

Predicting magnesium concentration in needles of Silver fir and Norway spruce—a case study

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Received 1 October 2002; received in revised form 13 January 2004; accepted 17 February 2004

Abstract

Different geostatistical methods are used to interpolate the spatial distribution of the foliar magnesium content of Silver fir and Norway spruce in the Black Forest. The data analysed are from a monitoring survey carried out in 1994 in the forest of Baden-Württemberg, a federal state in the south-west region of Germany. In this survey many potential explanatory variables are collected. The aim of this paper is to identify the best prediction method that can be useful in the future for cause–effect studies and environmental modelling. At the same time, causal relationships between the response variable and the predictors are investigated. Therefore, geostatistical methods with lowest prediction errors which simultaneously provide the highest explanation value had to be identified. The performance of different methods is measured using cross-validations techniques.

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Keywords: Kriging; Geostatistics; Spatial prediction; Spatial statistics; Linear model; Foliar magnesium content; Black Forest; Norway spruce; Silver fir

1. Introduction

In 1994 the forest health status has been monitored in Baden-Württemberg using different survey schemes where a number of different possible influential factors are recorded. A justification for these monitoring programmes is the hypothesis that the deterioration of forest crown condition is of a chronic nature. The deterioration is meant to be caused by acidification and washing out of essential alkaline macro nutrients in the root area which has a negative influence

on forest nutrition and this finally causes the loss of needles and leaves (see Anon, 1993). This acidification is caused by industrial emissions and affects soil chemistry including nutrient and metal availability. In some of the areas of Baden-Württemberg the soils are already acidic, e.g. in the Black Forest where the geology is mainly siliceous bedrock such granite and gneiss and does not have a high buffer capacity against the acids. When acid deposition occurs on not well-buffered soils, alkaline macro nutrients including potassium, calcium and magnesium are readily washed out, making them unavailable to the forest as nutrients. Especially, the supply of magnesium develops towards deficiency at the crystalline bedrock areas of the Black Forest, where the magnesium stock, is

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naturally low. Therefore, the magnesium supply of trees is supposed to be a key factor in forest deteriorations (Anon, 1993). Lots of efforts have been done in the last years to describe and justify the current state of deterioration of the forest in Germany and more in general in all Europe. In particular models have been developed to link the effect of soil acidification with the tree growth and the change in nutrients (see for instance Mohren and Ilvesniemi, 1995; Mohren et al., 1995 in which different models are proposed and analysed to study the effects of air pollution and soil acidification in the forest growth and indirectly in nutrient supply for Norway Spruce in Germany).

In this work, we suppose the following order of dependence among influencing factors: nature and magnitude of deposition of acidity and nitrogen → soil condition → forest nutrition → crown condition. In this sense we do not expect to find some acute impact of air pollutants rather than a chronic effect of step by step reduced buffering capacity and nutrient availability in soils, which leads at the end to forest damage (see Wilpert, 2002; Wilpert et al., 2000).

In this paper, we are investigating only a small part of the overall goal of the study. The aim is to establish a model for predicting magnesium contents in the needles (a) by using a trend function of soil condition, other site and tree characteristics, and/or (b) by exploiting spatial autocorrelation via geostatistical

methods. In particular, we will compare the prediction performances of different methods currently used in spatial studies, such as a model with independent errors, ordinary kriging, cokriging and kriging with external drift. The goals of each method are summarised in Fig. 1. Identifying a best prediction method can be useful in the future to predict the magnesium in the needles at unsampled locations. Maps of magnesium are needed for ecosystem managements purposes, for instance to decide which area of the forest needs some counteractions against soil acidification like liming.

2. The data

The data are from a monitoring programme carried out by the Forest Research Centre Baden-Württemberg (FVA) in 1994: the survey of emission impact and forest nutrition (Imissionsökologische Waldzustandserhebung und Ernährungsinventur (IWE)). The variable of interest is the magnesium (Mg) content (g/kg) in needles which were collected in the survey: 800 locations on a 4 km × 4 km grid needles of silver fir and spruce trees were sampled for the analysis of the main macro nutrients.

