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Statistical sampling approaches for soil monitoring

D. J. Brus
Alterra, Wageningen University and Research Centre, Environmental Science Group, PO Box 47, 6700 AA, Wageningen, The Netherlands

Summary

This paper describes three statistical sampling approaches for regional soil monitoring, a design-based, a model-based and a hybrid approach. In the model-based approach a space-time model is exploited to predict global statistical parameters of interest such as the space-time mean. In the hybrid approach this model is a time-series model of the spatial means. In the design-based approach no model is used: estimates are model-free. Full design-based inference requires that both sampling locations and times are selected by probability sampling, whereas the hybrid approach requires probability sampling of locations only. In a case study on soil eutrophication and acidification, a rotational panel design was implemented with probability sampling of locations and non-probability sampling of times. The hybrid and model-based predictions of the space-time means and trend of the mean for pH and ammonium at three depths in the soil profile were very similar. For pH the standard errors of the space-time means were about equal, but for ammonium the full model-based predictor was more precise than the hybrid predictor. For soil monitoring I advocate the selection of sampling locations by probability sampling so that the statistical inference approach is flexible. Selecting locations by a self-weighting probability sampling design ensures that the model-based predictor is not affected by selection bias.

Introduction

At many places in the world the soil is threatened, for instance by erosion, chemical pollution, salinization, decrease of organic matter or compaction (Lal *et al.,* 1989). As a consequence, the functioning of the soil for the production of food and fibres, as part of the ecosystem, for water storage and for other purposes is under pressure at these places. This is widely recognized by governments and other authorities, who react by commissioning the implementation of networks to monitor the soil. There are many scientific considerations in the design of a soil monitoring network, such as the selection of soil quality indicators, efficient measurement techniques, soil sampling devices and the use of soil process models (Morvan *et al.,* 2008; Arrouays *et al.,* 2012). There are also statistical considerations, such as the sampling design of the monitoring network (Conant *et al.,* 2011) and the statistical inference of the data. Recently an IUSS working group on soil monitoring has been established, under the auspices of, amongst others, the Pedometrics commission, to share expertise and motivate collaborative research on soil monitoring.

This paper focuses on the statistical aspects of monitoring, more specifically on the statistical sampling aspects, and related to this the statistical inference. A major decision in designing a monitoring network is the selection of the statistical sampling approach (de Gruijter *et al.,* 2006). Two fundamentally different sampling approaches can be distinguished, the design-based approach and the model-based approach (de Gruijter & ter Braak, 1990; Brus & de Gruijter, 1997). In a design-based sampling approach the estimation of the statistical parameter of interest, for instance the mean or the total, and its standard error is based on the inclusion probabilities of the sampling units. These probabilities are determined by the sampling design. This requires that the sampling units are selected by probability sampling, so that these inclusion probabilities are known. In a model-based approach the statistical inference is based on a model of the spatial variation. Randomness is introduced via the model, which is a stochastic model and therefore contains a random error term. As a consequence, selection of the sampling units by probability sampling is not strictly needed.

For soil monitoring, sampling times must be selected in addition to sampling locations. This leads to four combinations of probability (P) and non-probability sampling (NP): P-sampling in both space and time (P + P), NP-sampling in both space and time (NP + NP), P-sampling in space and NP-sampling in time (P + NP), and NP-sampling in space and P-sampling in time (NP + P). With P + P the statistical parameter of interest can be estimated with a fully design-based approach and without a model. With NP + NP, a model of the variation in space and time must be postulated to estimate the parameter of interest. In other words, the statistical inference is fully model-based. In P + NP a hybrid estimator is applied, involving both design-based and model-based inference (Brus & de Gruijter, 2012). The model in this hybrid approach is a time-series model, not a full space-time model. NP + P occurs rarely in practice and is not considered here.

Correspondence: D. J. Brus. E-mail: dick.brus@wur.nl
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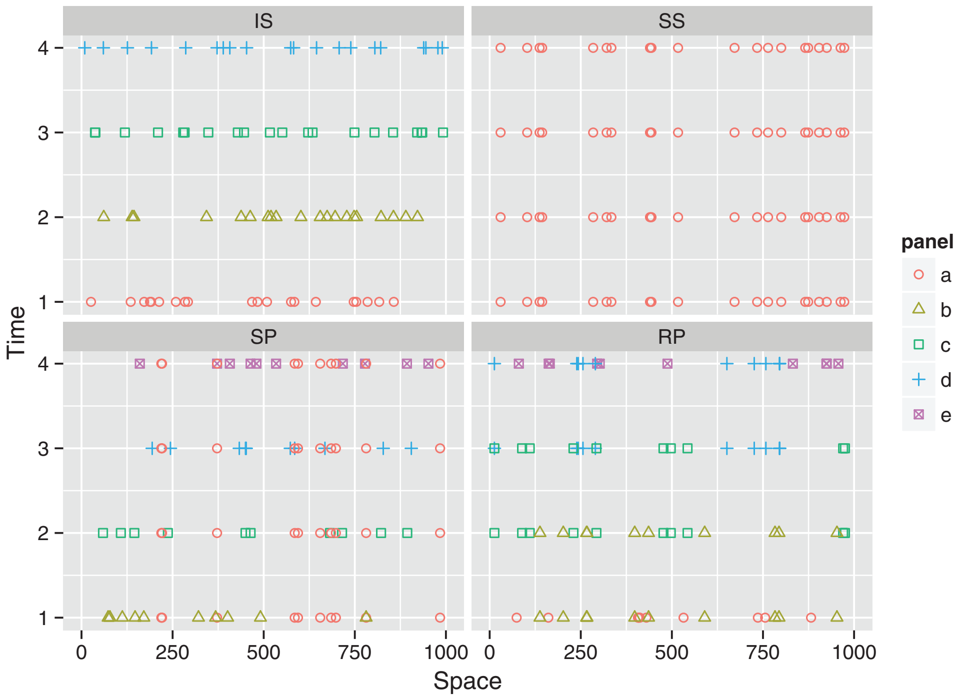

Figure 1 Notional examples of four space-time designs: SS, static-synchronous; IS, independent synchronous; SP, supplemented panel; RP, rotating panel design.

The aim of this paper is to explain, demonstrate and discuss the fully design-based approach, hybrid approach and fully model-based approach for space-time sampling and statistical inference of space-time parameters of interest. As a parameter of interest I will focus on the space-time mean. The space-time mean of a soil property is of interest when information is required at a spatial or temporal scale that is much larger than the support of a single measurement. For example, land managers might wish to know the total mass of nutrient lost through leaching or the mean rate of emission of greenhouse gases from all of the soil within a farm across an entire year. I will show how this mean and its variance can be predicted (i) using a model of the variation in space and time of the soil property of interest, (ii) using a model of the variation in time of the spatial means and (iii) without any model (model-free). The first two options will be demonstrated with a real-world case study on soil monitoring. In common with many soil monitoring networks the case study measures properties at only a small number of times. Therefore it can be a challenge to estimate a model of the temporal variation accurately. I use a novel approach based on regularized variograms that makes efficient use of the temporal information that is available. In the final section, the three sampling approaches will be discussed, and recommendations for soil monitoring applications will be given.

Theory

In this section the three main sampling approaches mentioned in the Introduction will be described. To highlight differences and similarities a common parameter of interest will be estimated with all three approaches, namely the space-time mean.

