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Mapping trace element deficiency by cokriging from regional geochemical soil data: A case study on cobalt for grazing sheep in Ireland

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ABSTRACT

Deficiency or excess of certain trace elements in the soil causes problems for agriculture, including disorders of grazing ruminants. Geostatistics has been used to map the probability that trace element concentrations in soil exceed or fall below particular thresholds. However, deficiency or toxicity problems may depend on interactions between elements in the soil. Here we show how cokriging from a regional survey of topsoil geochemistry can be used to map the risk of deficiency, and the best management intervention, where both depend on the interaction between two elements. Our case study is on cobalt. Farmers and their advisors in Ireland use index values for the concentration of total soil cobalt and manganese to identify where grazing sheep are at risk of cobalt deficiency. We use topsoil data from a regional geochemical survey across six counties of Ireland to form local cokriging predictions of cobalt and manganese concentrations with an attendant distribution which reflects the joint uncertainty of these predictions. From this distribution we then compute conditional probabilities for different combinations of cobalt and manganese index values, and so for the corresponding inferred risk to sheep of cobalt deficiency and the appropriateness of different management interventions. We represent these results as maps, using a verbal scale for the communication of uncertain information. This scale is based on one used by the Intergovernmental Panel on Climate Change, modified in light of some recent research on its effectiveness.

1. Introduction

Geochemistry is an important factor in many problems of soil management. The availability of particular trace elements in the soil to crops and grazing livestock can cause problems of either deficiency or toxicity. In this paper we consider the example of cobalt (Co) deficiency for sheep and other ruminants on pastures where the Co status of the grass may be inadequate because of soil geochemical factors. Ruminants depend on rumen bacteria to synthesise their supply of vitamin B_{12}, and these bacteria require a source of Co. Cobalt deficiency can therefore induce a deficiency of vitamin B_{12} which in turn causes various metabolic disorders (Stangl et al., 2000) which lead to conditions such as poor thrift and 'pine' in sheep (Coulter and Lalor, 2008). Small concentrations of blood vitamin B_{12} have been found among Irish cattle herds (Mee and Rogers, 1996), affecting 55% of herds sampled in 1993.

At farm-scale a decision on possible interventions to manage trace element deficiency or excess may be based on local soil information obtained by sampling the soil. However, at regional scale it would be possible to identify broader areas where there is a risk of a problem and where particular interventions are indicated. This information could be used both to identify regions where problems can be expected and to show where farmers would be advised to undertake local soil sampling to diagnose whether their particular soils require intervention. Such information is provided by systematic regional soil geochemical databases, which are available in many countries. In six counties of Ireland shown in Fig. 1 (Donegal, Sligo, Leitrim, Cavan, Monaghan and Louth) geochemical data on the topsoil are available from the recently-completed Tellus Border survey (Knights, 2013; Knights and Scanlon, 2013). Within the six counties of the Tellus Border survey are found 27% of all sheep farms and 22% of all sheep in Ireland, so the Co supply from the soil in this region is of considerable economic importance — data from Central Statistics Office (2012).

The mapping of trace element concentrations from topsoil geochemical data must take account of the considerable spatial variability which may be expected as a result of the multiple factors, operating at different spatial scales, which influence the concentration of trace elements in the soil. Because of this spatial variability, local predictions are subject to uncertainty. This can best be quantified through a geostatistical analysis in which the spatial variability of variables of interest is modelled explicitly and the local predictions are formed as an optimal combination of neighbouring observations which minimises and explicitly quantifies the mean squared error of the prediction (Webster and Oliver, 2007).

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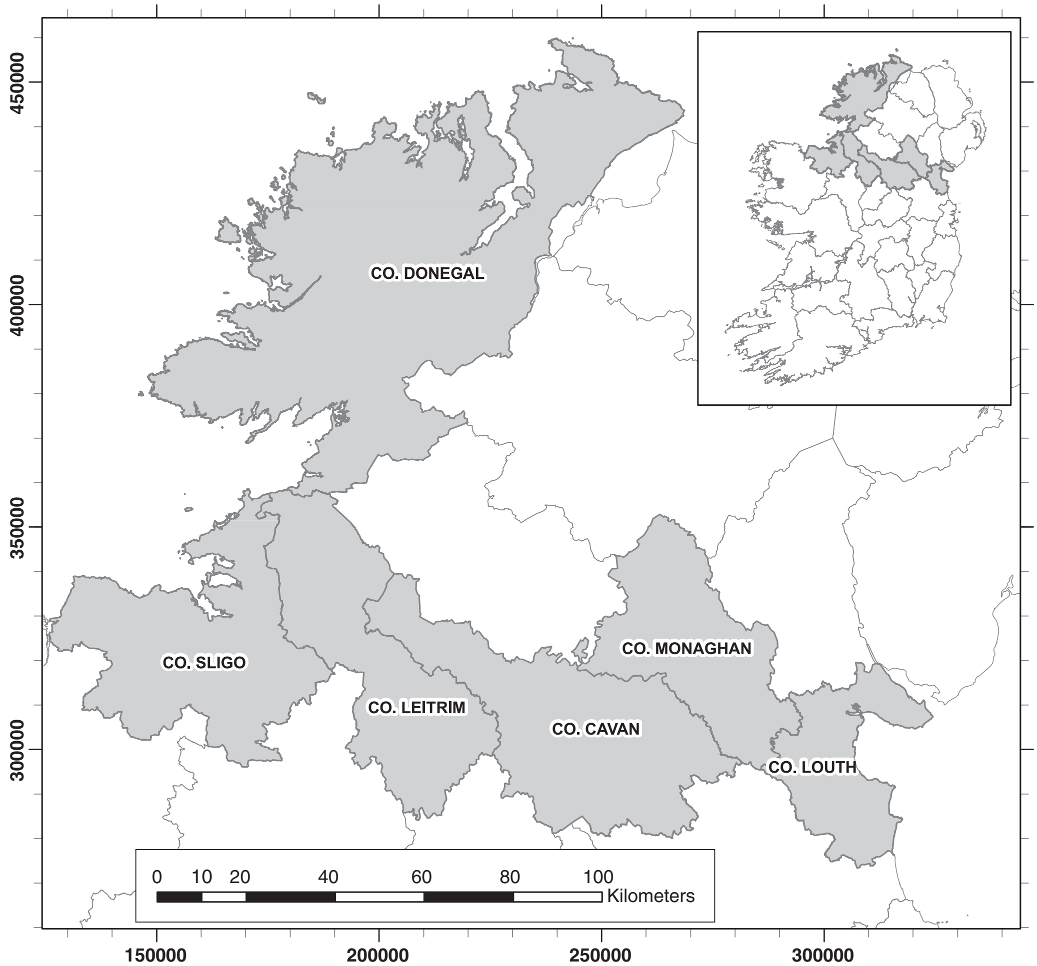

Fig. 1. Boundaries of the six Irish counties included in the Tellus Border survey. The inset map shows the whole of Ireland. Ordnance Survey Ireland Licence No. EN 0047213 ©Ordnance Survey Ireland/Government of Ireland. Units on the axes are metres relative to the origin of the Irish National Grid.

Geostatistical mapping by spatial prediction from regional data on soil geochemistry has been used to delineate areas at risk of trace element excess or deficiency (e.g. Van Meirvenne and Goovaerts, 2001; von Steiger et al., 1996; Webster and Oliver, 1989; Yang et al., 2008). What these studies have in common is that a toxicity or deficiency is inferred by comparing the predicted concentration of an element with a threshold value for that element. In practice, however, toxicity or deficiency of an element in soil depends not only on the absolute concentration of that element, but also on interactions with other elements and maybe on other factors of soil chemistry such as the pH or redox potential (Kabata-Pendias, 2001). Cobalt deficiency for grazing ruminants is a case in point.

It has long been recognised that Co deficiency in grazing ruminants can be linked to geochemistry and the underlying geology (Thornton and Alloway, 1974). However, the relationship is complex, and deficiencies may be found in plants growing on soils where the parent material has large Co concentrations. In particular it is known that Co in soil may be strongly associated with manganese oxide minerals (Jarvis, 1984), and it has been shown that this can reduce availability to plants (Li et al., 2004). Predictive relationships for available Co therefore include

Table 1
Soil indices for total Co and Mn and corresponding management classes for pasture Co deficiency for grazing sheep under the Teagasc system.
Taken from Coulter and Lalor (2008).

Soil Co index	Total Co concentration upper limit, mg kg^{-1}	Total Mn concentration upper limit, mg kg^{-1}		
		600	1000	>1000
1	3	High risk Soil treatment[a]		
2	5	Low risk Soil treatment[b]	High risk Animal treatment[c]	
3	10	No risk	No risk	Low risk Animal treatment[c]
4	>10	No risk	No risk	No risk

[a] Apply Cobalt sulphate (21% Co) at 3 kg ha^{-1} to one quarter of the grassland area every 4 years (annually at high pH).
[b] Apply Cobalt sulphate (21% Co) at 2 kg ha^{-1} to one quarter of the grassland area every 4 years (annually at high pH).
[c] Treat animals directly by oral Co drench, Co bullet or vitamin B_{12} injection.

manganese (Mn) as a covariate (Suttle et al., 2003). In Ireland advice about Co from Teagasc, the state agriculture and food development authority, is based on a consideration of soil index values for both Co and Mn which are shown in Table 1 (taken from Coulter and Lalor, 2008). The risk of Co deficiency, given the total Co and Mn concentrations in the soil, and appropriate interventions (fertiliser applications to the soil at different rates, or direct administration of supplements to the livestock) are indicated for particular combinations of the two sets of index values.