Possible *explanatory variables* which were collected in the IWE are: foliar nutrient contents such as calcium (Ca), potassium (K), manganese (Mn), phosphorus (P) and nitrogen (N), tree characteris-

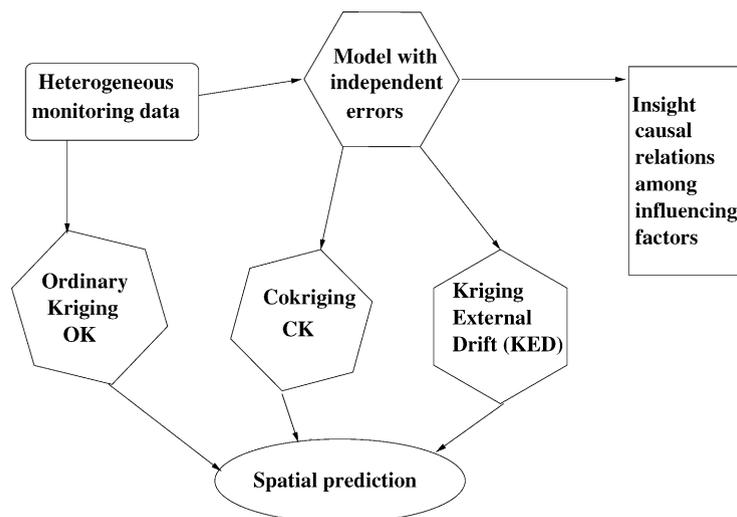


Fig. 1. Scheme of the goals and abilities of the different methods used for evaluation.

tics such as the age (BAter) and the tree species (fir/spruce) (BART), landscape and topographic characteristics such as geological substrate (Geol), direction of slope (Hang), gradient of slope (Hangneig), relief form (GForm), type of situation (Lage), soil characteristics such as soil texture (Boden), soil type (BTyp), soil depth (Gruend), soil water budget (Wasser), trophic class of the soil (Naehr) and humus form (Humus). In addition location, i.e. the x (Rechts) and y (Hoch) co-ordinates and the altitude (HoehenL), can be used to model the trend.

Most of these potential predictor variables were assessed by the survey personnel on an ordinal scale and therefore contain a subjective uncertainty. Nutrient data, age and co-ordinates were measured.

Due to its relative homogeneity in geology (e.g. no extra range substrates like lime stone areas with totally differing nutritional conditions exist there), we restrict the analysis to the region of the Black Forest (see Fig. 2). Additionally in this area the forest cover

amounts to a proportion of about 65% of the landscape and it is characterised by large rather than small patch-like stands.

3. Statistical methods

3.1. Model with independent errors

Initially, we use a model with independent errors to model the data using a trend function of the explanatory variables on soil condition and other characteristics. The model has the form:

$$E(y) = \beta_0 + \sum_k \beta_k x_k \quad (1)$$

Using such a model implies the assumption that the data are independent. Here independence of our spatially referenced data is not very likely. An alternative for interpolating and predicting the magnesium con-