This parameter is defined as:

$$\bar{\bar{z}}_{\mathcal{U}} = \frac{1}{|\mathcal{T}|\,|\mathcal{A}|}\int_{t\epsilon\mathcal{T}}\int_{\mathbf{s}\epsilon\mathcal{A}} z_{\mathbf{s},t}\mathrm{d}\mathbf{s}\mathrm{d}t = \frac{1}{|\mathcal{T}|}\int_{t\epsilon\mathcal{T}}\bar{z}_t\mathrm{d}t, \tag{1}$$

with $|\mathcal{T}|$ the length of the monitoring period, $|\mathcal{A}|$ the area of the study area, $z_{\mathbf{s},t}$ the value of the target variable at location $\mathbf{s}$ and time t, and $\bar{z}_t$ the spatial mean at time t. The universe of interest is the Cartesian product of the continuous temporal universe $\mathcal{T}$ and the spatial universe $\mathcal{A}$: $\mathcal{U} = \mathcal{T} \times \mathcal{A}$. The space-time mean is here defined as a population parameter for a continuous temporal universe of interest. If we discretise the universe of interest along the time-axis, for instance into days, the universe of interest becomes finite along the time-axis, and the space-time mean is defined as:

$$\bar{\bar{z}}_{\mathcal{U}} = \frac{1}{N}\sum_{t=1}^{N}\bar{z}_t, \tag{2}$$

with N the total number of times (days) in the monitoring period.

For the fully design-based approach and the hybrid approach the estimators of the space-time mean and its variance are determined by the type of spatial sampling design, type of temporal sampling design (not for the hybrid approach) and the type of space-time design. Figure 1 shows several basic types of space-time design (de Gruijter *et al.*, 2006). In a static design the sampling locations are fixed in space, but the observations are not synchronized in time (not shown). Conversely, in an independent synchronous design (hereafter referred to as IS-design) the observations are synchronized, but the sampling locations shift over time through the area. The spatial sample at a given time is selected independently from the spatial samples at the other times. No sampling locations are revisited. In a static-synchronous design (SS-design) the observations show a twofold alignment: all sampling locations are revisited at the same times. This design is also known as a pure panel. A supplemented panel design (SP-design) is a compromise between an independent synchronous and a static-synchronous design. Only a proportion of the sampling locations are revisited at the subsequent sampling times. The remaining proportion is replaced by new locations, selected independently from the revisited locations and all locations of other times. Another hybrid design type is the rotating panel (RP), in which sampling locations are revisited a restricted number of times (twice in Figure 1) and then replaced by new locations.

Full design-based approach

In this approach both locations and times are selected by probability sampling. Statistical inference is entirely based on the space-time sampling design, no model is involved. In other words this approach results in model-free estimates of the statistical parameter of interest and its sampling variance. This can be attractive when the validity of the result is of crucial importance, for instance in the case of compliance monitoring; see Brus & Knotters (2008) for an example of compliance monitoring of surface water quality. Brus *et al.* (2010) provide an application of this approach in soil monitoring.

I will elaborate now on estimation of the space-time mean with an independent-synchronous space-time design. A few remarks will be made on estimation for a static-synchronous space-time design.

Independent-synchronous design. With this design several times are selected randomly first, followed by selection of spatial samples at the selected times. The spatial samples are selected independently from each other (Figure 1). This implies that the estimated spatial means at the sampling times are design-independent by construction. The attractiveness of this type of space-time design is the simplicity of the estimators and the availability of an unbiased sampling variance estimator. The sample data can be treated as a two-stage random sample and the estimators for two-stage random spatial sampling can be applied (de Gruijter *et al.*, 2006). In the first stage sampling times are selected. This corresponds with the selection of the spatial primary sampling units in spatial sampling, for instance agricultural fields. In the second stage locations are selected at the selected times. This corresponds with the selection of secondary sampling units within the spatial primary sampling units in spatial sampling, for instance points within the selected agricultural fields. When sampling times are selected by simple random sampling or any other self-weighting design (a design with equal inclusion densities for all times), the unweighted average of the estimated spatial means is an unbiased estimator of the space-time mean:

$$\hat{\bar{\bar{z}}}_{\mathcal{U}} = \frac{1}{r}\sum_{j=1}^{r} \hat{\bar{z}}_j, \tag{3}$$

where r is the number of selected sampling times, and $\hat{\bar{z}}_j$ is the estimated spatial mean at sampling time t_j. For non-self-weighting temporal sampling designs, the Horvitz-Thompson-estimator or π-estimator of the space-time mean equals the weighted average of the estimated spatial means at the selected times, with weights inversely proportional to the inclusion probabilities of the sampling times (Särndal *et al.*, 1992). The estimator $\hat{\bar{z}}_j$ in Equation (3) is determined by the spatial sampling design.

With simple random sampling in time the sampling variance of the estimated space-time mean can be estimated by:

$$\hat{V} = \left(\hat{\bar{\bar{z}}}_{\mathcal{U}}\right) = \frac{\widehat{S^2}_{\mathcal{T}}}{r}, \tag{4}$$

with $\widehat{S^2}_{\mathcal{T}}$ the temporal variance of the estimated spatial means:

$$\widehat{S^2}_{\mathcal{T}} = \frac{1}{(r-1)}\sum_{j=1}^{r}\left(\hat{\bar{z}}_j - \hat{\bar{\bar{z}}}_{\mathcal{U}}\right)^2. \tag{5}$$

Neither the spatial variance nor the number of sampling locations is included in this variance estimator. The reason is that the error in the estimated spatial means is automatically accounted for by $\widehat{S^2}_{\mathcal{T}}$. Finally, note that this sampling variance accounts for variation resulting from repeated selection of locations and times.

Static-synchronous design. In circumstances where there are large costs associated with the installation of monitoring equipment, such as when using lysimeters to monitor soil pore water, it might not be cost-effective to observe different locations at the different times. In this situation it is generally much more efficient to observe all sampling locations at all selected sampling times, leading to a static-synchronous design (Figure 1).

An unbiased estimate of the space-time mean can be obtained in the same way as with independent synchronous sampling. However, no unbiased estimator of the sampling variance of the estimated space-time mean exists, because of the twofold alignment of the observations, and all sampling locations are revisited and observations are synchronized (de Gruijter *et al.*, 2006). The procedure described above for estimating the sampling variance does not account for temporal correlations between the estimated spatial means due to the fixed sampling locations. Treating the static-synchronous sample as an independent synchronous sample leads to an under-estimate of the sampling variance.

Hybrid approach

In the hybrid approach a time-series model of the spatial means is used in prediction. One reason for the use of such a model is that sampling times have not been selected by probability sampling, so that model-free, design-based inference of the space-time mean or another global parameter of interest is impossible. Even when times are selected by probability sampling, one might prefer to use such a model to predict the space-time mean, as it may increase its precision. Finally, another reason can be that we want to predict a discrete time-series of spatial means. To estimate or, more correctly, to predict statistically the space-time mean under the hybrid approach, a linear mixed model for the temporal variation of the spatial means is used (Brus & de Gruijter, 2012):

$$\overline{\mathbf{Z}} = \mathbf{D}\boldsymbol{\beta} + \boldsymbol{\eta}, \tag{6}$$

with $\overline{\mathbf{Z}}$ the r-vector with true spatial means at the sampling times $\overline{Z}_t$, $t = 1 \cdots r$, $\mathbf{D}$ the $r \times q$ matrix containing predictors, $\boldsymbol{\beta}$ the q-vector with regression coefficients and $\boldsymbol{\eta}$ the r-vector with model errors (model residuals). $\mathbf{D}$ can be, for instance, a vector with ones (spatial means constant over time), or a matrix with ones in the first column and the sampling time in the second column (linear trend of the spatial means). $\overline{\mathbf{Z}}$ is in upper case as, contrary to the fully design-based approach, in this hybrid approach the true spatial means are random quantities. The model errors $\boldsymbol{\eta}$ have 0 mean and an $r \times r$ covariance matrix $\mathbf{C}_\xi$. Note that these model covariances $\mathbf{C}_\xi$ are temporal covariances of spatial means, or in other words covariances on area-support (see section Case study). The Central Limit Theorem implies that the distribution of the spatial mean of a random space-time variable Z will be approximately Gaussian even when Z has a non-Gaussian distribution, depending on how strongly the distribution of Z deviates from Gaussian, the size of the area, and the strength of the spatial correlation.

