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The use of near infrared (NIR) spectroscopy to improve soil mapping at the farm scale

Johanna Wetterlind, Bo Stenberg and Mats Söderström

Division of Precision Agriculture, Department of Soil Science, SLU. PO Box 234, SE-532 23 Skara Sweden

bo.stenberg@mv.slu.se

Abstract

The creation of fine resolution soil maps is hampered by the increasing costs associated with conventional laboratory analyses of soil. In this study, near infrared (NIR) reflectance spectroscopy was used to reduce the number of conventional soil analyses required by the use of calibration models at the farm scale. Soil electrical conductivity and mid infrared (MIR) reflection from a satellite image were used and compared as ancillary data to guide the targeting of soil sampling. About 150 targeted samples were taken over a 97 hectare farm (approximately 1.5 samples per hectare) for each type of ancillary data. A sub-set of 25 samples was selected from each of the targeted data sets (150 points) to measure clay and soil organic matter (SOM) contents for calibration with NIR. For the remaining 125 samples only their NIR-spectra needed to be determined. The NIR calibration models for both SOM and clay contents resulted in predictions with small errors. Maps derived from the calibrated data were compared with a map based on 0.5 samples per hectare representing a conventional farm-scale soil map. The maps derived from the NIR-calibrated data are promising, and the potential for developing a cost-effective strategy to map soil from NIR-calibrated data at the farm-scale is considerable.

Keywords: Near infrared (NIR) spectroscopy · Soil electrical conductivity · Partial least squares regression · Satellite imagery · Mid infrared reflection (MIR)

Introduction

The most common sample density for soil mapping on farms in Sweden is approximately one sample per hectare, but some of the more expensive analyses, such as texture and soil organic matter (SOM), are generally done on every second sample only (0.5 samples per hectare) or not determined at all. Precision agriculture, however, requires a more detailed resolution of the variation in certain soil properties for site-specific liming or fertilizer application. In addition, if geostatistical techniques are to be applied, these should be based on a sufficient number of observations. For example, at least 100 observations have been recommended as a minimum to calculate a reliable variogram (Webster and Oliver, 1992). Kriging also requires spatially dependent data. Thus, to produce soil maps from kriged estimates for decision-support in precision agriculture a sampling intensity greater than that usually used for farm surveys is likely to be needed. It is not possible to specify a universally valid sampling density needed for a satisfactory resolution as the optimum value depends on the degree of spatial variation at the specific site, and also on the sample support (Oliver et al., 1997). A strategy to increase the accuracy of estimates from

more sparsely sampled soil data is the use of ancillary information that has been recorded intensively, and that is correlated with the soil properties of interest. Such data could come from combine harvesters equipped with yield monitors, devices that measure soil electrical conductivity (EC_a), detailed topographical surveys or possibly scans of biomass by tractor-mounted remote sensing equipment. Methods such as co-kriging, kriging with external drift, regression kriging or simple regression (e.g. Baxter and Oliver, 2005; Bhatti et al., 1991; Delin and Söderström, 2003; McBratney et al., 2000) can be used with such ancillary data to improve the accuracy of estimates, but they still require adequate data for the principle variable, which is seldom the case in practice. Therefore, it is important to find methods that increase the number of observations without increasing the cost.

The NIR spectroscopy techniques have the advantage of limited sample preparation and the potential to analyse many properties simultaneously. Several studies show the potential of NIR to predict clay (Bendor and Banin, 1995; Broge et al., 2004; Chang et al., 2001; Stenberg et al., 2002) and SOM content in soils (Mulla et al., 2001; Chang et al., 2001; Udelhoven et al., 2003). Neither regional (Udelhoven et al., 2003; Stenberg et al., 2002) nor national calibration models (Sørensen and Dalsgaard, 2005) for SOM seem to perform very well; possibly because of the large variation in other soil properties e.g. soil texture and mineralogy. Within-field calibrations appear to overcome such problems (Reeves et al. 1999; Stenberg et al. 2002). In addition, inaccuracies associated with the standardization of sample pre-treatment and differences in laboratory methods are reduced by local calibrations, as all samples can be analyzed in one batch.

The aim of this study was to use NIR-spectroscopy to reduce the number of samples analyzed by conventional laboratory methods by calibrating NIR for clay and SOM contents on a 97 ha farm. Additional aims were the development of strategies to distribute samples to resolve as much of the variation as possible with a limited sample size, and to select reference samples for the NIR calibrations. Electrical conductivity and mid infrared reflection (MIR) from a SPOT satellite image were used as ancillary data to target soil sampling and the selection of calibration samples. In this study we compared estimates for clay and SOM content based on NIR calibrations from data with 1.5 samples per hectare with traditionally analysed clay and SOM content at 0.5 samples per hectare representing conventional farm-scale soil mapping.