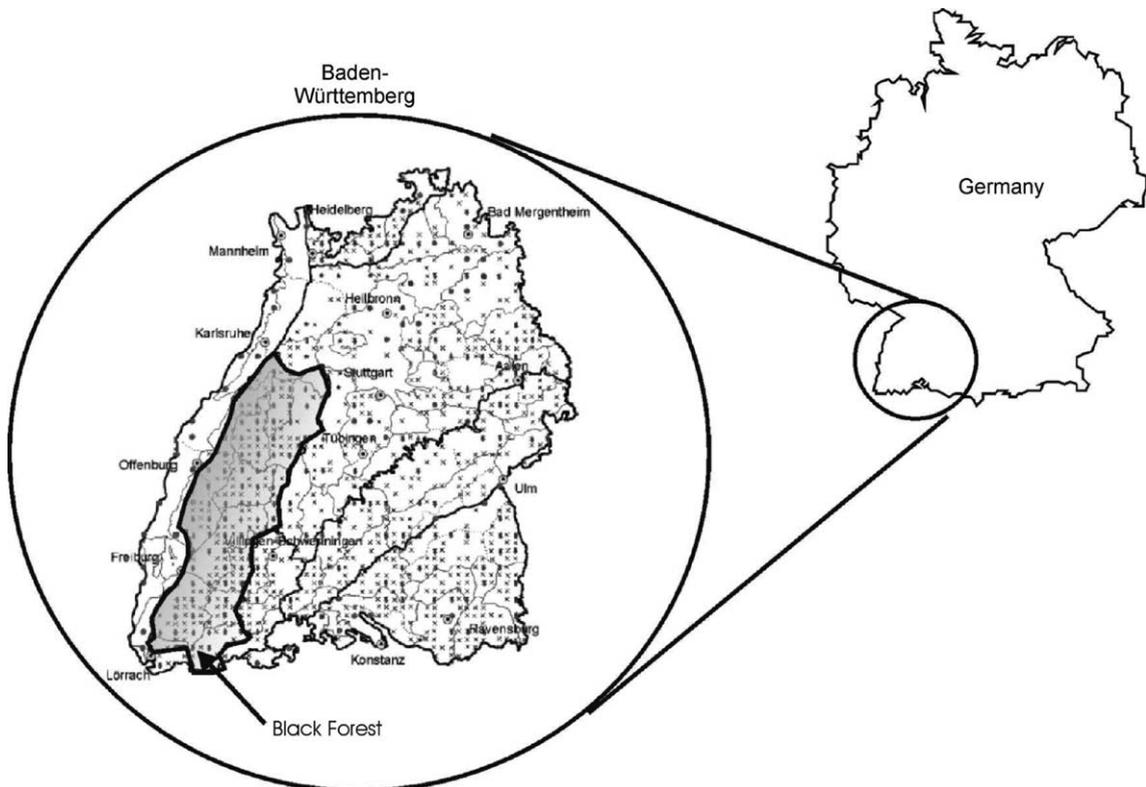


Fig. 2. Overview map. The area of the Black Forest grey shaded. The position of sampling points are marked with crosses and dots.

centrations in the needles taking into account the spatial correlation of the data is geostatistics (Matheron, 1963).

3.2. Geostatistical methods

The geostatistical approach is based on the assumption that sample values are related to one another in a way which is dependent on their distance. Then a primary aim of geostatistics is to estimate the spatial relationship between sample values. This estimate is used to make spatial prediction of unobserved values from neighbouring samples and to give an estimate of the variance of the prediction error.

In geostatistics (Cressie, 1993; Diggle et al., 1998) it is assumed that the data Y_i sampled at the locations $s_i, i = 1, \dots, n$, are partial realizations of a Gaussian random process $\{Y(s) | s \in D \subset R^d\}$ such that, $\forall s \in D$:

$$E[Y(s)] = \mu(s) \quad (2)$$

and the variance

$$\text{var}[Y(s_i) - Y(s_j)] = 2\gamma(s_i, s_j) \quad (3)$$

exists. The process is called intrinsic stationary if its *semi-variogram* $\gamma(s_i, s_j)$ depends only on the distance between s_i and s_j (and eventually on the direction of the vector $h = s_i - s_j$) but not on their locations.

The goal of kriging is to predict in an optimal way the value of the process $Y(\cdot)$, at an unsampled location s_0 from a linear combination of the observed values Y_i . $\hat{Y}(s_0) = \sum_{i=1}^n \omega_i Y_i$. The weights ω_i are chosen in order to minimise the mean square prediction error

$$\text{MSE} = E[(Y(s_0) - \hat{Y}(s_0))^2] \quad (4)$$

subject to the unbiasedness constraints $E[\hat{Y}(s_0)] = E[Y(s_0)]$. The resulting predictor has minimum variance, the so called kriging variance, within the class of unbiased predictors.

The kriging procedure is optimal in the sense that it gives optimal predictions when the covariance structure is known. The conventional kriging approach consists in *plug in* estimated parameter values and proceeds as if the estimates were the true values. In practice, the semi-variogram is estimated from the data using the empirical semi-variogram given by

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Y(s_i + h) - Y(s_i)]^2 \quad (5)$$

where $N(h)$ is the number of pairs of observations in D which are at distance h . If outliers are present we can use a robust semi-variogram estimator (see Cressie, 1993). It is necessary for the semi-variogram to be *conditionally negative definite* to guarantee the positiveness of the estimation variance (see Chilés and Delfiner, 1999). For this reason we need to fit a theoretical model to the empirical semi-variogram graph.

This theoretical curve is chosen from a class of idealised semi-variogram models. Here we consider the exponential model which has the form

$$\gamma(h, \alpha) = 1 - \exp\left(-\frac{h}{\alpha}\right), \quad h \geq 0 \quad (6)$$

One of the common methods for fitting the semi-variogram model is to fit *by eye* or by some *curve fitting algorithm* a theoretical curve to the empirical semi-variogram. An alternative approach is to compute the maximum likelihood estimator of the model parameters.