In practice, the spatial means are unknown, and in the hybrid approach these means are estimated from a probability sample. This leads to the following model for the estimated spatial means, $\hat{\overline{Z}}_t$, $t = 1 \cdots r$, in which besides the model error η there is an additional sampling error ε:

$$\hat{\overline{\mathbf{Z}}} = \mathbf{D}\boldsymbol{\beta} + \boldsymbol{\eta} + \boldsymbol{\varepsilon}, \tag{7}$$

with $\hat{\overline{\mathbf{Z}}}$ the vector with estimated spatial means, and $\boldsymbol{\varepsilon}$ the r-vector with sampling errors. The sampling errors have 0 mean and an $r \times r$ covariance matrix $\mathbf{C}_p$. The model errors and sampling errors are mutually independent, as these originate from independent stochastic processes. The overall covariance matrix of the estimated spatial means equals:

$$\mathbf{C}_{\xi p} = \mathbf{C}_\xi + \mathbf{C}_p. \tag{8}$$

The model parameters (the covariance function parameters and the regression coefficients) are unknown and must be estimated from the sample data. These model parameters can be estimated by residual maximum likelihood (Lark, 2000; Lark & Webster, 2006). Given the estimates of the covariance function parameters, the matrix $\hat{\mathbf{C}}_\xi$ can be computed and added to the matrix with estimated sampling covariances $\hat{\mathbf{C}}_p$ (see hereafter for how to obtain $\hat{\mathbf{C}}_p$). This matrix $\hat{\mathbf{C}}_{\xi p}$ can then be used to estimate the regression coefficients by generalized least squares:

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{D}'\hat{\mathbf{C}}_{\xi p}^{-1}\mathbf{D}\right)^{-1}\mathbf{D}'\hat{\mathbf{C}}_{\xi p}^{-1}\hat{\overline{\mathbf{Z}}}. \tag{9}$$

In the case of a linear trend model the second element of $\boldsymbol{\beta}$ in Equation (9) is the estimate of the linear trend of the spatial mean.

Under the model of Equation (7) the spatial mean at time t can then be predicted by (compare Diggle & Ribeiro, 2007):

$$\hat{\overline{Z}}_{t,\mathrm{hyb}} = \mathbf{d}'\boldsymbol{\beta} + \mathbf{c}'_\xi\mathbf{C}_{\xi p}^{-1}\left(\hat{\overline{\mathbf{Z}}} - \mathbf{D}\beta\right), \tag{10}$$

with $\mathbf{d}$ the q-vector with the predictors, and $\mathbf{c}_\xi$ the r-vector with model covariances between the spatial means at prediction time t and the sampling times. The predictor of Equation (10) will be referred to hereafter as the hybrid predictor. With the constant mean model $\mathbf{d}$ equals scalar 1, under the linear trend model $\mathbf{d} = \left(1, \bar{t}\right)'$, with $\bar{t} = \left(\mathcal{T}_s + \mathcal{T}_e\right)/2$, with $\mathcal{T}_s$ and $\mathcal{T}_e$ the start and end of the monitoring period, respectively. The hybrid predictor is similar to the universal kriging predictor for a one-dimensional universe (Cressie, 1993), except that the matrix of model covariances has been replaced by the matrix of the sums of the model and sampling covariances (Equation (8)).

The variance of the hybrid prediction error is (Corsten, 1989):

$$V\left(\hat{\overline{Z}}_{t,\mathrm{hyb}}\right) = \bar{c}_\xi\left(\mathcal{T}\right) - \mathbf{c}'_\xi\mathbf{C}_{\xi p}^{-1}\mathbf{c}_\xi + \mathbf{d}'_a\left(\mathbf{D}'\mathbf{C}_{\xi p}^{-1}\mathbf{D}\right)^{-1}\mathbf{d}_a, \tag{11}$$

with $\bar{c}_\xi\left(\mathcal{T}\right)$ the mean model covariance of spatial means within the monitoring period $\mathcal{T}$ bounded by T_s and T_e, and $\mathbf{d}_a = \mathbf{d} - \mathbf{D}'\mathbf{C}_{\xi p}^{-1}$. The mean model covariance $\bar{c}_\xi\left(\mathcal{T}\right)$ can be approximated by the Cauchy-Gauss method (Journel & Huijbregts, 1978). With this method, for a one-dimensional domain the mean covariance is approximated by a weighted sum of the covariances at four to six distances only.

The space-time mean for the space-time universe $\mathcal{U}$ and its variance can be predicted by replacing vector $\mathbf{c}_\xi$ in Equations (10) and (11) by $\bar{\mathbf{c}}_\xi$, the vector with mean model covariances of the spatial means between each sampling time and the monitoring period. The mean model covariance between a sampling time-point and all times in the monitoring period can be approximated by Gaussian quadrature, an approach that is similar to the Cauchy-Gauss method (Carr & Palmer, 1993).

Supplemented and rotating panel. For supplemented panel and rotating panel sampling the model of Equation (7) is reformulated such that multiple estimates of the spatial mean at a given time are accounted for. Each so-called panel of sampling locations gives an estimate of the spatial mean. A panel is a group of locations observed at the same set of sampling times. For the supplemented and the rotating panels depicted in Figure 1 at each sampling time two panels are sampled, leading to two panel-specific estimates per time, referred to as 'elementary estimates' (Brus & de Gruijter, 2011). This leads to the following model:

$$\hat{\overline{Z}}_\mathrm{e} = \mathbf{D}_\mathrm{e}\boldsymbol{\beta} + \mathbf{X}\boldsymbol{\eta} + \boldsymbol{\varepsilon}_\mathrm{e}. \tag{12}$$

Matrix $\mathbf{D}_\mathrm{e}$ now has dimension $E \times q$ with E the total number of elementary estimates (in Figure 1, $E = 4 \times 2$). $\mathbf{X}$ is a random-effect design matrix (dimension $E \times r$) with zeroes and ones selecting the appropriate element of $\boldsymbol{\eta}$. Vector $\boldsymbol{\eta}$ is as before, but vector $\boldsymbol{\varepsilon}_\mathrm{e}$ now has length E as we have multiple sampling errors per sampling time, one per elementary estimate. The overall covariance matrix of the estimated spatial means equals:

$$\mathbf{C}_{\xi p,\mathrm{e}} = \mathbf{X}\mathbf{C}_{\xi}\mathbf{X}' + \mathbf{C}_{p,\mathrm{e}}, \tag{13}$$

with covariance matrix $\mathbf{C}_{\xi}$ as before (dimension $r \times r$) and $\mathbf{C}_{p,\mathrm{e}}$ the sampling covariance matrix of the elementary estimates (dimension $E \times E$). See the case study for an example of $\mathbf{X}$ and $\mathbf{C}_{p,\mathrm{e}}$. The vector with model covariances must also be premultiplied by $\mathbf{X}$: $\mathbf{c}_{\xi,\mathrm{e}} = \mathbf{X}\mathbf{c}_{\xi}$. The hybrid predictor of the spatial mean at time t and its prediction variance can now be obtained by inserting the covariance matrix $\mathbf{C}_{\xi p,\mathrm{e}}$ and covariance vector $\mathbf{c}_{\xi,\mathrm{e}}$ into Equations (10) and (11).

Full model-based approach

With this sampling approach, prediction requires a stochastic model to describe the variation of the soil property of interest in time and space. The main advantages of this approach include a potential increase in the precision of the predicted global parameters of interest, the absence of a requirement to use probability sampling in either time or space and the ability to map the predictions at any locations in space or time.

In this approach it is assumed that the space-time distribution of the observations can be described by:

$$\mathbf{Z} = \mathbf{D}\boldsymbol{\beta} + \boldsymbol{\nu}, \tag{14}$$

with $\mathbf{Z}$ the n-vector with observations (n is total number of observations), $\mathbf{D}$ the $n \times q$ matrix with predictors, $\boldsymbol{\beta}$ the q-vector with regression coefficients and $\boldsymbol{\nu}$ the n-vector with model errors. Matrix $\mathbf{D}$ may contain spatial coordinates, the times of sampling and covariates that may vary in space and/or time. Note that I use a different symbol for the model error as compared with the model used in the hybrid approach, to stress that the distribution differs from that of $\boldsymbol{\eta}$ in Equation (6). The distribution of $\boldsymbol{\nu}$ is not necessarily Gaussian, and its variance will be larger.