Webster (1994) used geostatistical methods to map Co concentrations in soils of a part of south-east Scotland and to map the probability that the concentration fell below a particular threshold. However, as was seen above, the assessment of risk of Codeficiency cannot be based on the Co concentration alone. It is necessary to model the joint spatial variation of both Co and Mn in order to make appropriate geostatistical predictions of the risk of Co deficiency. In this paper we undertake cokriging of transformed Co and Mn concentrations, and then sample from the joint prediction distribution for the two variables to derive local estimates of the probability that particular combinations of the Co and Mn index values occur. This allows us to compute quantities such as the probability that there is no risk of Co deficiency at a site, or that a particular intervention is indicated. We represent these results using a scale for the communication of uncertain information used by the International Panel for Climate Change (Mastrandrea et al., 2010).

2. Materials and methods

2.1. The Tellus Border data

The sampled region is shown in Fig. 1 and is a little over 13,000 km^2 in extent. Topsoil samples were collected from 3475 sites across the geochemical survey area, at a target density of 0.25 samples per km^2. The sampling procedure was systematic and purposive, in the sense of de Gruijter et al. (2006). One sample site was selected from each 2×2-km grid square on the Irish National Grid. A sample site was chosen as close as possible to the centre of the square, and no closer than 250 m to any edge of the square. Sample sites were no closer than 100 m to features such as roads, tracks, pylons, buildings and water bodies shown on the Ordnance Survey Ireland map sheets at 1:50,000. Forested land was avoided, and field sampling teams avoided disturbed ground such as tips or spoil heaps, although ploughed land was sampled.

The soil sampling protocol at each site entailed collection of a composite sample from five auger holes, collected at the corners and centre of a 20×20-m square on the ground. Each core was 15 cm long, collected after removal of surface litter. An Edelman (Dutch-type) one-piece combination auger with a 5-cm diameter flight was used. A wide range of land use types were sampled, principally agricultural pasture and tillage, and rough grazing and moorlands (particularly on upland areas) which is sometimes commonage. At 81 of the sample sites a duplicate sample was collected by the same protocol 20 m from the initial sample site.

Samples were collected in paper bags and dried prior to sample preparation. Samples for multi-element analyses were dried and disaggregated by hand, and then sieved to pass through 2 mm using Sefar® Nitex® nylon sieve mesh of 2 mm aperture. The sub-2 mm fraction was milled using an agate planetary ball mill to produce a sample of predominantly <53 m fraction. A 1-g sub-sample of the milled material was treated by two-acid (ratio of 2:1 HNO_3:HCl *aqua regia* variant) sample digestion, and the digestate was analysed for concentrations of a range of major, minor and trace elements by multi-element ICP (-OES/-MS) analysis (Knights, 2013). The laboratory reports detection limits for the elements computed as three times the standard deviation of results from quality control blanks. For Co and Mn these were 0.1 mg kg^{-1} and 2 mg kg^{-1} respectively. None of the data on Co were smaller than the detection limit and just 2 of the data for Mn (Knights, 2013).

2.2. Soil indices and management decisions

Table 1 represents the Co and Mn indices used by Teagasc for advisory purposes with respect to managing risk of Co deficiency in sheep (Coulter and Lalor, 2008). The threshold concentrations of the elements which define the indices are total concentrations from *aqua regia* variant extraction of the soil. We therefore assumed that the Tellus Border soil data on Co and Mn concentrations could be used directly to identify the Co and Mn indices in this table. The table reflects the interaction of the total Co and Mn concentrations in controlling the Co available to grazing sheep. Thus, for example, the risk of deficiency on a Co index 2 soil is low if the Mn concentration is less than 600 mg kg^{-1}, but high when the Mn concentration is larger, because of the tendency for Mn oxides to reduce Co availability. The risk of Co deficiency in grazing sheep is never high when the Co index is 3 or 4, regardless of the Mn concentration, because of the amount of soil Co that sheep obtain directly through soil ingestion. Coulter and Lalor (2008) report that ingested soil may account for up to 25% of the stomach-contents of sheep.

We note that, in Table 1, Co index 1 soils with Mn concentrations larger than 600 mg kg^{-1} are not given an interpretation, and neither are Co index 2 soils with Mn concentrations more than 1000 mg kg^{-1}. Because Co and Mn concentrations are positively correlated, these combinations are very rare, only 16 (i.e. c. 0.5%) of the Tellus Border observations fall into these three categories. For the assessment of uncertainty we assumed that in all cases the risk of Co deficiency would be high, because the concentration of Co is less than 5 mg kg^{-1}, and that animal treatment would be indicated in these conditions.

2.3. Exploratory data analysis

Because the exploratory data analysis affects decisions on the statistical treatment of data, some results are reported in this section. Fig. 2 shows histograms of the log-transformed data on Co and Mn concentrations for the whole Tellus Border region and Fig. 3 shows the spatial distribution of the untransformed values of Co and Mn concentrations as a classified post-plot in which the classes are percentiles (quintiles) of the data values. The post-plots suggested marked variations, particularly in topsoil Co, between two broad geological subregions. The first, designated A, comprises soils formed over either Lower Palaeozoic (Ordovician–Silurian) sedimentary strata or glacial tills derived predominantly from these rocks. Subregion B consists of all other parent materials in the Tellus Border region. The subregions were defined from two sources: first, the all-Ireland 1:1,000,000-scale bedrock geology map (Geological Survey of Ireland, 2014) and second, the Teagasc subsoil geological parent material maps (mapped superficial deposits) — Fealy et al. (2009), Teagasc (2006). Concentrations of both Co and Mn are larger in subregion A than in subregion B, and the variability is smaller in subregion A. The spatial distribution of the subregions is shown in Fig. 4.

Table 2 presents summary statistics for both elements in both subregions, including the octile skewness which is a robust measure of the asymmetry of the distribution of data (Brys et al., 2003). In all cases a Box–Cox transformation of the data was considered. This takes the form

$$\begin{aligned} z &= \frac{y^{\zeta}-1}{\zeta} \quad \zeta \neq 0, \\ &= \ln(y) \quad \zeta = 0, \end{aligned} \tag{1}$$

where y is a value on the original scale and z is a transformed value. We used the Box–Cox procedure from the MASS package (Venables and Ripley, 2002) for the R platform (R Core Team, 2013) to find the likelihood profile of the ζ parameter and selected the value with maximum likelihood. In subregion A the transformation gave rise to data with symmetrical distributions (Fig. 5, Table 2) with conventional coefficient of skewness less than 1 and octile skewness less than 0.2 (Lark et al., 2006), possibly with some outliers in the upper tail of the distribution

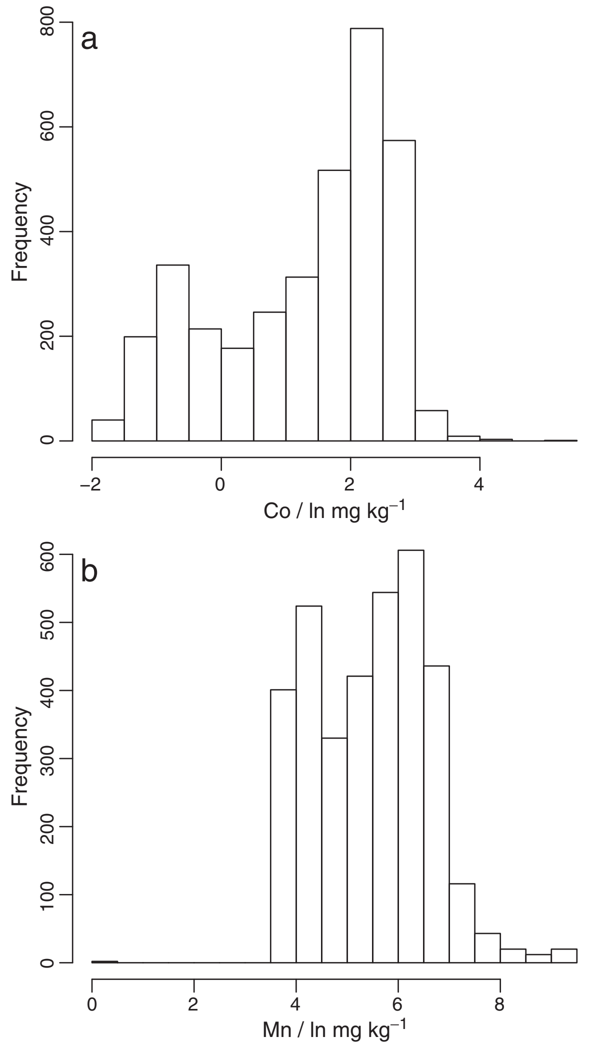

Fig. 2. Histogram of log-transformed data from across Tellus Border region: (a) Co, (b) Mn.

for Co. However, in subregion B the data on Co had a negative octile skew after the Box–Cox transformation. For this reason a normal-scores transformation was computed for both variables in subregion B. Under this transformation, widely used in geostatistics (e.g. Goovaerts, 1997; Journel and Huijbregts, 1978), a datum which corresponds to the p_k th quantile of the empirical distribution of the data is replaced with the same quantile of a standard normal distribution. Histograms of the transformed data for subregion A are shown in Fig. 5. Histograms of the normal-scores transformed data for subregion B are not shown since these necessarily correspond to a standard normal distribution.

Because of the clear differences between the subregions with respect to the summary statistics and the transformations it was decided to undertake geostatistical modelling and prediction within the subregions separately.

2.4. Cokriging and uncertainty

The next step in the analysis of the data was geostatistical prediction from the observations to a regular grid of target sites. This was done by ordinary cokriging — see, for example, Webster and Oliver (2007) — using a robustly estimated and validated linear model for the coregionalisation of the transformed data on Co and Mn concentrations.