3.3. Ordinary kriging and lognormal kriging

Ordinary kriging refers to spatial prediction under the assumptions that $\mu(s) = \mu$ is constant and

$$\sum_{i=1}^n \omega_i = 1 \quad (7)$$

(this last assumption guarantees unbiasedness). From standard theorems (see Cressie, 1993) we can easily derive the minimum mean square error predictor for $Y(\cdot)$ and the corresponding kriging variance.

If the stochastic process under study is non-Gaussian, we often try to make it Gaussian by a prior transformation of the variable. Then the kriging methodology is applied to the transformed variable. However the back-transformed value is usually biased and we have to use approximate expressions for the unbiased predictor and the mean-squared prediction error (see trans-Gaussian kriging in Cressie, 1993). In this paper we restrict our attention to the lognormal transformation, i.e. when the logarithm of the process under study $W(s)$ is Gaussian ($Y(s) = \log W(s)$). In this specific case, we have an exact expression for the unbiased predictor of our initial variable and for its mean-squared prediction error (see Cressie, 1993).

Other possible extensions relaxing the Gaussian assumptions are available in the literature (e.g. Diggle et al., 1998; Gotway and Stroup, 1997).

3.4. Universal kriging and kriging with external drift

Universal kriging refers to spatial prediction under the assumptions that there is a trend in the sample values $\mu(s) = \sum_{i=1}^n \beta_i f_i(s)$, where the β_i are fixed unknown parameters and the f_i are known functions of the spatial locations chosen to model the trend. Particular cases are a linear or a polynomial trend surface. The unbiasedness condition becomes

$$\sum \omega_i f_i(s_i) = f_i(s_0) \quad (8)$$

Universal kriging involves removing the trend from the sample values and study residuals variation. For details in the minimisation procedure see Cressie (1993) or Diamond and Armstrong (1984). If the trend is a function not only of the co-ordinates of the locations but also of other covariates the minimisation procedure is called kriging with external drift (KED) or kriging with a trend model. In this case we have:

$$E[Y|x_{i_1}, \dots, x_{i_n}] = \beta_0 + \beta_1 x_{i_1} + \dots + \beta_n x_{i_n} \quad (9)$$

where x_{i_1}, \dots, x_{i_n} are the observed covariates (for more details see Royle and Berliner, 1999; Gotway and Hartford, 1996; Deutsch and Journel, 1992). Here we use standard model selection techniques to select the appropriate trend function in the data, that is we use a linear model as in Eq. (1) to select the variables for the trend function. The coefficients in Eq. (9) are estimated within the kriging procedure.

3.5. Cokriging

If we want to consider several response variables simultaneously cokriging can be used. It accounts for the spatial cross correlation between primary and secondary variables. In contrast to KED, in cokriging the explanatory variables are not regarded as fixed, but are themselves considered as spatial random variables with an associated variogram. Besides fitting a semi-variogram model to the response variable, cokriging requires to fit a semi-variogram model to the secondary variable and a cross-semivariance model. We refer to Cressie (1993), Goovearts (1997), Wackernagel (1998) for details.

3.6. Cross-validation

Since we are mostly interested in how well the different methods perform in terms of prediction, an appropriate criteria of comparison is the prediction error. In order to estimate the prediction error reliably we use leave-one-out cross-validation to perform model validation. This procedure removes a single observation at a time from the data set and the model is fitted to the remaining observations. Then the actual outcome Y_i is compared with the predicted outcome \hat{Y}_i using the model based on the remaining $n - 1$ observations. The process is repeated n times to obtain an average accuracy that can be expressed by the mean squared prediction error $\sum (Y_i - \hat{Y}_i)^2$ at each location (see for instance Davison and Hinkley, 1997; Isaacs and Srivastava, 1989). The method which leads to the smallest estimated prediction error is preferred.