The space-time dependence of the model errors can be modelled by the summetric type of variogram (Dimitrakopoulos & Luo, 1994; Snepvangers *et al.*, 2003):

$$C\,(h,u) = C_s\,(h) + C_t\,(u) + C_{\mathrm{st}}(\sqrt{\left(h^2 + (\alpha u)^2\right)}, \tag{15}$$

with h the separation distance (lag) between two observations in space, u the separation distance in time, and α an anisotropy coefficient. So the space-time covariance function is the sum of a spatial covariance function $C_{\mathrm{s}}(\cdot)$, a temporal covariance function $C_{\mathrm{t}}(\cdot)$ and a geometric anisotropy space-time covariance function $C_{\mathrm{st}}(\cdot)$. This is a flexible covariance function that allows for differences in the range (distance parameter) between space and time (geometric anisotropy), as well as differences in sill-variance between space and time (zonal anisotropy).

In contrast to the hybrid approach, it is now possible to predict the value of Z at any location in the space-time universe $\mathcal{U}$. This value can be predicted by:

$$\widehat{Z}_{s,t,MB} = \mathbf{d}'\boldsymbol{\beta} + \mathbf{c}'_{\xi(\mathbf{Z})}\mathbf{C}^{-1}_{\xi(\mathbf{Z})}\,(\mathbf{Z} - \mathbf{D}\boldsymbol{\beta})\,, \tag{16}$$

with $\mathbf{d}$ the vector with predictor values at the prediction point ($\mathbf{s}$, t), $\mathbf{c}_{\xi(\mathbf{Z})}$ the n-vector with model covariances between the prediction point ($\mathbf{s}$, t) and the observations, $\mathbf{C}_{\xi(\mathbf{Z})}$ the $n \times n$ matrix with model covariances between the observations, $\mathbf{Z}$ the n-vector with observations, and $\mathbf{D}$ the $n \times q$ matrix with values of the predictors at the sampling points in the space-time universe. Note that I added subscript ($\mathbf{Z}$) to the symbols $\mathbf{c}_{\xi}$ and $\mathbf{C}_{\xi}$ to stress that, contrary to the hybrid approach, these are covariances of individual values of the target variable, not of spatial means. The predictor of Equation (16) will be referred to hereafter as the model-based predictor.

The spatial mean at time t can be predicted by replacing $\mathbf{c}_{\xi}$ in Equation (16) by a vector with mean covariances between the observations and the cross-section of the space-time universe U at time t. Similarly the space-time mean can be predicted by replacing $\mathbf{c}_{\xi}$ by a vector with mean covariances between the observations and the entire space-time universe U.

Case study

I will now demonstrate the sampling approaches with a case study on forest soil eutrophication and acidification. The study area is situated in forests on the Utrechtse Heuvelrug, an ice-pushed ridge of the Saalien ice-age (370 000–150 000 BP) in the Netherlands with gravelly sandy soils. In this area there is a forest monitoring network, the locations of which were selected by systematic unaligned random sampling. This network was sub-sampled by simple random sampling without replacement. At these locations the forest soil was sampled at three depths, in the topsoil, between the top- and subsoil, and in the subsoil. Sampling depth was not fixed, but soil horizons were sampled. pH and the ammonium concentration (NH_4 in mg kg^{-1}) were measured by weighing out 20 g of air-dried soil, adding 50 ml of 1 M KCl, mechanically shaking for 1 hour, filtering and measuring spectrophotometrically.

The sample size per sampling time n_t was 20. Sampling was repeated four times ($r = 4$), with an interval of approximately 1 year (2004–2007) according to a rotating panel design. Sampling times were not selected by probability sampling, but at a convenient time in the month of March. The matching proportion was 0.5, which means that ten randomly selected locations from a given sampling time were revisited at the next sampling time. At the fourth sampling time the ten new locations of the third sampling time were revisited, plus the ten locations of the first sampling time that were not revisited at the second sampling time (Figure 2). The total number of panels is thus four. The total number of sampling events (combinations of location and time) equals 80.

At some locations of the first sampling time, some soil horizons were erroneously not re-sampled at exactly the same depth at the second sampling time. The measurements at the first sampling time in the soil horizons that do not match were replaced by missing

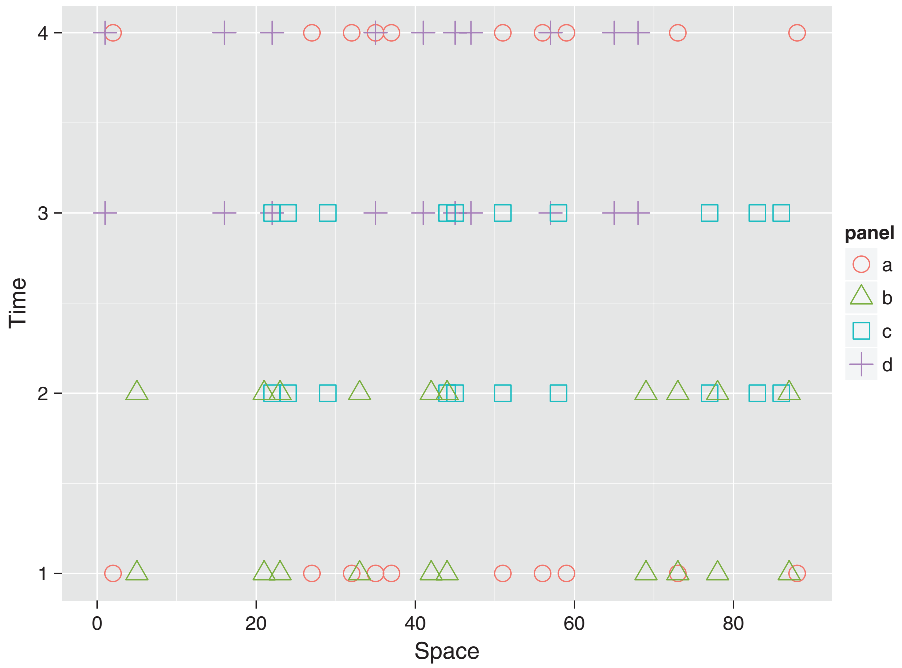

Figure 2 Schematic representation of the rotating panel sample to monitor forest soils of the Utrechtse Heuvelrug.

values. This resulted in four missing values in the topsoil, five in the middle soil horizon, and one in the subsoil.

The space-time means for universe U (Equation (1)) were obtained by both the hybrid and the model-based predictor. Also, time-series of the spatial means for a fine discretization of the monitoring period were obtained by these two predictors. Finally, the model-based predictor was used in space-time mapping, to predict the soil properties at the nodes of a fine space-time grid.

The NH_4 concentrations were log-transformed because the observations were skewed and therefore did not conform to the Gaussian model. Therefore all estimated spatial means and space-time means are means of log-transformed concentrations. While design-based estimation of means of untransformed NH_4 concentrations can be obtained in a straightforward manner by not transforming the data, hybrid and fully model-based estimation of these means is more complicated. The log-transformation generally improves the quality of the models and the predictions obtained with these models. However, back-transformation of the predicted means is not straightforward; see Paul & Cressie (2011).