Materials and methods

Site and sampling

The study was conducted over an area of 97 ha comprising five adjacent fields on Hacksta farm, in the south-east of Sweden about 70 km north-west of Stockholm (59°33' N, 17°02' E). The soil varies from loam to clay with only small topographical differences. The main crops were cereals, and no farmyard manure had been applied for many years.

Soil samples from the topsoil (0-20 cm) were taken in the autumn of 2005. At each sampling site, 20 sub-samples within a six meter radius were bulked to form a composite

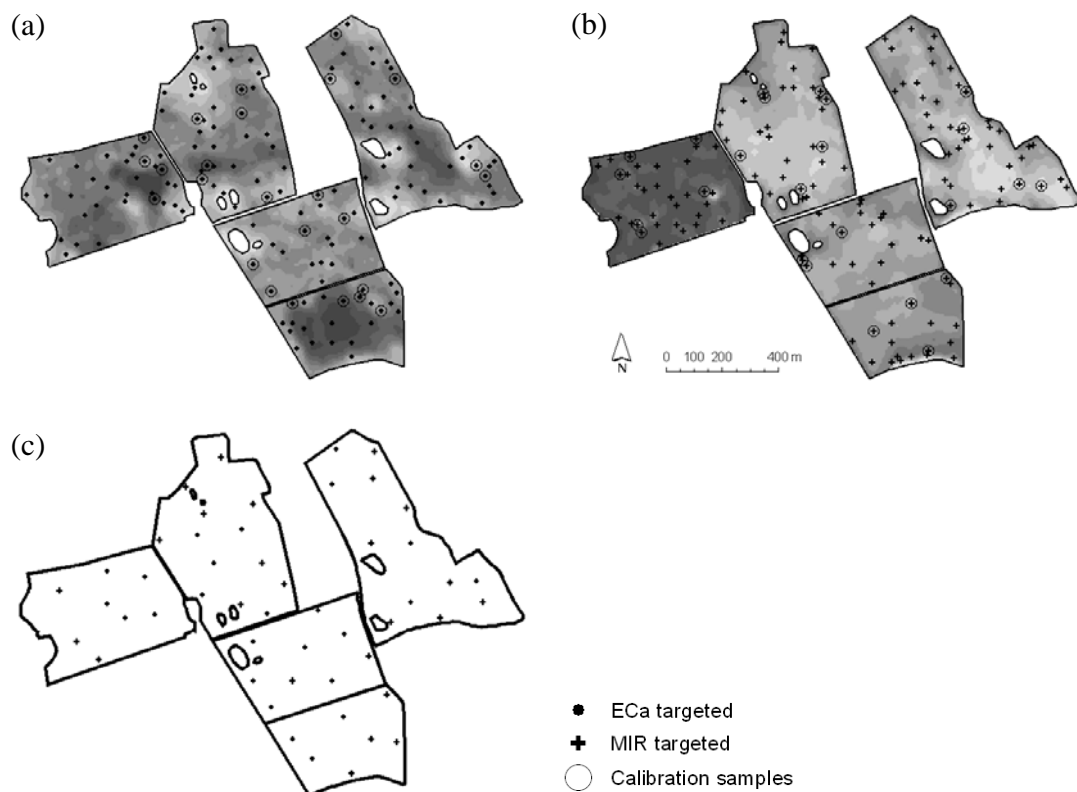


Figure 1. The three sampling strategies: Targeted samples and NIR calibration samples selected according to: (a) EC_a measurements, (b) MIR from a SPOT satellite image and (c) samples distributed according to a conventional sampling strategy with 0.5 samples per hectares (conventional sampling density). Large values for MIR and EC_a measurements are shown in dark gray and small values in light gray.

sample. One and a half composite samples per hectare were taken from the fields; their locations were targeted according to EC_a or MIR values and spaced to resolve as much of the variation as possible (Fig. 1a and b). The EC_a was recorded with an EM38 (Geonics Ltd., Mississauga, Ontario, Canada, www.geonics.com) at an interval of about 10 m along transects parallel to the tramlines which were 24-m apart. The MIR data (1580-1750 nm) from a SPOT 5 scene (10 m spatial resolution) recorded on 21st March 2003 was obtained from the Swedish Land Survey. The ground was free from snow and there was no interference from clouds. The crops in 2003 were winter cereals for all fields except for the eastern-most one.