2.4.1. The linear model of coregionalisation

The cokriging prediction of a variable is the best linear unbiased prediction conditional on neighbouring observations of the variable and of the coregionalised variable(s). The cokriging method is based on auto-variogram functions, which describe the spatial variability of the variables of interest, and the cross-variogram which describes their joint spatial variation. It is assumed that the observed values of two variables at location $\mathbf{x}$, $z_u(\mathbf{x})$ and $z_v(\mathbf{x})$, are realisations of intrinsically stationary random functions, $Z_u(\mathbf{x})$ and $Z_v(\mathbf{x})$ (Webster and Oliver, 2007), so the auto-variogram can be defined as:

$$\gamma_{u,u}(\mathbf{h}) = \frac{1}{2}\mathrm{E}\left[\{Z_u(\mathbf{x}) - Z_u(\mathbf{x}+\mathbf{h})\}^2\right] \tag{2}$$

where E[·] denotes the statistical expectation of the term in brackets and $\mathbf{h}$ is a lag vector which defines a separation in space between two observations. In this case there was no evidence for anisotropy in the observations (directional dependence of the variograms), and so all estimation and modelling were done with respect to the lag distance $h = |\mathbf{h}|$. The cross-variogram is similarly defined as

$$\gamma_{u,v}(\mathbf{h}) = \frac{1}{2}\mathrm{E}[\{Z_u(\mathbf{x}) - Z_u(\mathbf{x}+\mathbf{h})\}\{Z_v(\mathbf{x}) - Z_v(\mathbf{x}+\mathbf{h})\}]. \tag{3}$$

Variograms must be estimated from the data, $z_u(\mathbf{x}_j)$,$z_v(\mathbf{x}_j)j = 1,2,\ldots,n$ for discrete lags. The standard estimator is based on the method-of-moments estimator (Webster and Oliver, 2007), which for the cross-variogram is

$$\hat{\gamma}_{u,v}(\mathbf{h}) = \frac{1}{2N(\mathbf{h})}\sum_{i=1}^{N(\mathbf{h})}\{z_u(\mathbf{x}_i) - z_u(\mathbf{x}_i+\mathbf{h})\}\{z_v(\mathbf{x}_i) - z_v(\mathbf{x}_i+\mathbf{h})\}. \tag{4}$$

However, it is known that the method-of-moments estimator is susceptible to the effects of outlying observations in the data (e.g. Cressie and Hawkins, 1980; Lark, 2003); which may be marginal outliers, apparent in the histogram, or observations that are unusual in the context of their neighbours in space. Outliers can inflate estimates of the variograms, which will affect the measures of uncertainty attached to the cokriging predictions. For this reason we used both the method of moments estimator in Eq. (4) and a robust estimator, $\hat{\gamma}^{\mathrm{M}}_{u,v}(\mathbf{h})$, developed by Lark (2003). The robust estimator reduces the effect of outlying observations on the auto- and cross-variogram estimates. Each set of estimates was then fitted with a linear model of coregionalisation (LMCR) (Journel and Huijbregts, 1978) which is a model which allows the calculation of values of the auto- or cross-variogram for any particular lag interval. The LMCR is commonly recommended for modelling the auto- and cross-variograms (Webster and Oliver, 2007) because it ensures that all modelled linear combinations of the observations have non-negative variances. The LMCR was fitted to each of the sets of estimates by weighted least squares using the optimisation procedure of Lark and Papritz (2003).

It was then necessary to chose between the LMCR fitted to the method-of-moments estimates of the auto- and cross-variograms and the LMCR fitted to the robust estimates. To do this we followed Lark et al. (2012) and cross-validated the models by ordinary kriging of the values of the two transformed variables using the auto-variograms from the each fitted LMCR. For each observation the cross-validation procedure returns a prediction and a kriging variance of the prediction derived from all the remaining observations. The standardised squared prediction error can then be computed, for variable z_u at location x as

$$\theta_u(\mathbf{x}) = \frac{\{z_u(\mathbf{x}) - \widetilde{Z}_u(\mathbf{x})\}^2}{\sigma^2_{\mathrm{K},u}(\mathbf{x})}, \tag{5}$$

where $\widetilde{Z}_u(x)$ is the kriging prediction of $z_u(x)$ and $\sigma^2_{\mathrm{K},u}(x)$ is the kriging variance. With normal kriging errors and valid kriging variances θ_u is

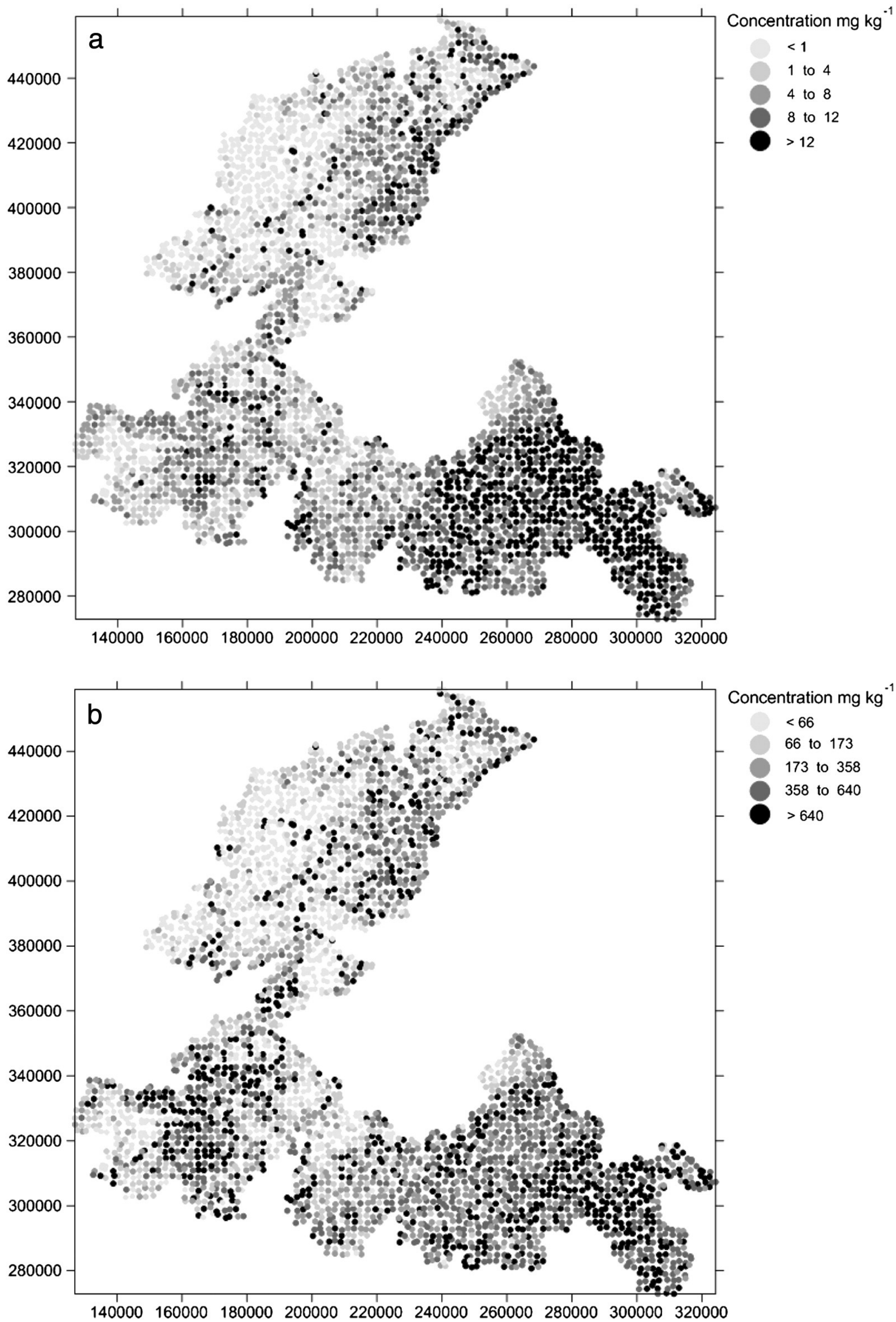

Fig. 3. Classified post-plot of the original data on (a) Co and (b) Mn topsoil concentration. The categories are quintiles (20th percentiles) of the data values.

expected to have a χ^2 distribution with 1 degree of freedom. In the presence of outliers the mean value of θ_u over the observations is not a good indicator of the validity of the kriging variances because the outliers may tend to inflate both the (non-robust) variogram estimates and the kriging errors. For this reason Lark (2000) recommended that the median of θ_u over all observations is used as a diagnostic, the expected value of this variable for the χ_1^2 variable is 0.455. This is now used as a diagnostic in robust spatial statistics (e.g. Lu et al., 2012; Pringle, 2013; Zimmermann et al., 2013).

2.4.2. Cokriging prediction

Once a LMCR for transformed Co and Mn was selected it was then used to predict these variables at locations on a 500-m interval grid across the Tellus Border region. The ordinary cokriging prediction of variable Z_u at location $\mathbf{x}_0$ is given by

$$\widetilde{Z}_u(\mathbf{x}_0) = \sum_{i=1}^{N} \lambda_{u,i}^{u} z_u(\mathbf{x}_i) + \sum_{i=1}^{N} \lambda_{v,i}^{u} z_v(\mathbf{x}_i), \quad (6)$$