Hybrid approach

The spatial means at time t for a fine discretization of the monitoring period and the space-time means, defined as the mean across the entire space-time universe of interest (Equation (1)), were obtained with the hybrid predictor (see Supplemented and rotating panel section). For all variables except pH in the subsoil, the estimated linear trends of the spatial means were small and according to the t-test not significant at 5%. Therefore, for all variables except pH in subsoil, I predicted the space-time mean under the constant mean model. For pH in subsoil the linear trend model was used. The eight elementary estimates were ordered as $(\hat{\hat{z}}_{a4}, \hat{\hat{z}}_{a1}, \hat{\hat{z}}_{b1}, \hat{\hat{z}}_{b2}, \hat{\hat{z}}_{c2}, \hat{\hat{z}}_{c3}, \hat{\hat{z}}_{d3}, \hat{\hat{z}}_{d4})$. For this ordering the design matrix $\mathbf{X}$ equals:

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and the sampling covariance matrix $\mathbf{C}_{p,\mathrm{e}}$ equals:

$$\begin{bmatrix} V_{a4} & C_{1,4} & 0 & 0 & 0 & 0 & 0 & 0 \\ C_{4,1} & V_{a1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{b1} & C_{1,2} & 0 & 0 & 0 & 0 \\ 0 & 0 & C_{2,1} & V_{b2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & V_{c2} & C_{2,3} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{3,2} & V_{c3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & V_{d3} & C_{3,4} \\ 0 & 0 & 0 & 0 & 0 & 0 & C_{4,3} & V_{d4} \end{bmatrix}$$

The sampling covariances of the estimated spatial means at two times ($C_{1,2}$, $C_{2,3}$, $C_{3,4}$, $C_{1,4}$) were estimated from the estimated correlation in the overlapping part of the samples, multiplied by the square roots of the spatial variances as estimated from all locations sampled at these times. This ensures that the matrix $\mathbf{C}_{\xi p}$ is positive definite and hence that its inverse can be calculated.

Brus & de Gruijter (2012) assumed a first-order autoregressive model for the spatial means, which is equivalent to an exponential variogram model without nugget. The distance parameter of this model was estimated with pairs of observations at the same location. For the rotational space-time design of the case study this resulted in an estimated correlation at time-lags of 1 and 3 years. No estimate of the correlation at a time-lag of 2 years was obtained, as there were no re-visits at this time-lag (Figure 2). Pairs of points with a time-lag of 2 years were also separated in space, so these pairs lead to biased (too small) estimates of the temporal correlation.

Here I followed a different approach for estimating the covariance function of the spatial means, which makes better use of the space-time data. Recall that this function is required to estimate the model covariance matrix $\mathbf{C}_\xi$ of the spatial means, Equations (8) and (9). The temporal variogram was obtained by regularization of the space-time variogram. In the next section I will explain how the space-time variogram was estimated. This variogram was regularized as described by Journel & Huijbregts (1978); see also Webster & Oliver (2007):

$$\gamma_{\mathcal{A}}(h,u) = \overline{\gamma}\left(\mathcal{A}, \mathcal{A}_{h,u}\right) - \overline{\gamma}(\mathcal{A}, \mathcal{A}), \tag{17}$$

with $\gamma_{\mathcal{A}}(h, u)$ the space-time semivariogram on block-support $\mathcal{A}$, $\overline{\gamma}\left(\mathcal{A}, \mathcal{A}_{h,u}\right)$ the mean semivariance on point support between two spatial blocks separated by distance h in space and distance u in time, and $\overline{\gamma}(\mathcal{A}, \mathcal{A})$ the mean semivariance on point support within spatial block $\mathcal{A}$. In our case block $\mathcal{A}$ is the study area. By taking $h=0$ we obtain the marginal temporal semivariogram of the spatial means for the study area. Both $\overline{\gamma}\left(\mathcal{A}, \mathcal{A}_{h,u}\right)$ and $\overline{\gamma}(\mathcal{A}, \mathcal{A})$ were approximated by random selection of 1 000 000 pairs of points. Finally, the covariance of two spatial means separated by time-lag u was obtained by computing the sill of the marginal temporal variogram on block-support, and subtracting the semivariance on block-support at this time-lag:

$$C_\xi(u) = \gamma_{\mathcal{A}}(0,\infty) - \gamma_{\mathcal{A}}(0,u). \tag{18}$$

$C_\xi(u)$ was computed for a range of values for u, and then a Matérn or an exponential variogram model without nugget was fitted to these values. Figure 3 and Table 1 show the result. Most striking is the very small sill variance for pH, especially in the middle soil horizon and subsoil, reflecting very small temporal fluctuations of the spatial mean pH. Ammonium at all three depths and pH in the subsoil showed meaningful temporal correlation, with effective temporal range varying from 1 to 2 years. For pH in the topsoil and middle soil horizon the effective temporal range was extremely small, so that the temporal variogram approximates a pure nugget variogram. The reliability of the fitted distance parameter is questionable, as it is much smaller than the smallest time-lag of 1 year in the dataset. Notice that the space-time covariogram itself is not used in hybrid prediction, but serves as a vehicle to derive the temporal covariogram of the spatial means.

Full model-based approach

I calibrated full space-time models, and used these models to predict the space-time means, to predict a time-series of spatial means for a fine discretization of the monitoring period, and in space-time mapping. A sum-metric model was fitted by maximum likelihood. For all three variograms of this sum-metric model an exponential model with nugget was used. The eight parameters of this model were fitted by minimizing the negative loglikelihood by differential evolution (Price *et al.*, 2006), using the R package DEoptim (Mullen *et al.*, 2011) (see Table 2). From comparison of the sill variances of the spatial and temporal variograms it is evident that for pH the spatial variation exceeds the temporal variation. The contribution of the geometric anisotropy variogram $\gamma_{st}(\cdot)$ was of the same order of magnitude as that of the spatial variogram. For ammonium (NH_4) the contribution of the geometric anisotropy variogram $\gamma_{st}(\cdot)$ outweighed those of the other two variograms. For NH_4 in the topsoil and middle soil horizon the spatial and temporal variation were of the same order of magnitude.

Design-based approach

Sampling times were not selected by probability, so model-free, design-based estimation of the space-time mean was impossible. For comparison I also computed the design-based generalized least squares estimates of the spatial means at the four sampling times as described by Brus & de Gruijter (2011). I then computed the average of these four GLS estimated spatial means, and its sampling variance. This average is not an unbiased estimate of the space-time mean (Equation (2)). However, it is interesting to see how much the hybrid and full model-based estimate differ from this design-based GLS estimate, and how different their variances are. In the latter estimator temporal variation of the spatial means within the monitoring period is ignored, and therefore I expected the sampling variance of the design-based GLS estimate to be smaller than the variance of the hybrid predictor.

Results

For all six variables the hybrid, model-based and design-based estimate/prediction of the space-time mean were nearly equal (Table 3). For pH the standard errors were also approximately equal, which can be explained by the very small temporal variances of the spatial means of pH. For NH_4 in the topsoil and subsoil the standard errors of the hybrid predictors were smaller than the design-based standard errors, despite the ignorance by the design-based estimator of temporal variation of the spatial means. For NH_4 the standard errors of the model-based predictor were smaller than for the hybrid predictor and the design-based estimator. This shows that the precision of the predicted space-time mean can be increased by exploiting a space-time model as in the fully model-based approach, or a time-series model of the spatial means as in the hybrid approach. The smaller standard error of the full model-based predictor compared with the hybrid predictor can be explained by the modelling of the spatial and spatio-temporal dependence of observations. These dependencies are not exploited by the hybrid predictor.