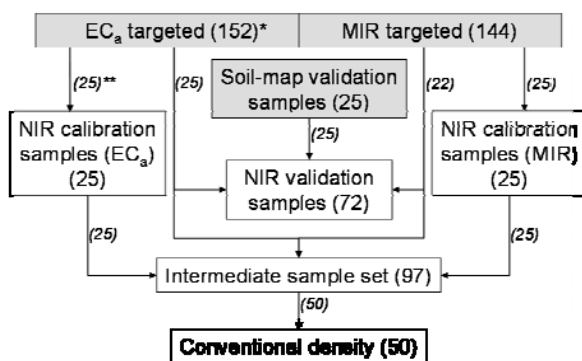
The strategy for targeted sampling adopted here was based on the principle that interpolation of an ancillary variable (in this study EC_a and MIR) measured at the selected sampling sites, should result in a map as similar as possible to one based on intensive sampling of the same ancillary variable. An automated method was used, described by Olsson and Söderström (2004) that minimizes the differences between these maps. In addition, it fulfils some other criteria, such as fairly even spatial coverage of sites and sampling no closer than 15 m to field borders and 12 m to locations already selected. This procedure of stratified, directed sampling includes the following steps:

creation of a map of the ancillary data, subdivision of the fields into 1.5 ha cells and an iterative process that inserted sampling sites successively in order to reach the desired number of samples or sampling density. The selection of sampling sites is based on the degree of variation in the ancillary map. This resulted in 152 targeted soil samples based on EC_a and 144 based on MIR.

Soil analyses

All soil analyses were done on the air-dried soil crushed to pass a 2 mm sieve. The NIR spectra were determined on all samples using a FieldSpec Pro FR scanning instrument (Analytical Spectral Devices Inc., Boulder, CO, USA, www.asdi.com). The instrument was equipped with a bare optic fibre connected to a probe with a 20 W Al-coated halogen tungsten light source placed 7 cm over the sample resulting in a field of view of ~7.5 cm². The spectral range was 350–2500 nm in 1.4–2.0 nm intervals with a band width of 3–10 nm. Both the NIR region between 780 and 2500 nm and the region from 450 to 2500 nm including visible light (VisNIR) were used. The shortest wavelengths were excluded because of excessive noise. Reflectance spectra from two sub-samples of each soil sample were recorded. Each spectrum comprised 100 averaged sub-spectra from a rotating sample, covering a total sample area of about 50 cm².

Twenty five samples from each of the EC_a and MIR targeted soil sampling schemes were selected for determining clay and total C contents (Fig. 1). The selections were done by choosing the first 25 of the samples selected by the automated sampling procedure described above. These two data sets (one for each sampling scheme) were used in the NIR calibrations and are hereafter referred to as NIR calibration data sets (Fig. 2). Total C was analysed by dry combustion at 1250 °C with a LECO[®] CNS-2000 analyser (LECO Corporation, St. Joseph, MI, USA, www.leco.com). As no carbonate was detected in these soil samples total C was transformed to SOM by multiplying with a factor of 1.724. Clay content was analysed by a sedimentation method modified from Gee and Bauder (1986).



* Numbers in parentheses are the number of samples in the sample sets.

** Italic numbers in parentheses are number of samples transferred to the next sample set

Figure 2. Diagram showing the relationship between the different soil sample sets. The grey boxes include all the samples taken from the fields. All samples in the EC_a and MIR targeted sample sets were measured with NIR. The samples in the other sample sets were in addition analysed for clay and SOM content by traditional laboratory soil analyses.

Analysis of NIR spectra

The registered NIR spectra from replicates were averaged and transformed to absorbance by $\log(1/\text{reflectance})$. The NIR data analysis and statistics were done with Unscrambler 9.7 (CAMO PROCESS AS, Oslo, Norway). To reduce light scatter effects influencing the baseline, enhance weak signals and reduce noise, each NIR-spectrum was transformed and smoothed by a first-order, eight points, Savitzky-Golay derivative (Savitzky and Golay 1964).

Spectra for the NIR region (780-2500 nm) and for VisNIR, which also includes visible light (450-2500 nm), were calibrated against SOM and clay content by the multivariate linear regression technique partial least squares (PLS) (Martens and Naes, 1989) using samples in the two NIR calibration data sets. Cross-validation through a leave-one-out procedure was used to optimize the calibrations. The prediction models produced in this way were validated on an independent set of 72 randomly selected samples (NIR validation data set) not included in either of the calibration samples (Fig. 2). The validations were evaluated by the r^2 -value of the relation between the NIR-estimate of the soil property and the reference measurement, the root mean squared error of prediction (RMSEP), the ratio of performance to deviation (RPD) (standard deviation (s.d.) divided by RMSEP) and by the range to error ratio (RER) (range divided by RMSEP). The best prediction models were then used to predict the clay and SOM content of the remaining soil samples (127 from the EC_a targeted samples and 119 from the MIR ones).

Conventional sampling density

To resemble a conventional sampling strategy a new soil data set of 97 samples was created by merging the 50 calibration samples (25 from the EC_a targeted and 25 from MIR targeted samples) with 47 of the reference samples in the NIR-validation data set that were not included in the soil-map validation sample set (Fig. 2). From this intermediate sample set, 50 sites were selected as close to a regular grid as possible representing a sample point density of about 0.5 samples per hectare (conventional density data set) (Fig. 1c). These 50 samples were all analysed for clay and SOM content by the laboratory methods described above.