4. Data analysis and results for the magnesium in the needles

4.1. Exploratory analysis

Magnesium content in the needles is not normally distributed. In order to apply kriging and fit a linear regression to these data we consider as the response variable the logarithm of the magnesium. The data set contains all survey locations in which magnesium in the needles was measured. In a first step we have screened the explanatory variables for correlation. If the correlation between two variables was higher than 0.5, we have chosen the variables which have a stronger effect on the response variable in terms of regression analysis in which the two correlated variables were used separately. Hence, we left out the factor tree species (Bart) which was strongly correlated with the calcium concentration in the needles (Ca). We also decided to leave out the factor geological area (Geol) because it was strongly correlated with x and y co-ordinates and had a prohibitively large number of different categories (18) for a reasonable model interpretation. Both factor inter-correlations have to be expected since Silver fir has systematically higher Ca contents in the needles than spruce and the geological areas of the Black Forest display a rather consequent order from the Triassic sandstones in the north to the

Table 1

Correlation between the response variable log(Mg) and possible explanatory variables containing tree specific characteristics calcium (Ca), manganese (Mn), potassium (K), phosphorus (P), nitrogen (N), age (BAlter) and tree type (BArt)

	log(Mg)	Ca	Mn	K	P	N	Balter	Bart
log(Mg)	1	0.73	0.09	0.25	0.24	-0.02	0.30	0.71
Ca	0.73	1	0.36	0.19	-0.007	-0.05	0.26	0.71
Mn	0.009	0.36	1	0.15	-0.16	-0.02	-0.08	0.36
K	0.25	0.19	0.15	1	0.26	0.16	0.13	0.38
P	0.24	-0.007	-0.16	0.26	1	0.37	0.12	0.13
N	-0.02	-0.05	-0.02	0.16	0.37	1	-0.19	-0.11
BAlter	0.30	0.26	-0.08	0.13	0.12	-0.19	1	0.33
BArt	0.71	0.71	0.36	0.38	0.13	-0.11	0.33	1

Table 2

Correlation between the response variable log(Mg) and possible explanatory variables containing geographic and stand conditions, x-ordinate (Rechts), y-co-ordinate (Hoch), soil depth (Gruend) trophic class of the soil (Naehr), relief (GForm), soil type (BTyp) and altitude (HoehenL)

	log(Mg)	Rechts	Hoch	Gruend	Naehr	GForm	Btyp	HoehenL
log(Mg)	1	-0.17	-0.17	-0.002	0.18	-0.07	-0.11	-0.09
Rechts	-0.17	1	0.76	0.01	-0.15	-0.1	0.3	-0.09
Hoch	-0.17	0.76	1	0.02	-0.05	0.05	0.3	-0.4
Gruend	-0.002	0.01	0.02	1	0.38	-0.08	0.08	-0.13
Naehr	0.18	-0.15	-0.05	0.38	1	-0.009	-0.25	-0.27
GForm	-0.07	-0.1	0.05	-0.08	-0.009	1	-0.02	-0.17
BTyp	-0.11	0.3	0.3	0.08	-0.25	-0.02	1	-0.005
HoehenL	-0.09	-0.09	-0.4	-0.13	-0.27	-0.17	-0.005	1

granite and gneiss bedrocks in the south. In Tables 1 and 2 we have the correlation of the response variable log(Mg) and some possible explanatory variables.

4.2. Model with independent errors results

The following model was fitted:

$$E(\log(\text{Mg}_i)) = \beta_0 + \beta_1 \text{Ca}_i + \beta_2 \text{P}_i + \beta_3 \text{Hoch}_i + \beta_4 \text{Mn}_i + \beta_5 \text{K}_i + \text{Gruend}_{k_1} + \beta_6 \text{N}_i + \text{Naehr}_{k_2} \quad (10)$$

where the observation i is at location y_i with levels k_1 for the soil depth and k_2 for the nutrient balance.

This model choice was the result of a backward model selection process (e.g. Burnham and Anderson, 2003). More precisely we started from a general model containing all the explanatory variables retained from the preliminary selection and then used backward elimination for model selection. The idea of backward elimination is to fit all models obtainable by deleting a single term from

an initial model and computing the *Bayesian Information Criterion (BIC)* for each of them ($BIC = -2 \text{ maximised log likelihood} + p \log(n)$ where n is the sample size and p is the number of parameters). At each step the model with the lowest *BIC* is preferred. The estimated coefficients of model in Eq. (10) are given in Table 3. Calcium content in the needles is the

Table 3

Parameter estimates for the selected model with independent errors (drift parameters of KED)

	Estimate	Standard error
Intercept	9.752	2.428
Ca	0.144	0.006
P	0.265	0.040
Hoch	-0.002	0.000
Mn	-0.036	0.012
K	0.020	0.007
Gruend 2	0.066	0.038
Gruend 3	-0.057	0.054
N	-0.017	0.007
Naehr 2	-0.013	0.039
Naehr 3	0.112	0.051