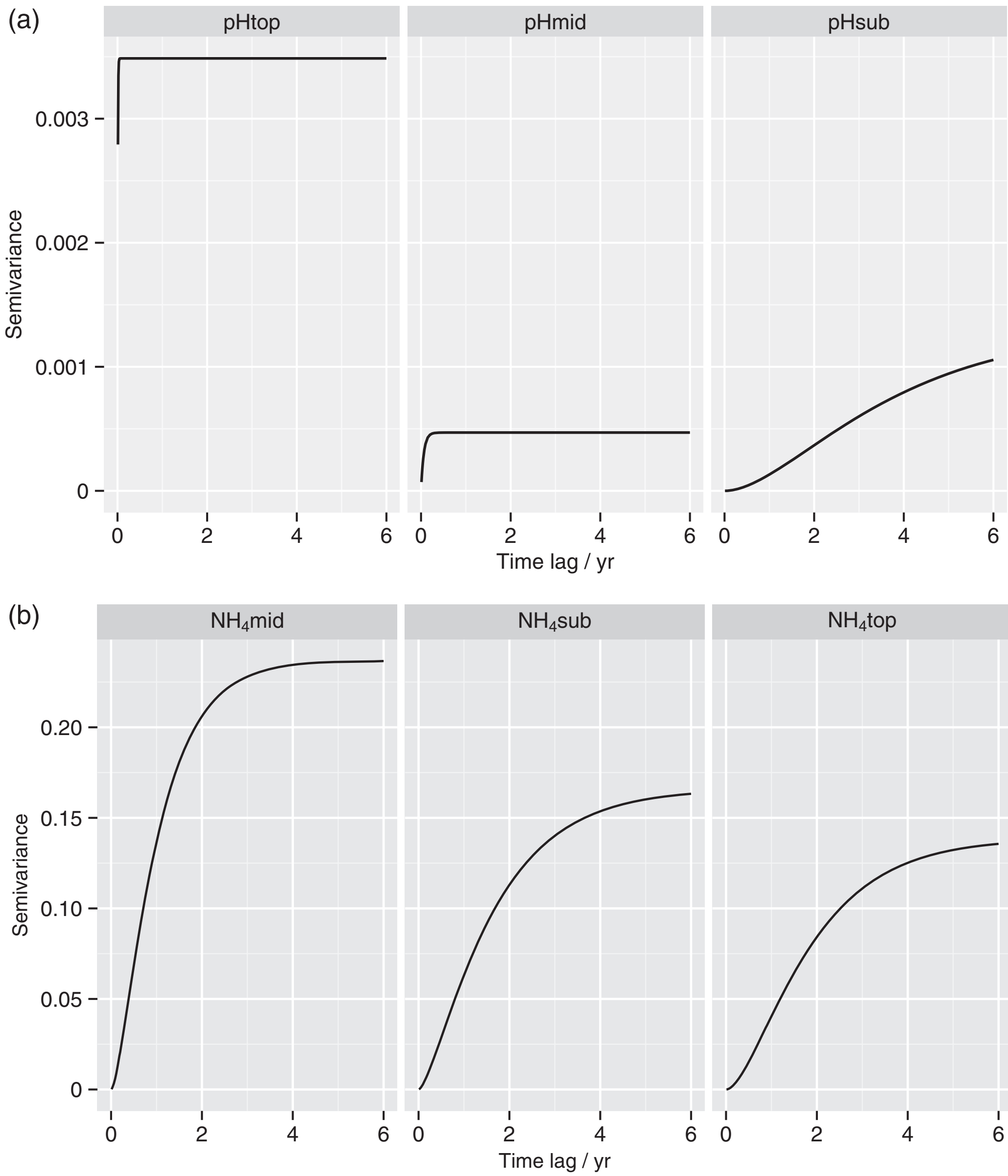

Figure 3 Regularized variograms and fitted models for pH (a) and log(NH_4) (b) in topsoil (top), the middle soil horizon (mid) and subsoil (sub). For model parameters, see Table 1.

The three estimates of the linear trends for pH in subsoil were comparable (Table 3). The hybrid and model-based standard errors were slightly larger than the design-based standard error.

For pH in the topsoil and middle soil horizon the 'time-series' of hybrid and fully model-based predicted spatial means are horizontal lines, with small spikes at the sampling times for topsoil pH (Figure 4). The temporal variograms for these two variables showed very weak structure only, so that the predicted spatial mean equalled the constant model mean, except at times very close to the sampling times. For pH in the subsoil the hybrid and model-based predicted spatial means also equalled approximately the estimated model means, but for this variable these

Table 1 Fitted model for the temporal variogram of the spatial means of pH and log(NH_4), used in the hybrid approach, as obtained by regularization of the sum-metric space-time variogram (Table 2)

	Model type	c(t)	a(t) / year	κ
pHtop	Exponential	0.00349	0.0062	–
pHmid	Exponential	0.00047	0.0612	–
pHsub	Matérn	0.00131	2.090	1.347
NH_4top	Matérn	0.139	1.140	1.172
NH_4mid	Matérn	0.237	0.710	0.932
NH_4sub	Matérn	0.166	1.220	0.839

c(t), sill variance; a(t), distance parameter; κ, order (shape parameter).

Table 2 Fitted parameters of the sum-metric space-time variogram for pH and log(NH4)

	c_0 (s)	c(s)	a(s) / km	c_0 (t)	c(t)	a (t) / year	c_0 (st)	c(st)
pHtop	5.70×10^{-2}	4.58×10^{-2}	2.65	2.12×10^{-3}	1.28×10^{-3}	0.0120	3.54×10^{-2}	1.03×10^{-3}
pHmid	2.02×10^{-2}	2.31×10^{-2}	2.08	1.21×10^{-8}	1.29×10^{-9}	0.0298	2.29×10^{-2}	6.79×10^{-3}
pHsub	2.85×10^{-2}	9.26×10^{-3}	3.48	3.18×10^{-8}	1.09×10^{-9}	2.32	8.55×10^{-3}	9.87×10^{-3}
NH_4top	4.34×10^{-6}	$7.40 \times 10^{-1}8$	8.99	1.17×10^{-6}	6.33×10^{-8}	1.32	4.87×10^{-6}	3.86×10^{-1}
NH_4mid	6.25×10^{-3}	4.35×10^{-3}	9.19	7.04×10^{-3}	6.21×10^{-6}	0.726	8.19×10^{-3}	6.22×10^{-1}
NH_4sub	3.86×10^{-8}	1.70×10^{-7}	7.65	7.42×10^{-3}	1.52×10^{-7}	1.12	1.79×10^{-6}	4.98×10^{-1}

c_0(s), spatial nugget variance; c(s), spatial partial sill variance; a(s), spatial distance parameter, and corresponding parameters for the temporal and spatiotemporal variograms.

Table 3 Hybrid predictions $\left(\hat{\bar{\bar{Z}}}_{\mathcal{U},\mathrm{hyb}}\right)$, fully model-based predictions $\left(\hat{\bar{\bar{Z}}}_{\mathcal{U},\mathrm{MB}}\right)$ and design-based GLS estimates $\left(\hat{\bar{\bar{z}}}_{\mathrm{GLS}}\right)$ of the space-time mean and their standard errors (se) for pH and log(NH_4) at three depths in forest soils on the 'Utrechtse Heuvelrug'

	$\hat{\bar{\bar{Z}}}_{\mathcal{U},\mathrm{hyb}}$	se $\left(\hat{\bar{\bar{Z}}}_{\mathcal{U},hyb}\right)$	$\hat{\bar{\bar{Z}}}_{\mathcal{U},\mathrm{MB}}$	se $\left(\hat{\bar{\bar{Z}}}_{\mathcal{U},\mathrm{MB}}\right)$	$\hat{\bar{\bar{z}}}_{\mathrm{GLS}}$	se $\left(\hat{\bar{\bar{z}}}_{\mathrm{GLS}}\right)$
pHtop	3.39	0.0623	3.36	0.0617	3.37	0.0562
pHmid	3.99	0.0396	3.97	0.0393	3.99	0.0398
pHsub	4.28	0.0352	4.22	0.0386	4.29	0.0358
NH_4top	0.00141	0.0724	0.00304	0.0546	0.0437	0.0770
NH_4mid	−0.985	0.129	−0.957	0.0990	−0.986	0.103
NH_4sub	−1.73	0.0983	−1.70	0.0668	−0.986	0.103
	$\hat{\beta}_{2,\mathrm{hyb}}$	se $\left(\hat{\beta}_{2,\mathrm{hyb}}\right)$	$\hat{\beta}_{2,\mathrm{MB}}$	se $\left(\hat{\beta}_{2,\mathrm{MB}}\right)$	$\hat{b}_{2,\mathrm{GLS}}$	se $\left(\hat{b}_{2,\mathrm{GLS}}\right)$
pHsub	−0.0428	0.0183	−0.0473	0.0184	−0.0497	0.0166

Last row: estimates of the linear trend of the spatial mean.

model means were not constant, but a linear function of time. For NH_4 at all three depths the time-series of hybrid predictions are smooth lines, passing nearly through the design-based estimated means at the sampling times. The time-series of model-based predicted spatial means are a little bit less smooth. The hybrid predictions of the spatial means in the observation years were in most cases about equal to the design-based estimated means. The differences between the model-based predicted spatial means and the design-based estimated means were occasionally somewhat larger, for instance for NH_4 in the middle soil horizon at 2004.