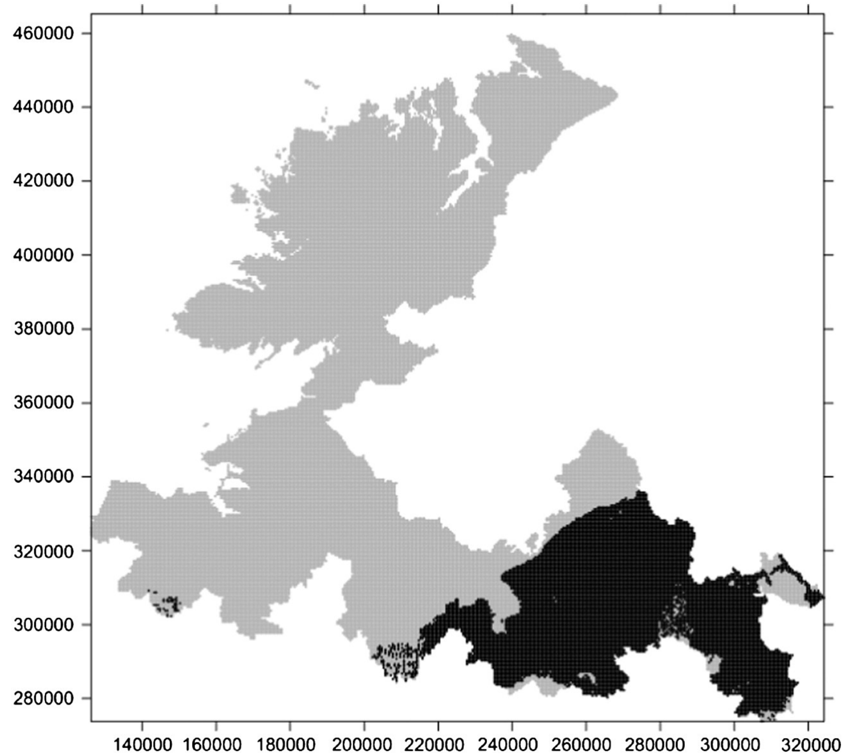

Fig. 4. Parent material sub-regions of the Tellus Border region. Subregion A (black) is Lower Palaeozoic (Ordovician–Silurian) sedimentary strata or tills derived predominantly from these rocks. Subregion B (grey) comprises all other parent materials.

where the values of $\lambda^u_{u,i}$ and $\lambda^u_{v,i}$ are ordinary cokriging weights. The superscript, u, in each case indicates that the weight is for the prediction of Z_u, and the subscript u or v indicates whether the weight is applied to observed values of the transformed Co and Mn concentrations respectively at the ith neighbouring location. A cokriging predictor of Z_v is defined similarly. Given a set of values of the cokriging weights and the LMCR one may define $\mathbf{C}(\mathbf{x}_0)$ — a 2×2 covariance matrix of the cokriging errors of $Z_u(\mathbf{x}_0)$ and $Z_v(\mathbf{x}_0)$ such that $\mathbf{C}(\mathbf{x}_0)[1,1]$ is the expected squared error of $\widetilde{Z}_u(\mathbf{x}_0)$, $\mathbf{C}(\mathbf{x}_0)[2,2]$ is the expected squared error of $\widetilde{Z}_v(\mathbf{x}_0)$ and $\mathbf{C}(\mathbf{x}_0)[1,2] = \mathbf{C}(\mathbf{x}_0)[2,1]$ is the expected product of the errors of $\widetilde{Z}_u(\mathbf{x}_0)$ and $\widetilde{Z}_v(\mathbf{x}_0)$ (Pawlowsky-Glahn and Olea, 2004). The weights $\lambda^u_{u,i}$ and $\lambda^u_{v,i}, i = 1,2,\ldots N$ are found which minimise the value of $\mathrm{C}(\mathrm{x}_0)[1,1]$ subject to the constraint that $\sum_{i=1}^{N} \lambda^u_{u,i} = 1$ and $\sum_{i=1}^{N} \lambda^u_{v,i} = 0$. The weights for the ordinary cokriging estimate of $Z_v(\mathbf{x}_0)$ are found in the same way.

In this study we undertook cokriging of transformed Co and Mn concentrations using the cokriging programme COKB3D from the GSLIB Fortran library (Deutsch and Journel, 1992).

Table 2
Summary statistics of the data on Co and Mn for subregions A and B before and after the Box–Cox transformation. The maximum-likelihood estimator of the parameter, ζ of the Box–Cox transformation is also reported, and the number of observations, n, in each subregion.

Statistic	Untransformed data		Transformed data	
	Co	Mn	Co	Mn
Subregion A				
Mean	12.3	551.4	7.97	9.06
Median	12.5	499.0	8.15	9.1
Standard deviation	4.1	299.1	2.51	1.08
Skewness	0.51	2.02	0.13	−0.08
Octile skewness	−0.1	0.20	−0.13	−0.05
ζ			0.79	0.12
n	815		815	
Subregion B				
Mean	5.1	434.2	1.12	3.35
Median	3.4	166.0	1.33	3.34
Standard deviation	6.6	931.4	1.45	0.43
Skewness	9.73	6.12	−0.06	−0.04
Octile skewness	0.41	0.69	−0.21	0.03
ζ			0.13	−0.18
n	2660		2660	

2.4.3. Uncertainty

It is assumed that the co-kriging predictions of variables Z_u and Z_v at location $\mathbf{x}_0$ are jointly normally distributed with mean equal to the unknown true values, $z_u(\mathbf{x}_0)$ and $z_v(\mathbf{x}_0)$ and covariance matrix $\mathrm{C}(\mathbf{x}_0)$ as defined above. Given this, it is possible to draw a sample from this distribution by computing

$$\boldsymbol{\eta} = \mathbf{L}\varepsilon, \tag{7}$$

where $\boldsymbol{\eta}$ is a vector containing the samples of the variables $Z_u(\mathbf{x}_0)$ and $Z_v(\mathbf{x}_0)$, ϵ is a vector containing two independent values drawn from a standard normal random variable and $\mathbf{L}$ is the upper-triangular factor of $\mathbf{C}(\mathbf{x}_0)$ in its Cholesky decomposition

$$\mathbf{C}(\mathbf{x}_0) = \mathbf{L}\mathbf{L}^{\mathrm{T}}, \tag{8}$$

(where superscript T denotes the matrix transpose) which can be computed because $\mathbf{C}(\mathbf{x}_0)$ is positive definite if both variables have positive variances. The simulated values in $\boldsymbol{\eta}$ can be back-transformed to the original scales of measurement.

In this study our objective is to produce a map of the interventions indicated for the management of the risk of cobalt deficiency for grazing sheep. At some unsampled location, $\mathbf{x}_0$ the soil concentrations of Co and Mn are unknown, but from the cokriging and simulation procedures described above one may draw a sample from the joint distribution of the transformed values of these variables. For any sample it is then possible to identify the corresponding cell in Table 1 by comparing the sample values with the transformed values of the thresholds for the Co and

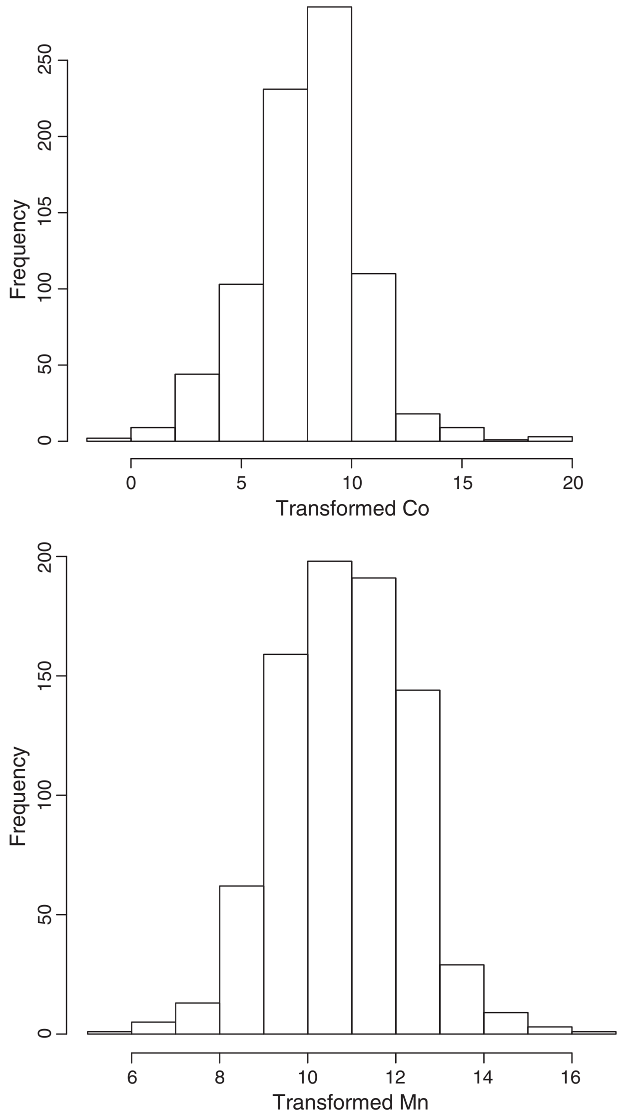

Fig. 5. Histogram of Box–Cox-transformed data from subregion A: (a) Co, (b) Mn.

Mn indices. These thresholds can be found for Box–Cox transformed values by direct application of Eq. (1), and for the normal-scores transformed variables by linear interpolation between observations in the original dataset. By repeated sampling from the joint distribution at x_0 one may estimate the conditional probability that any particular combination of Co and Mn indices from Table 1 occurs at that location, by the proportion of the sample for which the random values correspond to that combination. This provides an estimate of the conditional probability that the particular corresponding management intervention would be indicated at x_0 if the true Co and Mn concentrations were known.

This procedure was followed for locations on the 500-m grid for which cokriging predictions had been derived. At each location the Cholesky decomposition of the covariance matrix was obtained with the CHFAC subroutine in the IMSL library (Visual Numerics, 2006). Five thousand realisations of the random variate η were then generated with the RNMVN subroutine from the IMSL library, and from these a probability estimate was assigned to each management scenario for Co deficiency in Table 1: no risk; low risk, soil treatment at 2 kg ha^{-1} indicated; low risk, animal treatment indicated; high risk, soil treatment at 3 kg ha^{-1} indicated; high risk, animal treatment indicated. In addition, each simulated value was back-transformed to the original scale of measurement (by algebraic inversion of the Box–Cox transform in the case of subregion A, and by inversion of the original normal-scores transform using linear interpolation in the case of subregion B). The mean of all realisations of the back-transformed values was treated as an approximation to the conditional expectation of the concentration of the element at the grid node. This could be mapped as an expectation-type prediction of the concentration.