Soil maps

Experimental variograms for clay and SOM content were computed from the 50 conventional density samples (analysed by traditional laboratory methods) as well as from the NIR predicted clay and SOM contents of the EC_a and MIR targeted samples, respectively. The experimental variograms were computed and modelled using the geostatistical software GS⁺ 5.1 (Gamma Design software, www.gammadesign.com). The model parameters were then used for interpolation by ordinary block kriging to a 5-m grid with the GIS-software ArcGIS 9.1 (ESRI, www.esri.com) and the Geostatistical and Spatial Analyst extensions. For validation of the soil maps, we used 25 randomly selected samples, not included in either the EC_a or the MIR targeted data sets, that were analysed for clay and SOM content by traditional laboratory measurements (soil-map validation data set) (Fig. 2). The validation was done by interpolating the values for all data sets at the locations of the validation samples. The interpolated clay and SOM maps from the

three strategies (EC_a and MIR targeted samples and the conventional density samples) were compared by calculating the difference between the maps on a 5-m grid.

Results

Table 1 gives selected descriptive statistics for SOM and clay content analysed by traditional laboratory methods for the different calibration and validation data sets, and for samples at the conventional sampling density. There were only small differences in mean SOM and clay contents between the data sets. It is noticeable, however, that none of the NIR calibration data sets nor the data at the conventional density included samples with as large an SOM content as the validation ones. Only NIR calibration samples selected by the EC_a method had SOM contents over 7%. The data at the conventional density have a considerably smaller standard deviation than the other selected data, suggesting that it does not fully represent the total SOM content variation present. The smallest range in clay content is for the MIR calibration data and the soil-map validation data. The correlation between SOM and clay content is weak, the coefficient of determination $r^2 = 0.27$.

Table 2 shows the validation results for the NIR and VisNIR calibrations when predicting SOM and clay content of the 72 NIR-validation samples. There are small differences only between the methods. The predictions of SOM content are better than those of clay according to the RPD and RER values regardless of calibration data set and spectral range. In general, exclusion of the visible bands slightly improves the predictions, except

Table 1. Results from laboratory analysis of clay and SOM contents by traditional methods for the different data sets

	n	Clay (%)				SOM (%)			
		Mean	Min.	Max.	s.d.	Mean	Min.	Max.	s.d.
NIR calibration data set (EC_a)	25	49	22	62	7.9	4.1	2.4	7.1	1.09
NIR calibration data set (MIR)	25	47	32	62	8.3	3.9	2.3	6.0	0.96
Conventional density data set*	50	47	25	62	8.1	3.8	2.3	5.8	0.89
NIR validation data set	72	47	25	66	8.7	3.9	2.4	7.7	0.97
Soil-map validation data set	25	48	34	62	8.3	3.9	2.5	7.7	1.16

* 0.5 samples hectares.

n is number of samples

s.d. is standard deviation

Table 2. Validation of NIR and VisNIR calibration models for the prediction of SOM and clay content using the 25 NIR calibration samples selected according to EC_a or MIR.

	Clay				SOM			
	r^2	RMSEP	RPD	RER	r^2	RMSEP	RPD	RER
EC_{aNIR}	0.80	3.9	2.2	10.5	0.89	0.32	3.0	16.6
$EC_{aVisNIR}$	0.81	3.7	2.3	11.0	0.89	0.32	3.0	16.4
MIR_{NIR}	0.81	3.8	2.3	10.9	0.88	0.33	2.9	15.9
MIR_{VisNIR}	0.74	4.4	2.0	9.4	0.87	0.35	2.8	15.4

Validations were done with the 72 independent NIR-validation samples

for the prediction of clay by the EC_a NIR calibration data set. Therefore, the VisNIR calibration was used for predicting clay content with the EC_a targeted samples in all subsequent analyses, whereas the NIR calibrations were used for all the other predictions.

The experimental variograms and fitted models are shown in Fig. 3 and the model parameters used for kriging are given in Table 3. Note that the variograms for the data at the conventional density are based on only 50 samples and are likely to be unreliable. For example, the first points of the experimental variograms are based on few sample pairs. The effective ranges for the conventional data are two to three times longer for both clay and SOM, compared with ranges for the MIR and EC_a targeted data, respectively. This indicates that 0.5 samples per hectare probably fails to resolve the more detailed variation in the soil properties. Nevertheless, the overall appearance of the resulting SOM maps is

