesting a smooth spatial process. The smooth process is because each observation refers to an average yield within a plot of 3360 m^2. Fig. 13 shows the response functions of the fertiliser application on the cotton lint yield for the 3 management zone. As seen, the 3 zones have a different maximum yield, zone 1 is the highest, followed by

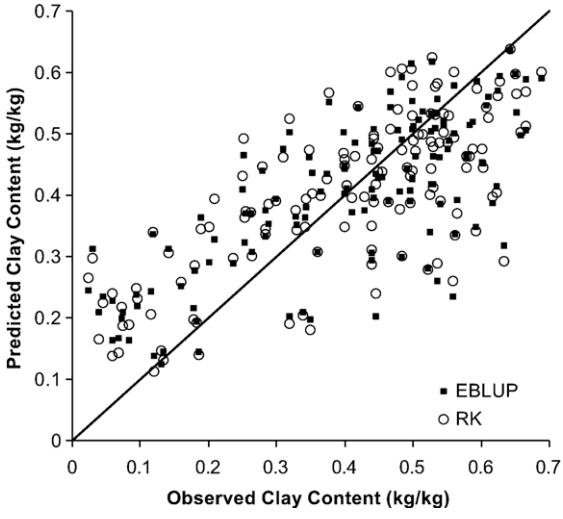

Fig. 11. Comparison between observed and predicted topsoil clay content in the Edgeroi area.

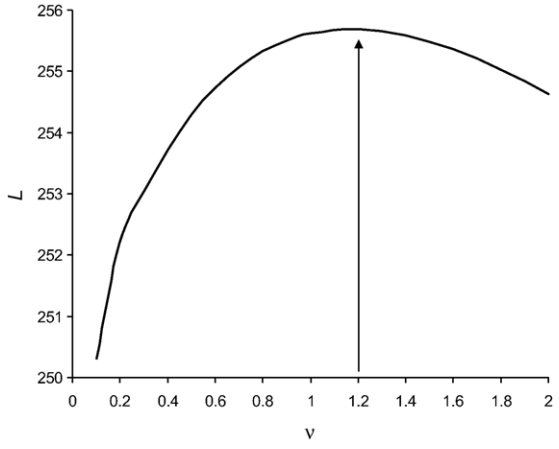

Fig. 12. Profile likelihood determining the optimum smoothness parameter ν of the Matern covariance function.

zones 2 and 3, respectively. The difference between the quadratic response function from EBLUP and OLS is small. Optimum fertiliser rates giving the maximum yield estimated by EBLUP and OLS do not differ much. Using leave-one-out cross validation we evaluated the performance of the 3 methods in predicting yield. Table 5 shows that REML-EBLUP outperformed RK and OK. This is the only example in this paper that shows the advantage of REML-EBLUP, increasing the precision about 24 times compared with RK. The inadequacy of the $\theta(\mathbf{x})$ statistics is demonstrated again, favouring kriging and implying the overestimation of variance for EBLUP.

5. Discussion

Theoretically RK should not perform better than REML-EBLUP as it assumes an independent fixed model and the random effect. It has been shown that the estimation of variogram of the residuals may be biased by using RK especially at large lags, and the prediction variance is underestimated (Cressie, 1993). Although results presented here show slight improvement of

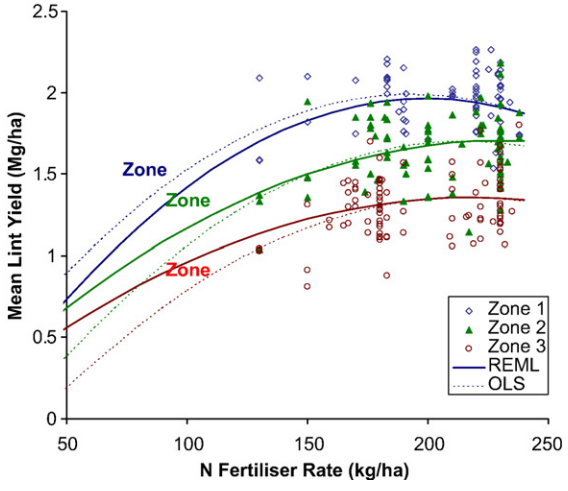

Fig. 13. Response function for the nitrogen field trial experiment, dots represent observations, curves represent estimated quadratic response function.