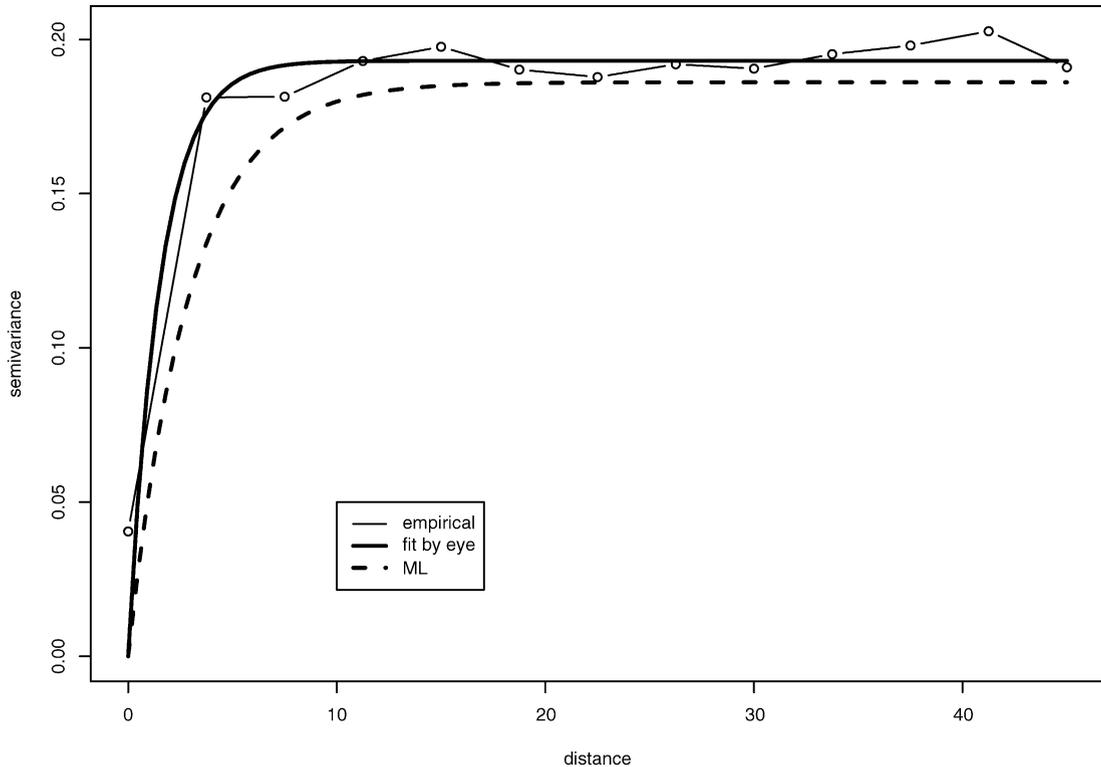


Fig. 3. The empirical semi-variogram of log(Mg) with fitted semi-variogram models using maximum likelihood (ML) and the fit by eye.

strongest predictor for the magnesium contents in the needles. The model explains about 67% of variation (*R*-squared value) in the data.

4.3. Cross-validations results

We use the log kriging, i.e. we apply kriging procedures to the logarithm of the magnesium in the needles. In order to reveal the possible spatial structure of the response variable, we have computed its semi-variogram. The empirical semi-variogram is fitted using an exponential model. Fig. 3 shows the empirical semi-variogram of the original data and the two theoretical semi-variogram fitted by eyes and using the maximum likelihood estimation method. As you can see in the picture, the semi-variogram reaches a limiting value (the sill) at about 0.2. This means that for a distance (the range) bigger then 3 km the data are not correlated. The behaviour of the semi-variogram does not suggests the presence of a trend in the geographical co-ordinates. This observation suggests us

to use ordinary kriging for prediction and we compare it with the kriging with external drift. For the drift we use the results of the model selection procedure for the model with independent errors in Eq. (10) (the corresponding semi-variogram is shown in Fig. 4). To confirm the hypothesis of absence of a strong trend in the geographical co-ordinates, we compare the prediction results reached with ordinary kriging with those of universal kriging. Covariance parameters are estimated using the maximum likelihood method and the estimates for OK, UK and KED are shown in Table 4. We also consider cokriging including in the kriging procedure the continuous variables Ca, P and