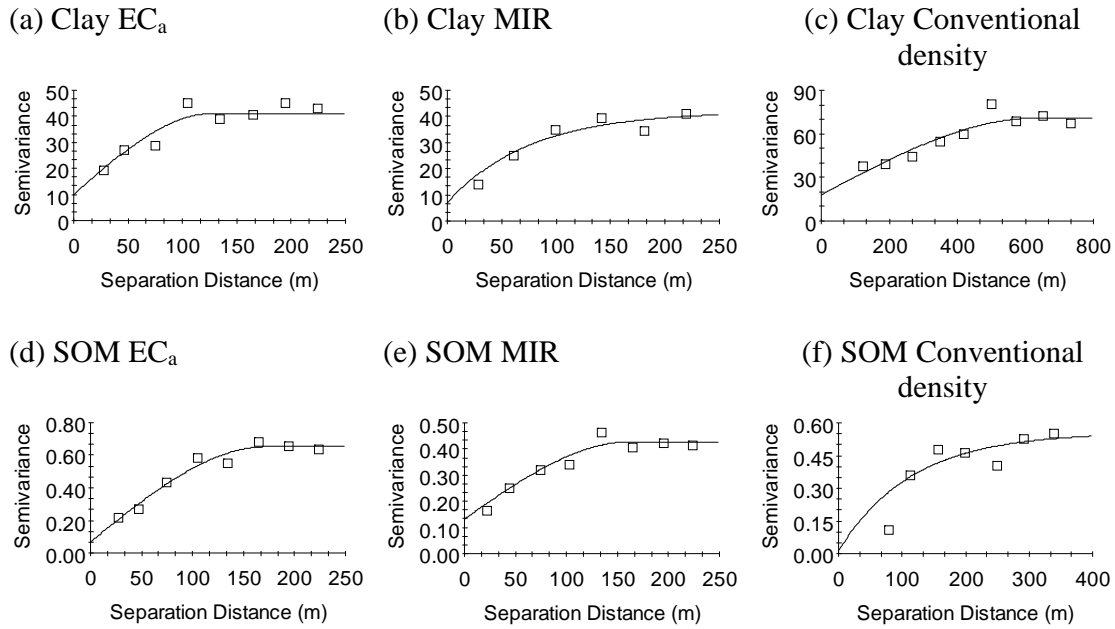


Figure 3. Variograms for the different datasets

Table 3. Model parameters for the fitted variograms in Figure 4.

	Model	c_0	c_0+c	a (m)
Clay EC _a	Spherical	10	41	127
Clay MIR	Exponential	7	42	228
Clay Conventional density	Spherical	18	71	638
SOM EC _a	Spherical	0.069	0.653	173
SOM MIR	Spherical	0.133	0.428	163
SOM Conventional density	Exponential	0.013	0.556	345

c_0 = nugget variance

c_0+c = sill

a = the range for the spherical model and the effective range ($a=3r$) for the exponential model, where r is the distance parameter.

fairly similar in spite of the sampling strategy (Fig. 4). However, the map of clay based on the conventional data set (Fig. 5c) lacks details and shows only the general pattern of variation.

Figure 6 shows maps of the differences between the interpolated maps of the MIR and EC_a targeted samples. Table 4 gives descriptive statistics of the differences between the interpolated values of SOM and clay from the three strategies. For clay, the maps derived from the EC_a and MIR targeted samples (Fig. 4a and b) are fairly similar, according to the distribution in difference classes (Table 4), whereas that based on the conventional density (Fig. 4c) is somewhat different. For SOM content, on the other hand, the map derived from the EC_a targeted samples deviates from the other two (Table 4).

The validation results of the SOM and clay estimates derived from the different sampling strategies according to the 25 soil-map validation samples are given in Table 5. For SOM, the EC_a strategy shows a clear improvement in the accuracy of the estimates from the validation statistics compared to those from both the conventional density and the MIR strategies. However, both the EC_a and MIR targeted samples resulted in more detailed maps and were more accurate according to the validation results than the map from the