2.4.4. Representing uncertain information

From the output of the procedures described above one can map directly the probabilities of particular management scenarios. These probabilities will indicate where particular interventions are likely to be required by the land manager, and also where further soil sampling is required in order to resolve uncertainty about local conditions and make a more robust decision. This information can be used by individual land managers to decide whether to undertake an intervention, or to sample the soil on their farm for analysis. It can also be used strategically or commercially, e.g. by regional advisors to decide where producers should be encouraged to consider interventions or local, targeted, soil sampling.

The raw probability maps are not necessarily useful for non-specialists, it is well-known that numerical probabilities are often misunderstood by a target audience (Galesic and Garcia-Retamero, 2010; Spiegelhalter et al., 2011). For this reason the Intergovernmental Panel on Climate Change (Mastrandrea et al., 2010) uses a standard verbal scale for the attachment of probabilistic information to uncertain outcomes. If the probability of an outcome is P_o and $P_o \geq 0.66$ then the outcome is described as 'Likely'. This may be intensified to 'Very likely' if $P_o \geq 0.9$ and to 'Virtually certain' if $P_o \geq 0.99$. If $0.33 \leq P_o < 0.66$ then the outcome is described as 'About as likely as not'. If $P_o < 0.33$ then the outcome is described as 'Unlikely'. This may be intensified to 'Very unlikely' if $P_o < 0.1$ and to 'Exceptionally unlikely' if $P_o < 0.01$.

The IPCC verbal scale for communicating uncertainty about unknown outcomes has been evaluated in empirical studies and criticised as a result. Harris and Corner (2011) showed that the interpretation of a verbal uncertainty for some outcome could be biased by the severity of that outcome. Considerable variability has been found among individuals in their interpretation of the verbal scale and a tendency to over-estimate the uncertainty attached to a prediction (Budescu et al., 2009). Budescu et al. (2009) recommend that some numerical information is conveyed along with the verbal scale. They also propose that any ambiguity in the interpretation of quantitative statements about an outcome (e.g. what is a 'large' event?) should be distinguished from the uncertainty attached to whether that outcome occurs or not. It is also important to specify, as far as possible, the sources of uncertainty in statements about outcomes.

Given these results, we report the geostatistical predictions as follows. First, we use the basic IPCC scale with intensifiers, but we also indicate the corresponding probabilities (as percentages) as recommended by Budescu et al. (2009). Second, we make it clear that the source of uncertainty in these predictions is the spatial variability of soil Co and Mn. The outcome under consideration is therefore that a particular soil management scenario would be indicated if the soil properties were known without error, possible uncertainty about the implications of particular soil conditions for the Co status of grazing livestock is excluded. Third, we frame the management outcomes without the use of quantifiers which are potentially ambiguous (Budescu et al., 2009) or which may introduce severity bias (Harris and Corner, 2011). Specifically we did not refer to the 'low' or 'high' risk of a cobalt deficiency indicated for particular combinations of Co and Mn indices in Table 1. Rather we consider the following possible outcomes:

1. 'Soil Co and Mn indicate a risk of Co deficiency' (the Co and Mn index correspond to any cell in Table 1 not designated 'None').
2. 'Soil Co and Mn indicate that soil treatment at 3 kg ha^{-1} Cobalt sulphate is required.'
3. 'Soil Co and Mn indicate that soil treatment at 2 kg ha^{-1} Cobalt sulphate is required.'
4. 'Soil Co and Mn indicate that animal treatment is required to avoid Co deficiency.'

3. Results

The estimated variograms and fitted LMCRs for the two regions, and robust and method-of-moments estimators, are shown in Fig. 6. In most cases, and always at the shorter lag distances, the robust estimator produces smaller estimates than does the method of moments. The mean and median standardised squared prediction errors from cross-validation by ordinary kriging of each element are reported in Table 3a. The median values are closest to 0.455 for the model fitted to the robust estimator, except for Mn in subregion A. The mean values are somewhat larger than 1.0 for the robust estimator, which is expected because of inflation of the numerator of Eq. (5) by outlying observations. For this reason the models fitted to the robust estimator were used in further analyses. The summary statistics of the cross-validation errors in Table 3b, and their histograms (Fig. 7) suggest that these errors may reasonably be treated as normal variables, with some outlying values. Note that the histograms in Fig. 7 have the probability density functions with robust parameters (median and absolute median deviation from the median) overprinted.

Fig. 8 shows the conditional expectations of topsoil Co and Mn concentrations across the Tellus Border region. Note the large concentrations of both elements within subregion A, predominantly Co. Louth,

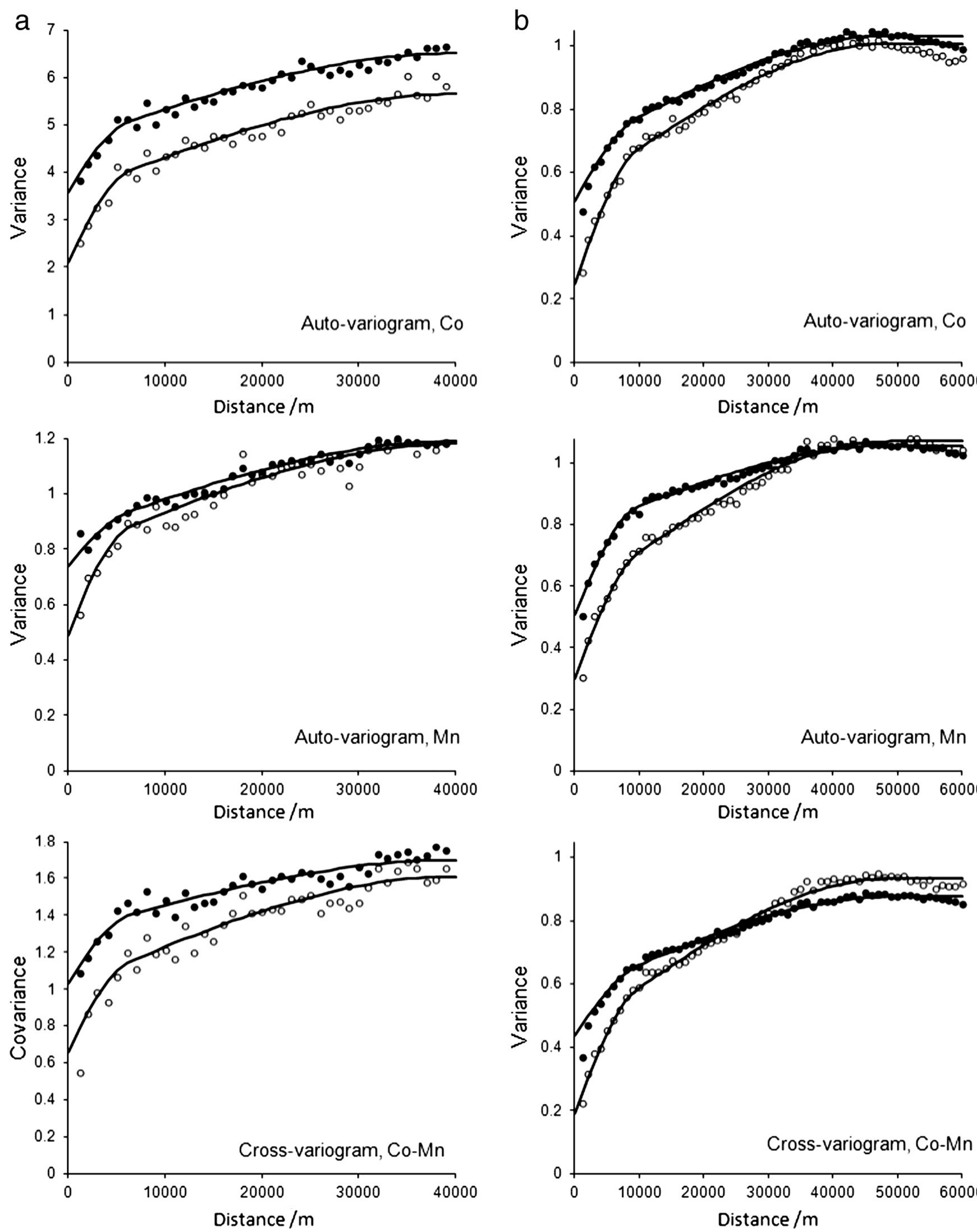

Fig. 6. Auto- and cross-variograms of transformed Co and Mn concentrations by method of moments estimator (solid disc, ●) or the robust estimator (open circle, ○) for (a) region A and (b) region B. Solid lines show the fitted LMCR.

Table 3a
Statistics on θ, standardised squared prediction error, from cross-validation of the models fitted to the method of moments and robust variogram estimates for transformed concentrations of Co and Mn.

Estimator	Subregion A				Subregion B			
	Method of moments		Robust		Method of moments		Robust	
	Co	Mn	Co	Mn	Co	Mn	Co	Mn
Mean θ	0.98	1.02	1.45	1.30	0.95	0.98	1.56	1.46
Median θ	0.33	0.44	0.50	0.53	0.32	0.31	0.53	0.48

Co. Monaghan and eastern Co. Leitrim. Larger concentrations of Mn are also found in eastern parts of Co. Sligo and north and west Co. Leitrim. The smallest concentrations of Co are found in Co. Donegal, particularly in the west, and over much of the west of Co. Sligo.

The management classes designated by Teagasc and shown in Table 1 are mapped in Fig. 9(a) where the most probable class is delineated. Note that class 'No risk' and 'High risk, soil treatment 1' are the classes of maximum probability over almost all the region, class 'Low risk, soil treatment 2' is indicated at fewer than 0.1% of the nodes of the kriging grid, a small cluster in the south of Co. Sligo. Fig. 9(b) indicates the uncertainty attendant on these indicated classes, the probability of the class of maximum probability is indicated. The class of maximum probability may have a large probability (e.g. in most of subregion A, and in much of the west of Co. Donegal), but it can be as small as 0.28, particularly in zones of transition between geochemically contrasting areas. This shows that, while over much of the western Tellus Border area it is most likely that the risk of Co deficiency is high, as indicated by the soil, there can be significant uncertainty due to the spatial variability of the geochemistry of the soil. This variability is predominantly caused by variation in the Mn concentrations (Fig. 2). As noted above class 'Low risk, soil treatment 2' is the most probable class in a small area of Co. Sligo, but Fig. 9(b) shows that the probability that this class is indicated there is still small, if larger than for any other class.