Table 4
Estimates of covariance parameters for OK, KED and UK

	Partial sill	Range	Nugget
OK	0.1861	2.948	0
UK	0.1801	2.798	0
KED	0.0642	1.914	0

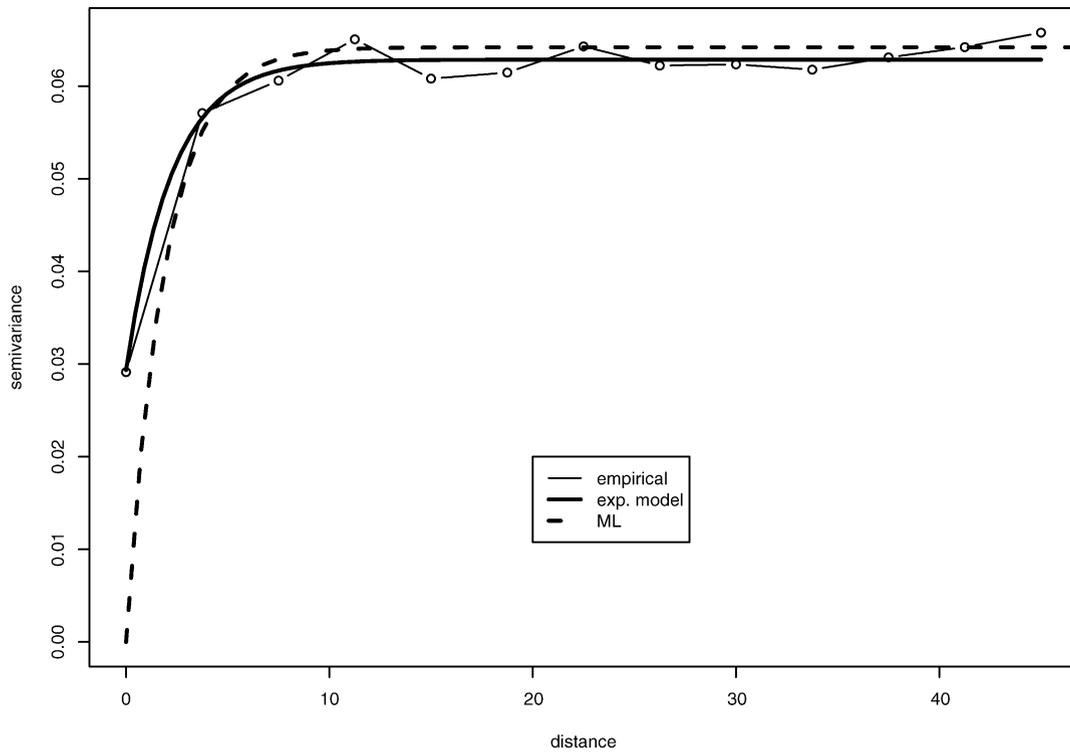


Fig. 4. Empirical and fitted semi-variogram of the residuals of model (10).

K. Fig. 5 show the cross-semivariogram models fitted for the cokriging method. The results of the mean squared prediction errors with the various methods were estimated using leave-one-out cross-validation and are displayed in Table 5. The leave-one-out cross-validation using the model with independent errors results in a mean squared prediction error of 0.096. All the kriging methods reduce the mean squared prediction error. Ordinary kriging yields only a small improvement compared to the model with independent errors. Including more than one variable in the kriging process reduced the error to 0.07 (CK). KED gives

the lowest mean square prediction error (0.048). As expected UK does not improve the prediction with respect to OK. Table 3 shows the values of the Bayesian Information Criteria (BIC) computed for OK, UK and KED. Once again the overall conclusion is that “best” results are reached using kriging with external drift and that universal kriging is not preferred to ordinary kriging.

For OK, UK and KED the R package *geoR* (Ribeiro and Diggle, 2000) was used and for cokriging the ISATIS package was used (Bleines et al., 2000).

Table 5

Mean squared prediction error for log(Mg) from the model with independent errors, ordinary kriging (OK), universal kriging (UK), kriging with external drift (KED) and cokriging (CK)

	Independent errors	OK	UK	KED	CK ^a
mean squared error	0.096	0.091	0.092	0.048	0.070

^a Cokriging was performed with variables Ca, P and K.