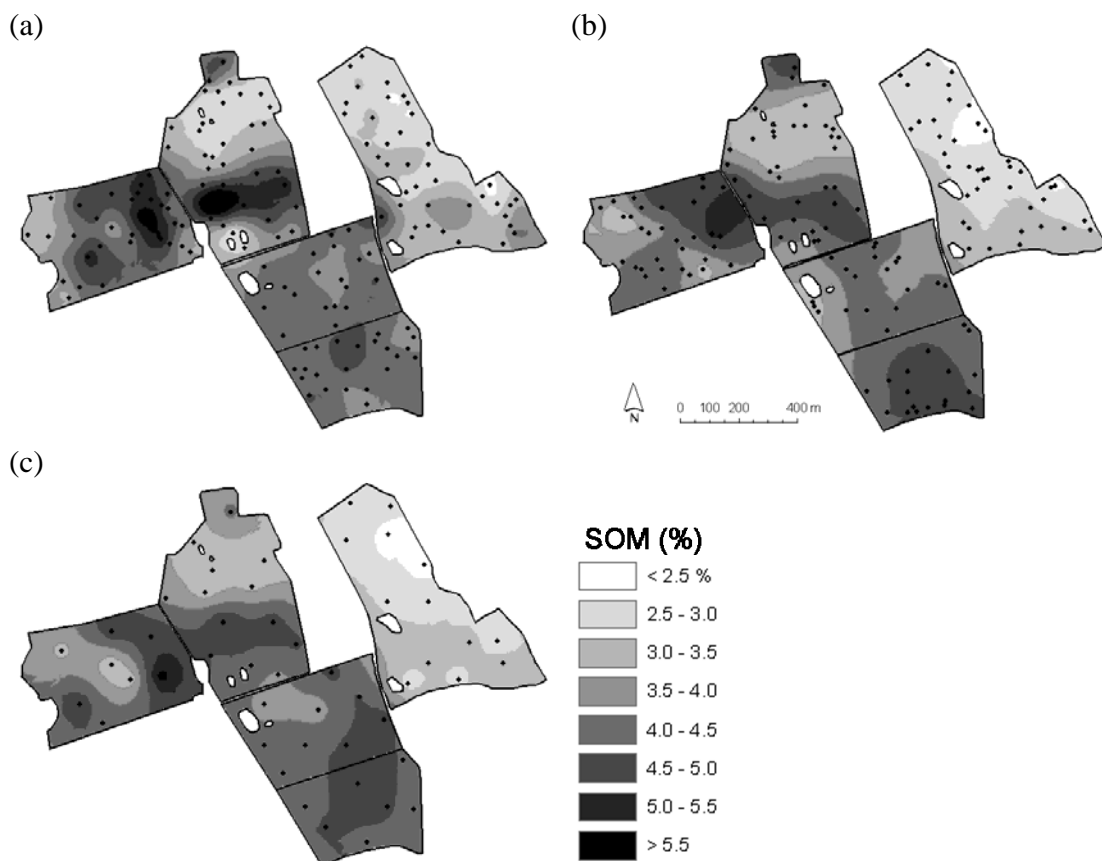


Figure 4. The NIR predicted SOM content interpolated from: (a) EC_a targeted soil sample data and (b) MIR targeted soil sample data. (c) Traditionally analysed SOM content interpolated from 50 samples that represent conventional sampling density with 0.5 samples per hectares.

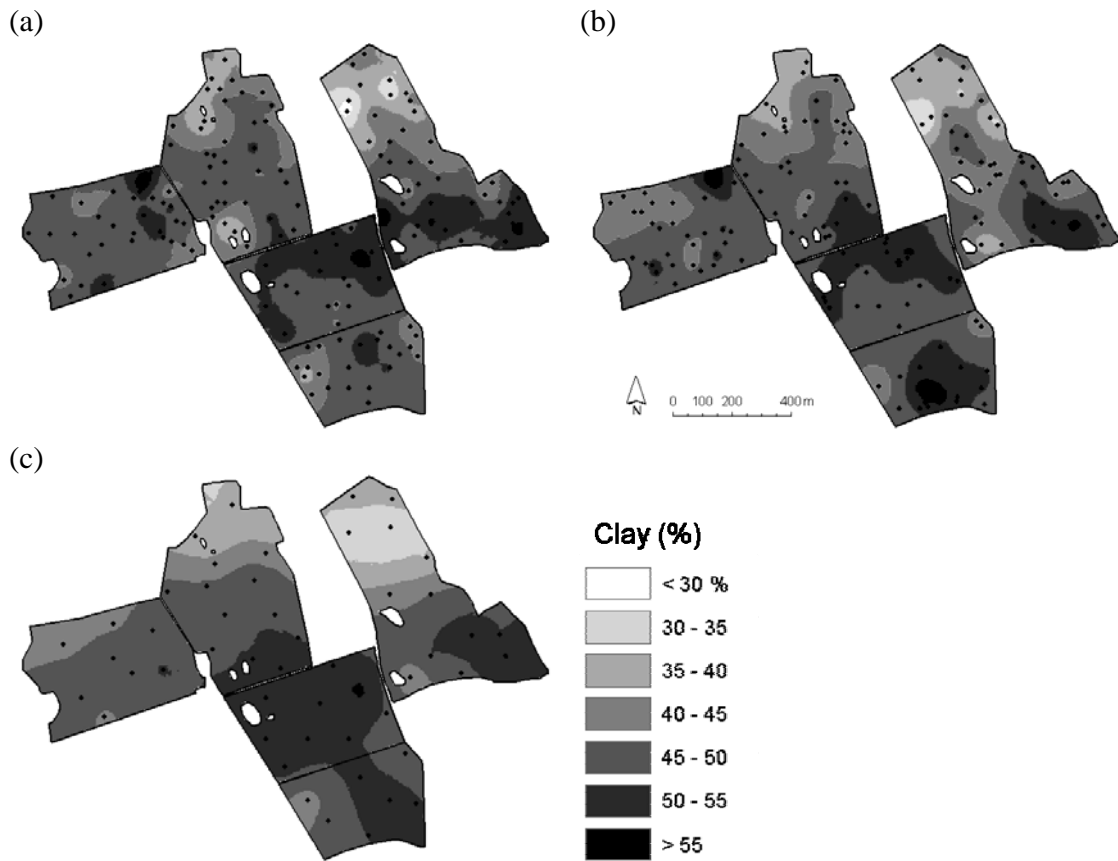


Figure 5. The NIR predicted clay content from: (a) EC_a targeted soil sample data and (b) MIR targeted soil sample data. (c) Traditionally analysed clay content interpolated from 50 samples that represent the conventional sampling density with 0.5 samples per hectares.