Given this, we now turn to maps produced specifically to convey the uncertainty about the risk of Co deficiency, and the indicated intervention, given topsoil Co and Mn concentrations at unsampled sites. Note that we consider here only the uncertainty due to the fact that Co and Mn concentrations are spatially variable, and have been interpolated to the nodes of the 500-m grid, which are not directly sampled. We do not attempt to account for any uncertainty about how grazing livestock can respond to local soil conditions. Fig. 10 shows the map of probability that topsoil Co and Mn concentrations indicate a risk of Co deficiency. The red colours indicate that this is 'likely' on the IPCC scale, with the intensifiers distinguished by variations of hue. Similarly blue colours indicate where the risk of deficiency is unlikely, and grey where it is 'about as likely as not'. The actual probabilities are also indicated (as percentages) on the colour scale, in accordance with the recommendations of Budescu et al. (2009). Fig. 11 uses the same scale to display the probability that the intervention indicated by local soil conditions is soil treatment 1 (application of Co fertiliser at 3 kg ha^{-1}), and Figs. 12 and 13 show the probabilities for soil treatment 2 and animal treatment. Animal treatment is as likely as not to be indicated in a small area in south-west Donegal where Mn concentrations are locally large, but otherwise is unlikely to be indicated. Note that animal treatment may be a suitable intervention anywhere where Co is deficient. When we say here that animal treatment is indicated we mean that animal treatment rather than a soil treatment is necessary because of the combination of Co and Mn indices (Coulter and Lalor, 2008). Animal treatment may be more appropriate than soil treatment over areas of commonage where producers do not have ownership or tenancy of the land. Commonage accounts for 17% of land in Co. Donegal, but rather less (0–3%) in other counties of the Tellus Border region (Central Statistics Office, 2012).

Table 3b
Summary statistics of cross-validation kriging errors (kriging with the models fitted to robust estimates).

Statistic	Subregion A		Subregion B	
	Co	Mn	Co	Mn
Mean	0.005	0.000	0.000	0.000
Median	−0.007	−0.017	0.057	0.036
St Dev	2.115	0.956	0.770	0.796
Skewness	−0.621	0.091	−0.587	−0.422
Octile skew	0.026	0.072	−0.105	−0.038

4. Discussion

These results show how data from a regional geochemical survey, through an appropriate multivariate geostatistical analysis, can be used to map variations in the concentrations of topsoil Co and Mn against recognised thresholds, and so the susceptibility of grazing sheep to Co deficiency. At any unsampled location there is uncertainty about the true concentration of Co and Mn, and so the management intervention. This is due to the spatial variability of these properties. This uncertainty can be represented by mapping the probability that pasture soils have Co and Mn concentrations expected to lead to deficiency, and mapping separately the probabilities that particular interventions would be deemed appropriate, given the soil information.

As noted above, we have considered uncertainty due to soil variability, given the Teagasc index values. Further work is necessary to address the uncertainty in these diagnostic concentrations, given the environmental factors that affect trace element concentration in forage and resulting availability to the rumen microflora and the variability of animal responses. It is known that response to animal treatment on pastures where the soil has small Co concentrations may be variable, and it is possible that this reflects differences in the rumen fermentation (Gruner et al., 2004). One possible area for future research is to combine regional geochemical data with comparable data on flock blood vitamin B_{12} concentrations both to refine the diagnostic values and to quantify their uncertainty. Such a study would need to account for the difference in sample support between the soil and physiological data. Another approach would be to elicit opinions from experienced veterinarians and other consultants on the probability of the occurrence of vitamin B_{12} deficiency over a range of soil conditions, management systems and breeds.

The information presented in this study could be used for various purposes. At a regional scale it can be used for an overall assessment (e.g. by county) of the importance of Co deficiency for farmers, particularly where sheep and cattle production are economically important. This could be used to target extension work, or to help the veterinarian in the interpretation of diagnostic results from particular flocks so as to decide whether Co deficiency is the most likely explanation of problems.

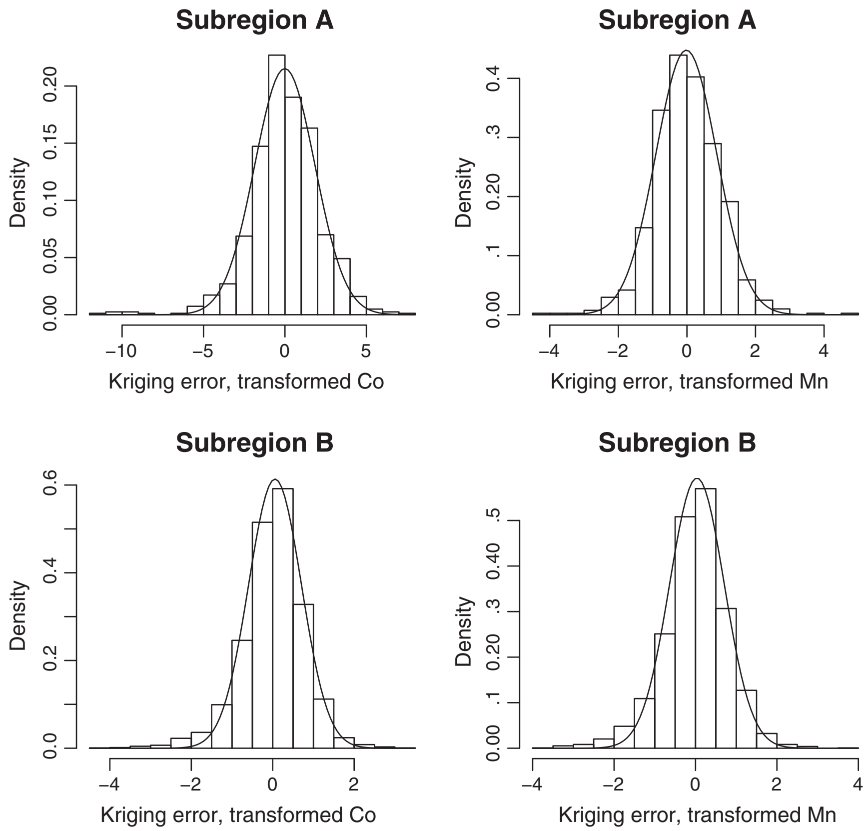

Fig. 7. Histograms of cross-validation errors (kriging with the models fitted to robust estimates). The continuous curves are normal probability densities, with robustly estimated parameters.

Locally the information could also be used for decision making. For example, in a location where it is judged 'exceptionally unlikely' that Co is deficient then the costs of local soil sampling, let alone any intervention, are unlikely to be justified. Similarly, if it is 'virtually certain' that Co is deficient then it may be decided to take an appropriate intervention without costly local soil investigation. Where there is greater uncertainty — for example, where it is only 'likely' that there is a deficiency, or 'as likely as not', then local soil sampling should be undertaken to support a decision on a particular farm.

The joint probability distribution for Co and Mn concentrations could be used in a formal decision analysis to compute the expected loss to a farmer of alternative decisions, and the benefits of additional soil sampling to reduce local uncertainty. This would require further information about the costs of alternative interventions, and the costs to farmers of lost production which could be attributable to Co deficiency. Let $L_I(\mathbf{s})$ denote the net loss incurred by a producer as a result of following intervention I at a location where soil conditions are described by $\mathbf{s}$, a vector containing values of variables such as total concentrations of Co and Mn. The loss represents total costs to the producer of following the intervention given the actual soil conditions (variable costs of implementing the intervention and any disbenefits resulting from the intervention) over any benefits from following the intervention. The expected loss to the producer who follows intervention I at a location where the joint probability distribution for the Co and Mn concentrations is $f(\mathbf{s})$ would be given by

$$\overline{L}_I = \int L_I(\mathbf{s}) f(\mathbf{s}) \, \mathrm{d}\mathbf{s}, \tag{9}$$

where the integral is over both variables in $\mathbf{s}$. One may then select an intervention on the basis of, for example, minimum expected loss. The value of additional soil information obtained locally to reduce the uncertainty about local soil conditions could then be estimated by calculating the expected loss under a new distribution $f_n(\mathbf{s})$ conditional on the local information. As a first approximation, with the shortest lag distance in the empirical variograms at about 1000 m, the nugget (co) variances for Co and Mn would provide reasonable values from which to estimate the joint density function of the farm mean Co and Mn estimated by simple random sampling at specified intensity. On this basis one might compare the marginal costs of additional soil sampling effort and its marginal benefit in order to decide how much effort it is rational to deploy locally.

5. Conclusions

Measured topsoil Co and Mn concentrations show marked spatial variation in the region of the Tellus Border survey in Ireland. This was modelled geostatistically for two distinct geological domains, subregions A and B. The geostatistical models were used to generate cokriging predictions of topsoil Co and Mn and to compute conditional probabilities that the concentrations at unsampled sites indicated a risk of Co deficiency for grazing livestock, and that particular management interventions are appropriate. While over most of the Tellus Border region the most probable situation is either that there is no risk of Co deficiency, or that there is a high risk with soil treatment an appropriate intervention, the uncertainty about this designation is variable and may be large. It has been shown how the probabilities obtained from the geostatistical model can be represented visually on a verbal scale, accounting for recent research on the effective communication of uncertainty.