Figures 5–8 show maps of the model-based predictions of pH and NH_4 in the subsoil at the observation times and midway between them (September 2004–2007) and their kriging variances, respectively. The pH maps clearly show the temporal trend of the spatial means. The spatial patterns of pH were very persistent, whereas for NH_4 the spatial patterns clearly changed over time. The strong persistence of the spatial patterns for pH can be explained by the very weak contribution of the geometric anisotropy variogram to the total variation. If this contribution had been zero, the patterns would have been exactly equal, only the levels would have been different. Cross-validation of the predictions at points showed that the fully model-based predictions are nearly unbiased (negligibly small mean error) and that the kriging variance is an approximately unbiased estimate of the prediction error variance (Table 4). The mean standardized squared prediction error (MSSE) was close to the desired value of one for all six variables, showing that the computed prediction error variance is, on average, a good quantification of our uncertainty about the predictions. This was a bit surprising as the number of observations used to calibrate the space-time model was only 80. An under-estimation of the prediction error variance could have been expected as the uncertainty about the model parameters is not accounted for in the computed variance.

General discussion and conclusions

For statistical space-time mapping, calibration of a space-time model is required. To predict a time-series of spatial means, either a space-time model or a time-series model of spatial means is required. The case study demonstrated that such space-time models can also be beneficial when the space-time mean is predicted because they lead to a reduction in the uncertainty of such a prediction. With a model-based and a hybrid-sampling approach it is important to validate the model. It is necessary to confirm that the assumptions underlying these models are appropriate. Validation of predictions at points in space-time using a space-time model can be done by computing, for instance, summary statistics of the standardized squared prediction errors. In the case study the mean of this error, MSSE, was surprisingly close to the desirable value of 1, despite the small number of observations (80). In compliance monitoring, discussions on the validity of the estimated space-time mean can be avoided by design-based inference, requiring selection of both times and locations by probability sampling.

One might argue that comparing the standard errors of the model-based, hybrid and design-based predictors/estimators is like comparing cheese and chalk. The sources of randomness accounted for by the standard errors differ between the statistical approaches. In the design-based approach this is the random selection of sampling units, whereas in the model-based approach this is the random term in the model, reflecting our imperfect knowledge about the variation in space and time of the soil property of interest. In the hybrid approach both sources of random selection of locations and uncertainty about the temporal variation of spatial means are combined. Despite this, I think it is still useful to compare these

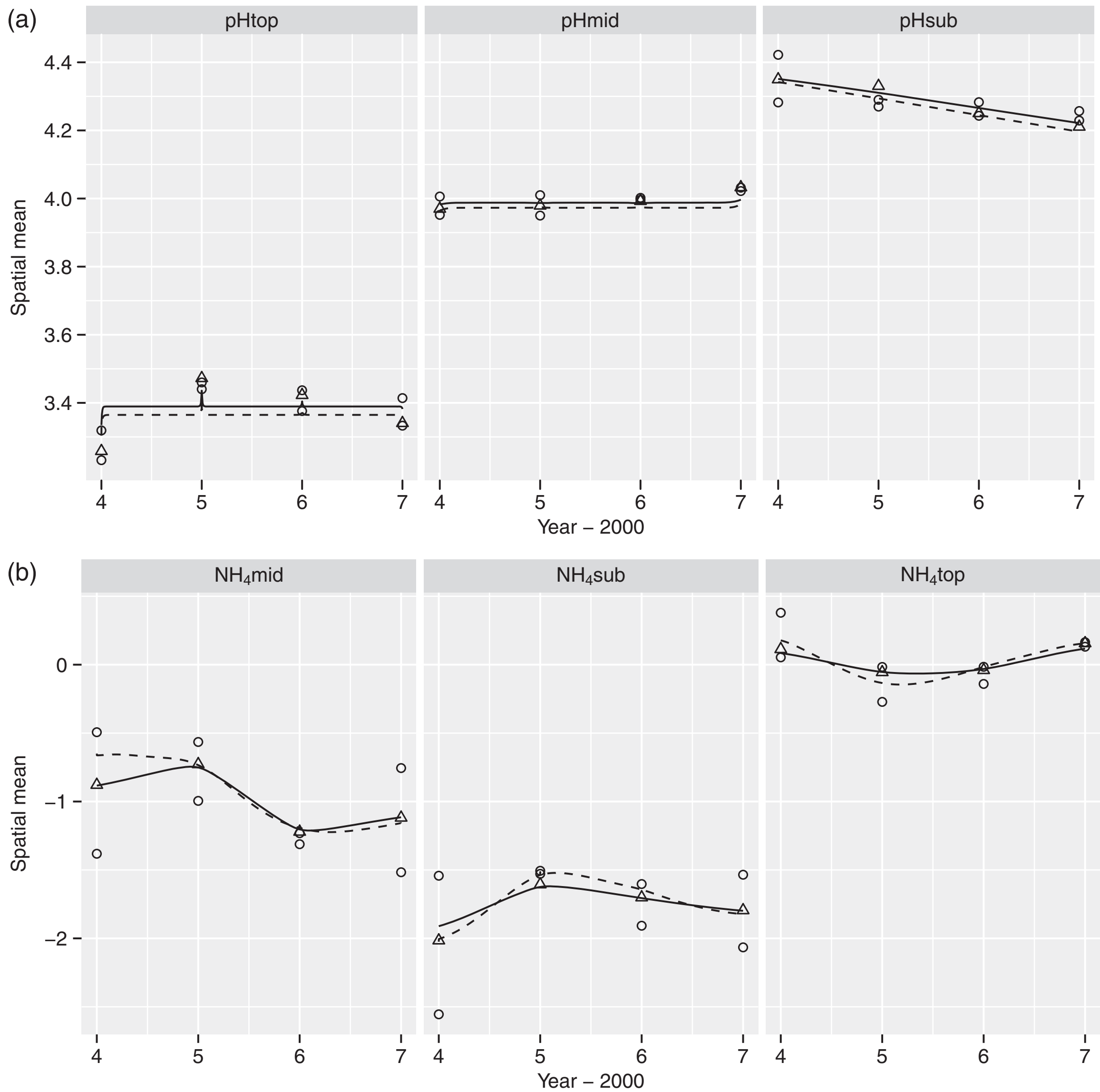

Figure 4 Time-series of hybrid (solid line) and model-based (dashed line) predictions of spatial means of pH (a) and log(NH_4) (b) in topsoil (top), the middle soil horizon (mid) and subsoil (sub). Open circles, elementary estimates of the spatial means; triangles, design-based, GLS estimates of the spatial means.

standard errors, as in some way these all express our uncertainty about the parameter of interest.

The negligible difference in estimated space-time mean between the design-based and hybrid predictor on the one hand and the model-based predictor on the other hand in the case study, is at least partly due to the self-weighting spatial sampling design. This means that the inclusion density of the sampling locations is constant throughout the study area. There are no differences in spatial sampling density. I expect larger differences between the design-based and hybrid predictors on the one hand and the model-based predictor on the other when the inclusion densities differ strongly, as for instance in stratified random sampling with disproportional allocation (different sampling densities in the strata). The design-based and hybrid predictor correct for the selection bias, but there is no guarantee that the model-based predictor does also.