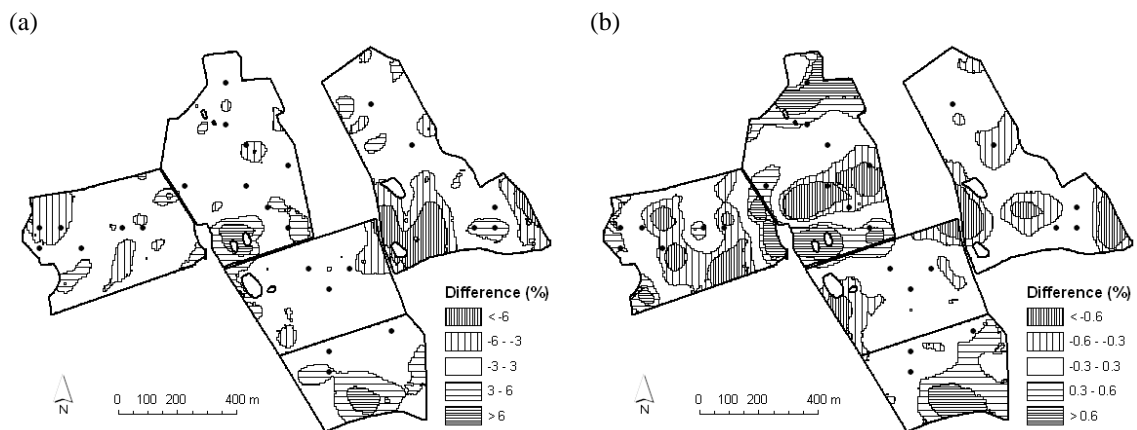


Figure 6. Maps of the differences between the interpolated maps of the MIR and EC_a targeted sample data, (a) clay MIR - clay EC_a, and (b) SOM MIR - SOM EC_a.

data at the conventional density. For clay content, there were minor differences only between the performances of the different methods (Table 5).

Table 4. Differences in percentage points between the three soil maps for clay and SOM content.

	Min	Max	Mean	s.d.	% in class ^a		
					1 ¹	2 ²	3 ³
Clay							
Conventional density - EC _a targeted	-14	14	0.2	3.3	61	30	9
Conventional density - MIR targeted	-14	10	0.4	3.2	66	28	6
MIR targeted - EC _a targeted	-12	11	-0.2	2.9	74	21	6
SOM							
Conventional density - EC _a targeted	-2.1	1.9	0.0	0.4	56	28	16
Conventional density - MIR targeted	-1.1	1.1	0.1	0.3	76	22	2
MIR targeted - EC _a targeted	-2.2	1.6	-0.1	0.4	56	28	16

^aPercentage of total area in one out of three classes:

¹ no difference (absolute difference less than 3 or 0.3 percentage units for clay and SOM, respectively)

² small difference (absolute difference of 3-6 or 0.3-0.6 percentage units for clay and SOM, respectively)

³ large difference (absolute difference over 6 or 0.6 percentage units for clay and SOM, respectively).

Table 5. Validation of soil maps for SOM and clay content derived from NIR predictions using either the EC_a or MIR targeted samples compared to maps derived from traditionally analyzed SOM and clay content in a 0.5 sample per hectare grid (conventional sampling density).

	n	Clay				SOM			
		R ²	RMSEP	RPD	RER	R ²	RMSEP	RPD	RER
EC _a targeted	152	0.60	5.6	1.4	7.2	0.72	0.64	1.6	7.6
MIR targeted	144	0.53	5.5	1.5	7.3	0.44	0.86	1.2	5.7
Conventional density	50	0.51	5.7	1.4	7.0	0.36	0.94	1.1	5.2

n is the number of samples used for interpolation

Validations were done with the 25 independent soil-map validation samples

Discussion

In general, the validation statistics indicate that the NIR calibrations for both SOM and clay are reliable. The RMSEP values of between 3 and 4 for the prediction of clay content (Table 2) are comparable to those for other Swedish and Danish calibrations (Stenberg et al., 2002; Sørensen and Dalsgaard, 2005). In spite of the difficulty of calibrating general prediction models for SOM, the validation statistics for this relatively small area were good (Table 2) and are comparable with, for example, those from a Swedish farm of 60 ha with a clay content of between 30 and 40% (Wetterlind et al., 2006), a 13 ha field in Germany (Udelhoven et al., 2003) and an agricultural district in NSW, Australia (Islam et al., 2003). Including the visible range of the spectra in the calibrations had little effect, although it improved the prediction of clay with the EC_a targeted samples to some extent and it has been beneficial in some earlier studies (Fystro, 2002; Islam et al., 2003). Stenberg et al., (2002) and Sørensen and Dalsgaard (2005) found that the calibrations for SOM gave better predictions for soil with a low sand content, therefore, there is also a risk that small scale calibrations such as the ones in this study might be more unreliable on farms dominated by more sandy soil than in the example described here.