5. Discussion

For predicting the logarithm of magnesium contents in the needles of spruce trees in the Black Forest we have used four models:

1. a model with independent errors,
2. ordinary kriging (OK),

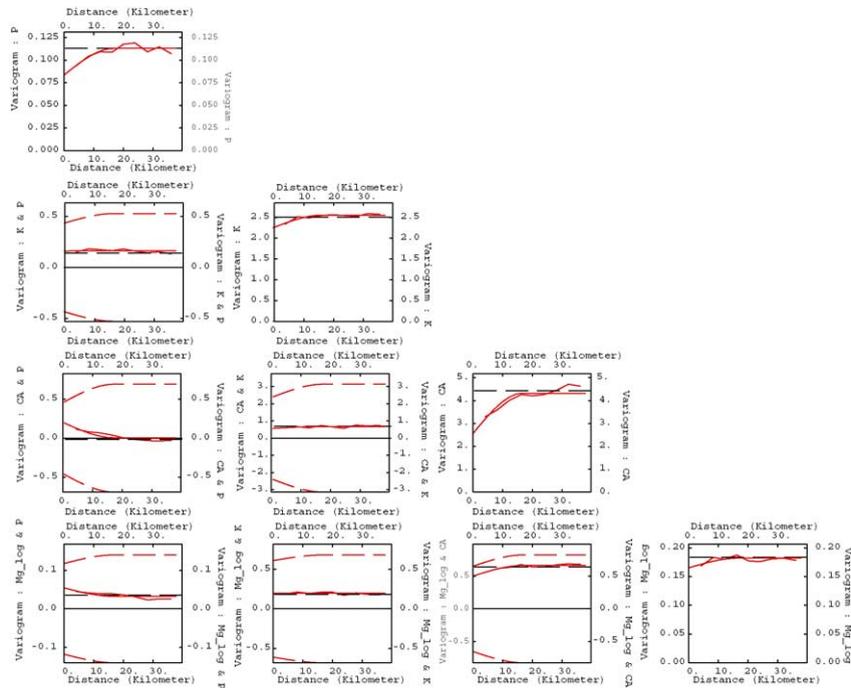


Fig. 5. Cross-semivariogram models fitted for the cokriging.

3. kriging with external drift/kriging with a trend model (KED),
4. cokriging (CK).

In comparison to OK, the model with independent errors, KED and CK allow to incorporate explanatory information such as other nutrients, tree characteristics, soil characteristics or locational variables. The semi-variogram of the logarithm of magnesium in Fig. 3 showed that spatial correlation is present, but no strong spatial trend exists. This hypothesis is validate by the fact that UK does not improve the prediction compared with OK. This observation suggests to use geostatistical methods such as OK, KED and CK, which take into account the spatial correlation. It still seems worthwhile to utilise the variables selected for the model with independent errors to establish the trend function in KED which also considers spatial correlation. KED performed best in terms of prediction; it halved the mean squared prediction error in comparison to OK and the model with independent errors. The prediction error of CK is smaller than for OK. But compared to KED, CK does not

have the benefit of allowing for a trend function with categorical variables. The model with independent errors and OK yield similar mean squared prediction errors. The great advantage of OK compared to the other methods is that explanatory information, which might be expensive to measure is not required. The advantage of OK and CK is that fine grid map predictions can be produced for a particular variable without need of further information. Maps of magnesium contents in needles are further needed for forest management purposes, for instance to decide which areas of the forest need some treatment, e.g. fertilisation or liming with dolomite. For the model with independent errors and KED this is not easily accomplished since to predict such maps the explanatory information must be available on a fine grid (in addition to the survey location used for fitting the trend model).

Although we set ourselves the goal of identifying the best prediction method, we have also identified a procedure which allows the investigation of causal relationships at the same time. That is carrying out a model selection procedure for a model with indepen-

dent errors as an initial step and then using the selected model in KED.

The fact that the model with independent errors procedure identified the Ca contents of needles as strongest and positively correlated predictor for the Mg contents was unexpected concerning an uptake antagonism between these elements as commonly postulated in the literature on tree nutrition (Fiedler et al., 1973; Hüttl, 1991). Our contradictory finding may be interpreted as an indicator for the existence of an external factor as for instance the deposition load which is afflicting the health of the trees, e.g. by lowering the effectiveness of roots in nutrient uptake as a whole and is thus disturbing the natural reaction patterns. This example should explain the power of KED for causal interpretation besides its high performance in prediction.

Acknowledgements

The research was partially supported by the BMBF-research project number 0339985.

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