With non-probability sampling of both locations and times there is no other option than calibrating a full space-time model, and to use this space-time variogram in fully model-based prediction. Therefore, for soil monitoring the selection of sampling locations by probability sampling is a safe choice as it leads to flexibility with regard to the statistical inference. Probability samples of locations can also be used in fully model-based prediction of the global parameters of interest and in model-based space-time mapping. Probability sampling for model-based inference has an important advantage over non-probability sampling. When a self-weighting sampling design is implemented, this ensures that the predictor is not affected by selection bias.

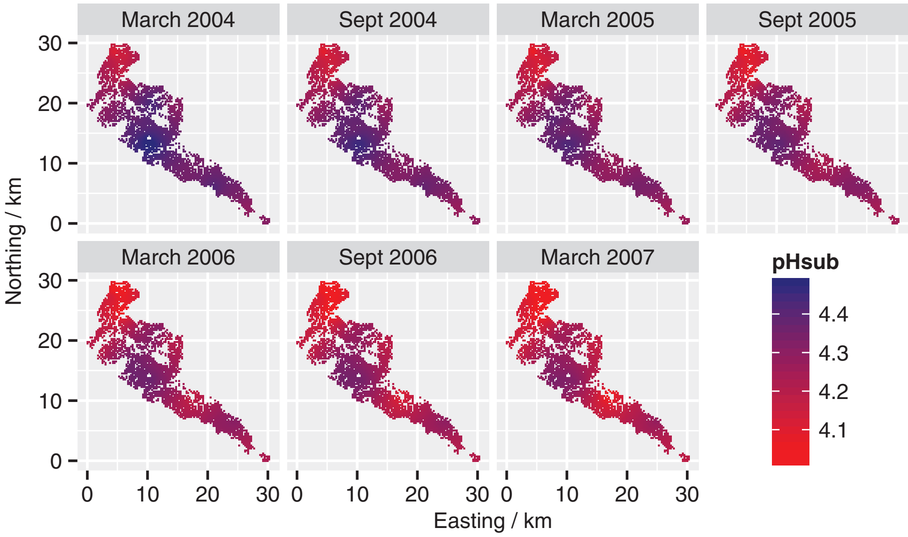

Figure 5 Model-based predictions of pH in the subsoil, as obtained with the space-time model.

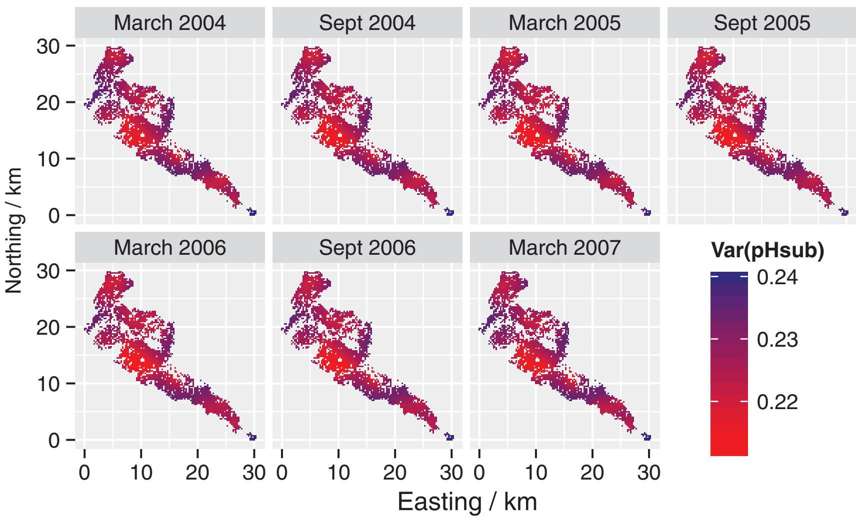

Figure 6 Kriging variance of model-based predictions of pH in the subsoil.

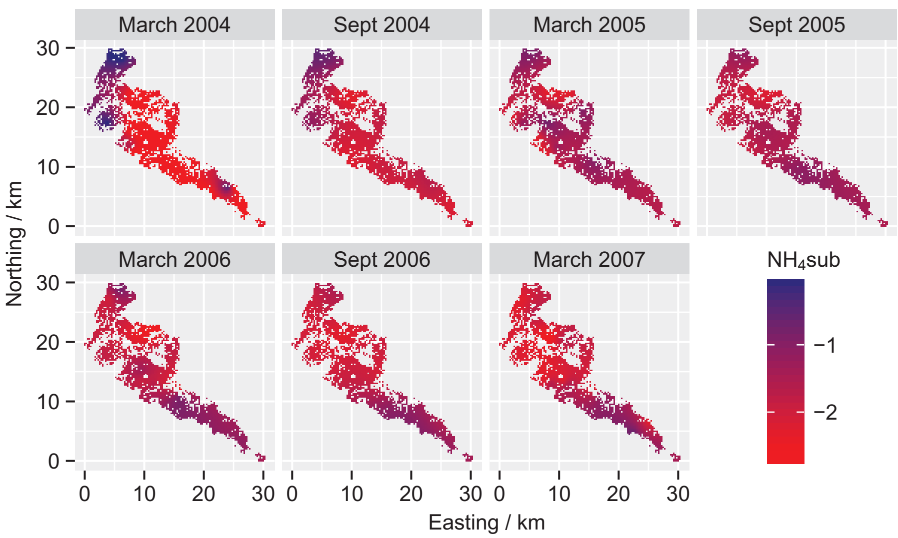

Figure 7 Model-based predictions of log(NH_4) in the subsoil, as obtained with the space-time model.

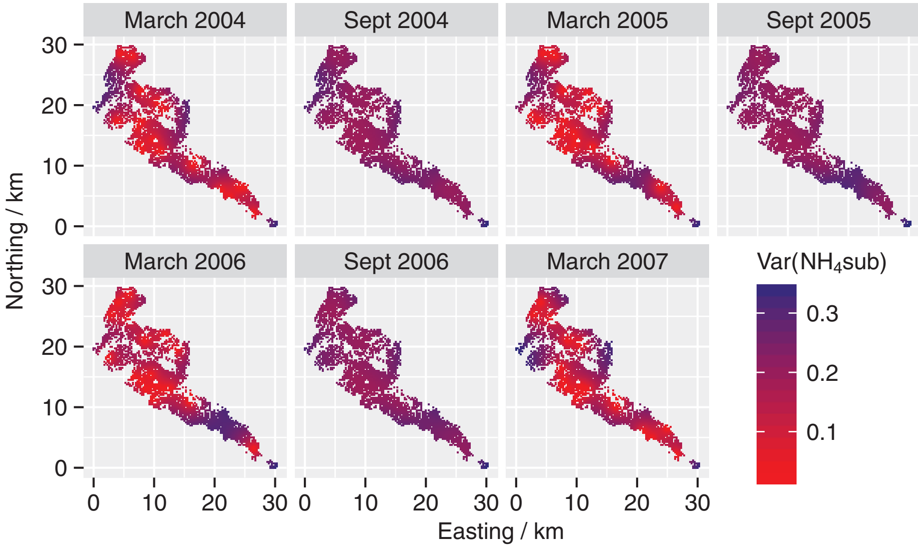

Figure 8 Kriging variance of model-based predictions of $\log(NH_4)$ in the subsoil.

Table 4 Cross-validation statistics of the fully model-based predictions at points

	ME	MAE	RMSE	MSSE
pHtop	-5.12×10^{-4}	0.202	0.264	1.002
pHmid	3.68×10^{-3}	0.181	0.224	1.010
pHsub	-1.42×10^{-3}	0.128	0.15	0.989
NH_4top	-9.39×10^{-3}	0.438	0.602	1.046
NH_4mid	-8.64×10^{-3}	0.657	0.800	1.018
NH_4sub	8.24×10^{-3}	0.538	0.665	0.992

ME, mean error; MAE, mean absolute error; RMSE, root mean squared error; MSSE, mean standardized squared error.

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