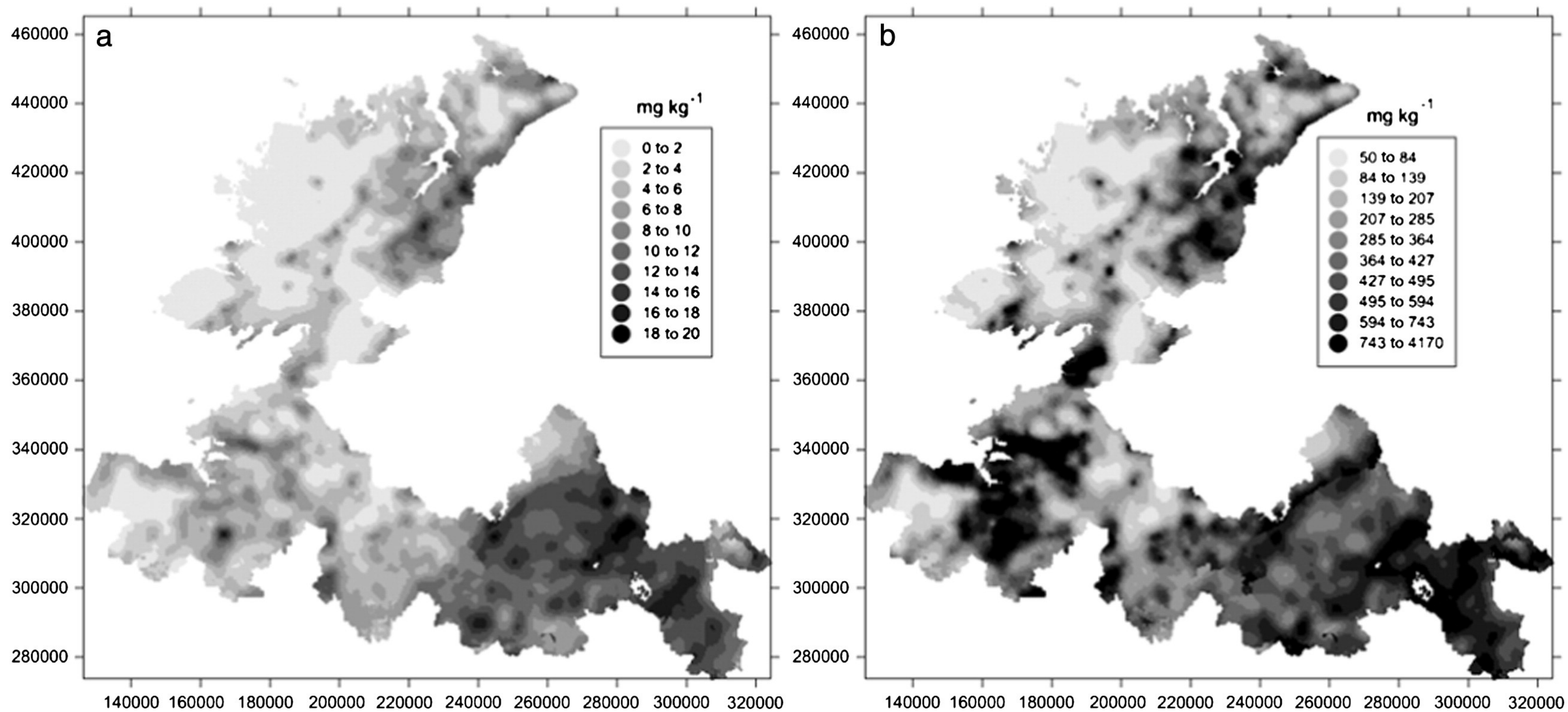

Fig. 8. Cokriging predictions of the conditional mean concentration in topsoil of (a) Co and (b) Mn.

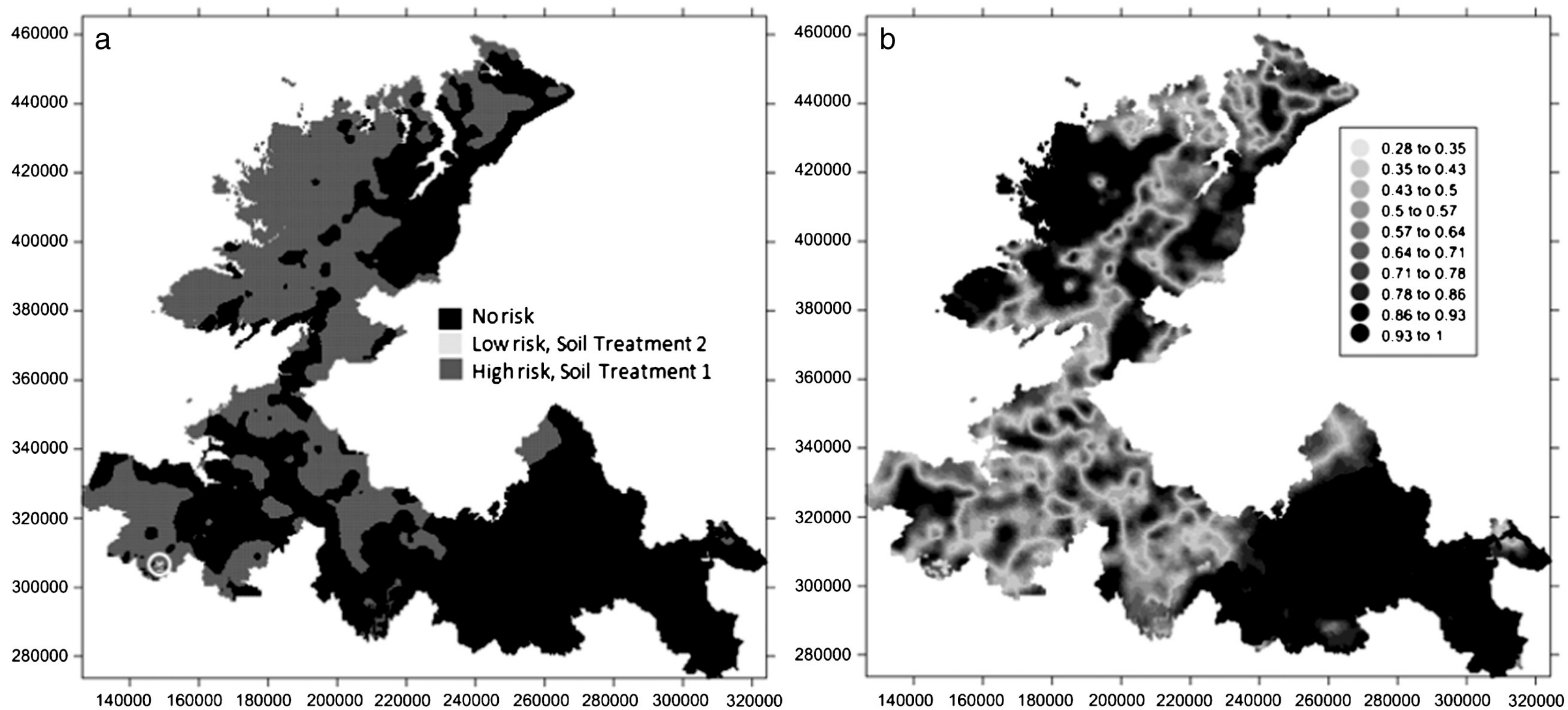

Fig. 9. Map of (a) most probable management class and (b) probability of the most probable management class. N.B. Class 'Low Risk, Soil Treatment 2' is the most probable class over a very restricted area in the south-west of Co. Sligo, indicated by a circle in panel (a).

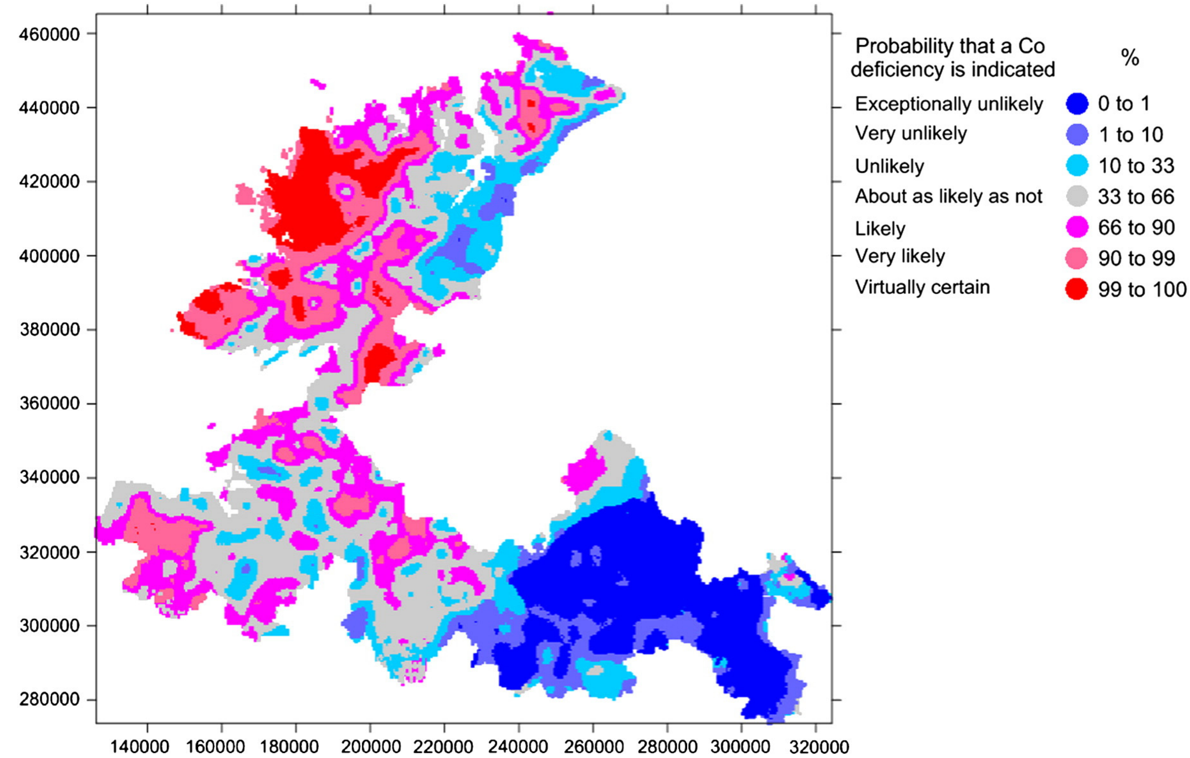

Fig. 10. Map on verbal probability scale (with probabilities indicated as percentages) of the probability that local topsoil Co and Mn concentrations would indicate a risk of Co deficiency.