Table 5
Prediction of cotton lint yield from N fertiliser field experiment using leave-one-out cross validation

Prediction methods	RMSD (Mg/ha)	Mean $\theta(\mathbf{x})$	Median $\theta(\mathbf{x})$
REML-EBLUP	0.126	0.31	0.08
Regression Kriging	0.157	1.03	0.32
Kriging	0.163	1.86	0.54
Ordinary LS (Trend only)	0.188		

prediction when using REML-EBLUP, the advantage does not appear to be large. Table 6 shows the relative improvement of using REML-EBLUP compared with RK and OK in terms of the reduction in RMSD. We see that for soil properties, the improvement over RK is quite small 0.5–3.5%. The improvement over OK is about twice of RK. We are surprised to find that practically RK performs as well as EBLUP. The advantage of EBLUP is only shown in the field experiment data where the yield is clearly affected by the N fertiliser and management zones. Cressie (1993) noted substantial bias at large lags of variogram when the residuals are estimated based on OLS (as done in RK), however in a local neighbourhood kriging predictor mainly used variogram model at small lags and the discrepancy is more pronounced in the predictor variance. There are mixed results with regard to the use of standardised squared deviations $\theta(\mathbf{x})$, from the Meuse Zn data which has a strong trend, the mean and median of $\theta(\mathbf{x})$ suggests similar performance of EBLUP and RK. Results on the pH and clay content prediction suggest that REML-EBLUP performed worse than RK and OK. This appropriateness of using this statistics for kriging with trend need further investigation as it favours the use of OK and RK, where the variance mostly comes from the spatial component. Meanwhile the variance of REML-EBLUP is a combination of both trend and the residuals (Eq. (5)).

The Matérn covariance function is useful for characterising the nature of the spatial process. As seen in the Meuse Zn data and Nitrogen fertiliser experiment, the Matérn function identifies the smooth spatial process which is difficult to determine with the method of moments. However this information does not provide a significant advantage in spatial prediction over RK.

We have shown that in some cases the prediction incorporating ancillary variables can improve the prediction; in some instances the improvement is quite small. We demonstrated that when the trend model only explains a small part of the variation, there is a slight improvement in prediction when using RK or EBLUP (as in clay content in Edgeroi and Hunter Valley pH data). Thus as an initial inspection, we suggest examination of the variograms of the data, and residuals using the method of

Table 6
Relative improvement of prediction using REML-EBLUP compared with regression kriging (RK) and ordinary kriging (OK) in terms of RMSD reduction

	Improvement over RK (%)	Improvement over OK (%)
Meuse Zn data	2.1	15.2
Pokolbin pH (50 observations)	3.5	6.0
Pokolbin pH (250 observation)	1.2	2.2
Edgeroi clay content	1.7	5.0
Cotton yield	24.6	29.4

moments. When the trend model constitutes a large proportion of the variance (as in the Meuse Zn concentration data, and N field experiment) BLUP and RK can help to improve the prediction. On the other hand, for the purpose of digital soil mapping, the inclusion of ancillary variables adds more information to the produced map compared to using kriging. With kriging the resulted soil maps will be too smooth especially when the interpolation covers large areas. Incorporating the ancillary variables which represent the soil forming factors adds content to the map. The information content produced from such maps compared with just kriging need to be accounted when comparing the prediction performance.

6. Conclusions

Although statistically inappropriate, RK is easy and has proven to be a robust technique for practical application. Furthermore various linear and nonlinear trend models can be incorporated. When a large number of data is present (eg. proximally sensed data) local regression kriging, which involves estimating a local trend model and combination with local kriging of the residuals (Walter et al., 2001) should present a unique and robust technique with good results. REML-EBLUP is useful when there is a strong trend, we need to understand the underlying spatial process, and when the number of observations is small (<200). We conclude that improvement in the prediction of soil properties does not rely on more sophisticated statistical methods, but rather on gathering more useful and higher quality data.

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