In spite of the differences in the ranges of values covered by the calibration data sets (Table 1), the small differences between the performances of the NIR calibrations for

SOM (Table 2) might be because there were few samples with SOM contents exceeding those in the NIR calibration sets. Two samples only, of all the samples analysed by traditional laboratory measurements, exceeded 6% SOM. The sample with the largest SOM content of 7.7% in the NIR validation data set was predicted with half the error by the EC_a NIR calibration compared to the MIR NIR calibration (0.35% and 0.72% SOM, respectively). This difference can probably be explained by the smaller extent of extrapolation by the EC_a NIR calibration. However, this single sample of 7.7 % did not have a great influence on the NIR validation statistics. A similar reasoning could be applied to clay content for which the EC_a NIR calibration data set covered the lower range of values better than the MIR NIR set; four samples only had <32% clay in the NIR validation data set. However, on average these four values were predicted equally well by both NIR calibrations and only the sample with the smallest clay content (25%) was predicted badly.

Validation of the estimates based on the soil map validation samples showed that the conventional sampling approach performed quite well for clay when compared with the other strategies (Table 4). The conventional approach seems to have resolved the main aspects of the variation in clay on this farm. The locations of the validation samples were not optimal, however. For clay, the soil map validation samples did not include areas where there were large differences between the different strategies (Figs. 4 and 6). If there had been some validation samples in these latter areas, the results possibly would have shown larger differences between the three strategies.

The maps of differences (Fig. 6) show that some areas differ markedly between the different sampling strategies for both SOM and clay contents. This is especially the case close to the non-arable areas in the central area where the short-range variation in the soil is considerable. Another area with differences in both soil maps is the southernmost field where the sampling strategies resulted in very different sampling patterns. The MIR targeted samples are located mainly in the southern part of that field, whereas the EC_a strategy resulted in denser sampling in the northern part of the field. The differences between the two sampling strategies are also large between the non-arable areas in the southwestern area of the easternmost field and at the corner of the adjacent field where there is both considerable short-range soil variation and a sparse sampling density for the MIR targeted samples. This indicates that some of the differences between the resulting clay and SOM maps from the MIR and EC_a strategies relate to differences in sample location. This accords with the findings of Frogbrook and Oliver (2000) who showed that sample location had a large effect on the resulting variation described in interpolated maps when the sampling was sparse.

As a consequence of the small differences between the methods of sample selection, practical aspects might determine which method to choose. The MIR-based strategy has the potential to be cost-effective compared to EC_a since the price per hectare of a satellite scene is small. Its benefit, however, depends on the availability of satellite imagery from a suitable time of year when the fields of interest are free from snow, dense vegetation and cloud cover, for example. In addition, it might be necessary to combine several images to create the ancillary data required. The EC_a data are easier to obtain at present at

the farm level. The EC_a targeted sampling also performed slightly better than the MIR targeted sampling in this study, particularly for SOM, therefore, it is reasonable to recommend this approach at present.

Although the various sampling strategies have resulted in somewhat different outcomes, it is important to consider what effects these differences might have on practical agriculture. Clay and SOM are, for example, used to estimate lime requirement where there is a need to raise the soil pH. In our example, if the conventional density approach is compared with the EC_a targeted sampling, the within-field differences in the amount of lime required to increase the soil pH by one unit (estimated according to Gustafsson, 1999) in the two northwestern fields is up to +/- 5 tons per hectare in some parts. Hence, the combined effects of differences in both clay and SOM estimates from the different sampling strategies could be of economic significance.

Recent regulations for receiving certain subsidies from the Swedish Board of Agriculture state that soil texture should be analysed at an intensity of one sample per three hectares. This would be of limited use for precision agriculture unless these traditional analyses are supplemented with NIR measurements from additional samples and used for the calibration of SOM and clay as described in this research.

Conclusion

The results from this study demonstrate that there is considerable potential for developing a cost-effective farm-scale soil mapping strategy for SOM and clay content based on NIR calibrations. The results for the different sampling strategies indicate the importance of covering as large a part of the variation as possible in the calibration samples. This means that the use of only 25 samples for creating the NIR calibration model might not be enough to cover the upper and lower extremes of the distribution for several properties. Moreover, it is important that sample locations cover the spatial variation in the fields. In this study, EC_a was more responsive to the variation in the field and performed slightly better than MIR for targeting soil sample locations and selecting NIR calibration samples.

To make farm-scale soil mapping of SOM and clay content with today's recommended sampling density of one sample per two or three hectares useful for precision agriculture, including NIR measurements of additional samples is a feasible strategy. The additional cost would be limited, especially if samples at a density of one sample per hectare are already taken for other analyses.

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