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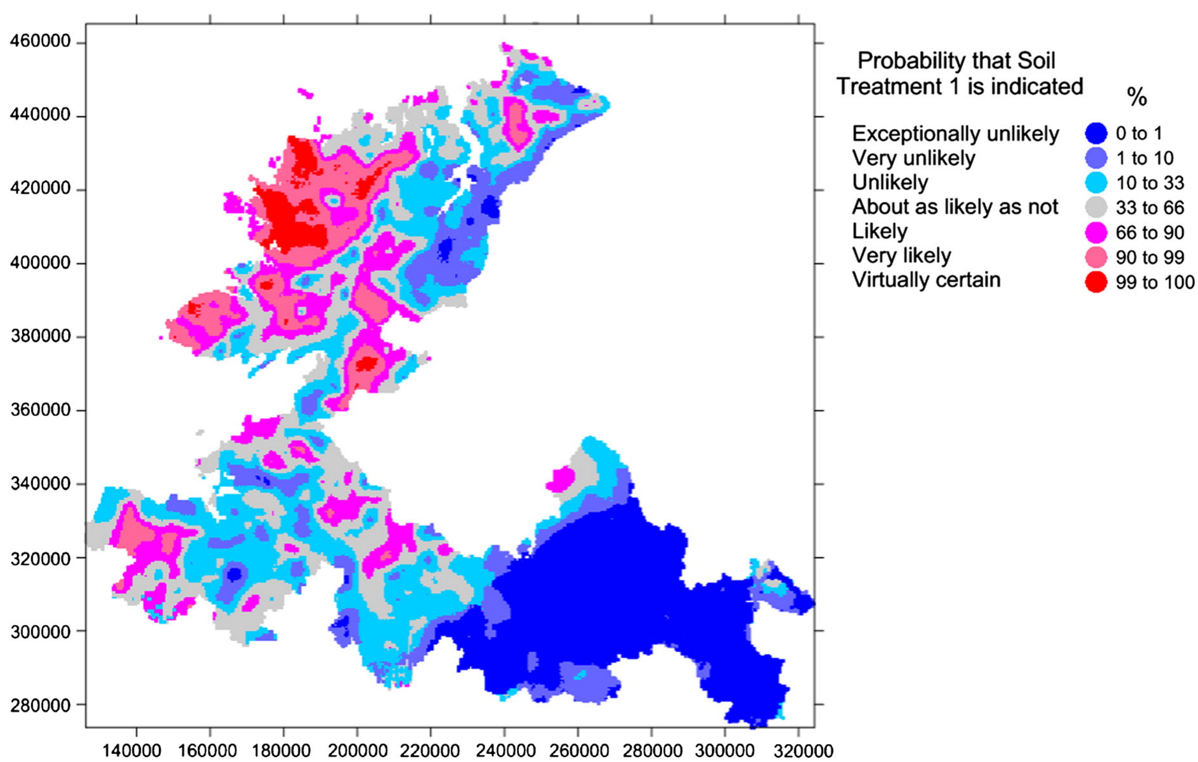

Fig. 11. Map on verbal probability scale (with probabilities indicated as percentages) of the probability that the intervention indicated by local soil conditions is soil treatment 1 (application of Co fertiliser at 3 kg ha^{-1}).

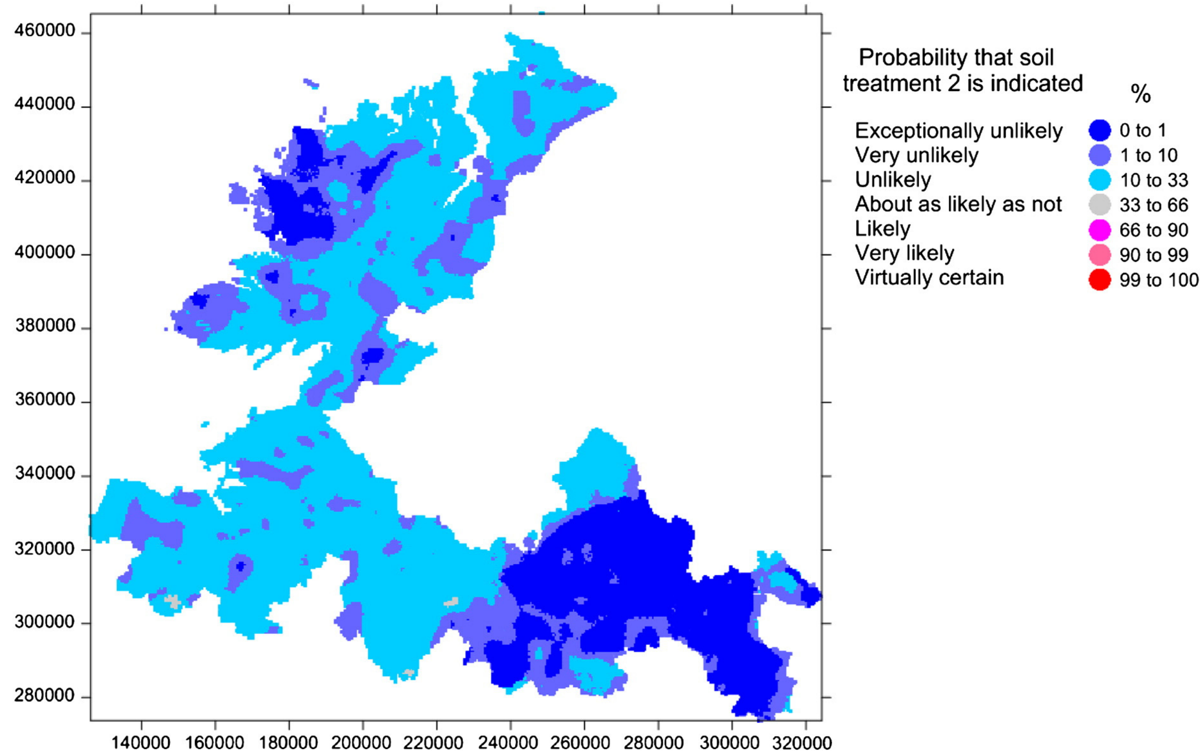

Fig. 12. Map on verbal probability scale (with probabilities indicated as percentages) of the probability that the intervention indicated by local soil conditions is soil treatment 2 (application of Co fertiliser at 2 kg ha^{-1}).

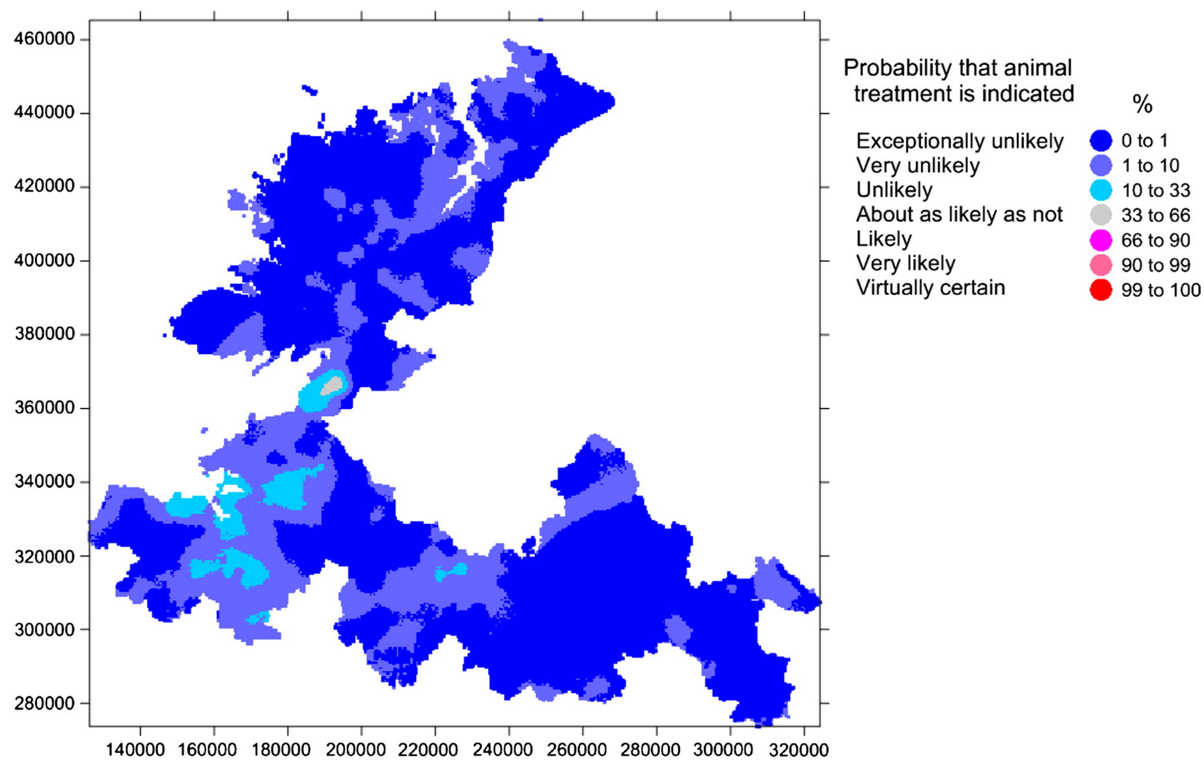

Fig. 13. Map on verbal probability scale (with probabilities indicated as percentages) of the probability that the intervention indicated by local soil conditions is animal treatment because of the concentration of Mn in soil.

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