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Corresponding Author: Dr. G. Cadisch,

Corresponding Author's Institution: Uni Hohenheim

First Author: Juan Guillermo Cobo

Order of Authors: Juan Guillermo Cobo; Gerd Dercon; Tsitsi Yekeye; Lazarus Chapungu; Chengetai Kadzere; Amon Murwira; Robert Delve; G. Cadisch

Abstract: Knowledge of soil spatial variability is important in natural resource management, interpolation and soil sampling design, but requires a considerable amount of geo-referenced data. In this study, mid-infrared spectroscopy in combination with spatial analyses tools is being proposed to facilitate landscape evaluation and monitoring. Mid-infrared spectroscopy

(MIRS) and geostatistics were integrated for evaluating soil spatial structures of three land settlement schemes in Zimbabwe (i.e. communal area, old resettlement and new resettlement; on loamy-sand, sandy-loam and clay soils, respectively). A nested non-aligned design with hierarchical grids of 750, 150 and 30 m resulted in 432 sampling points across all three villages (730-1360 ha). At each point, a composite topsoil sample was taken and analyzed by MIRS. Conventional laboratory analyses on 25-38% of the samples were used for the prediction of concentration values on the remaining samples through the application of MIRS - partial least squares regression models. These models were successful (R2>89) for sand, clay, pH, total C and N, exchangeable Ca, Mg and effective CEC; but not for silt, available P and exchangeable K and Al (R2<82). Minimum sample sizes required to accurately estimate the mean of each soil property in each village were calculated. With regard to locations, fewer samples were needed in the new resettlement area than in the other two areas (e.g. 66 versus 133-473 samples for estimating soil C at 10% error, respectively); regarding parameters, less samples were needed for estimating pH and sand (i.e. 3-52 versus 27-504 samples for the remaining properties, at same error margin). Spatial analyses of soil properties in each village were assessed by constructing standardized isotropic semivariograms, which were usually well described by spherical models. Spatial autocorrelation of most variables was displayed over ranges of 250-695 m. Nugget-to-sill ratios showed that, in general, spatial dependence of soil properties was: new resettlement > old resettlement > communal area; which was potentially attributed to both intrinsic (e.g. texture) and extrinsic (e.g. management) factors. As a new approach, geostatistical analysis was performed using MIRS data directly, after principal component analyses, where the first three components explained 70% of the overall variability. Semivariograms based on these components showed that spatial dependence per village was similar to overall dependence identified from individual soil properties in each area. In fact, the first component (explaining

49% of variation) related well with all soil properties of reference samples (absolute correlation values of 0.55-0.96). This suggested that MIRS data could be directly linked to geostatistics for a broad and quick evaluation of soil spatial variability. It is concluded that integrating MIRS with geostatistical analyses is a cost-effective promising approach, i.e. for soil fertility and carbon sequestration assessments, mapping and monitoring at landscape level.

Integration of mid-infrared spectroscopy and geostatistics in the assessment of soil spatial variability at landscape level

Juan Guillermo Cobo[1,2], Gerd Dercon[1,3], Tsitsi Yekeye[4], Lazarus Chapungu[4], Chengetai Kadzere[2], Amon Murwira[4], Robert Delve[2,5], Georg Cadisch[1,*]

[1] *University of Hohenheim, Institute of Plant Production and Agroecology in the Tropics and Subtropics, 70593 Stuttgart, Germany*

[2] *Tropical Soil Biology and Fertility Institute of the International Center for Tropical Agriculture (TSBF-CIAT), MP 228, Harare, Zimbabwe*

[3] *Present address: Soil and Water Management and Crop Nutrition Subprogramme, Joint FAO/IAEA Division of Nuclear Techniques in Food and Agriculture, Department of Nuclear Sciences and Applications, International Atomic Energy Agency – IAEA, Wagramerstrasse 5 A-1400, Vienna, Austria*

[4] *University of Zimbabwe, Dept. of Geography and Environmental Science, MP 167 Harare, Zimbabwe*

[5] *Present address: Catholic Relief Services, P.O. Box 49675-00100, Nairobi, Kenya*

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* Corresponding author: E-mail address: georg.cadisch@uni-hohenheim.de; Tel.: +49 711 459 22438; Fax: +49 711 459 22304.

Abstract

Knowledge of soil spatial variability is important in natural resource management, interpolation and soil sampling design, but requires a considerable amount of geo-referenced data. In this study, mid-infrared spectroscopy in combination with spatial analyses tools is being proposed to facilitate landscape evaluation and monitoring. Mid-infrared spectroscopy (MIRS) and geostatistics were integrated for evaluating soil spatial structures of three land settlement schemes in Zimbabwe (i.e. communal area, old resettlement and new resettlement; on loamy-sand, sandy-loam and clay soils, respectively). A nested non-aligned design with hierarchical grids of 750, 150 and 30 m resulted in 432 sampling points across all three villages (730-1360 ha). At each point, a composite topsoil sample was taken and analyzed by MIRS. Conventional laboratory analyses on 25-38% of the samples were used for the prediction of concentration values on the remaining samples through the application of MIRS - partial least squares regression models. These models were successful (R^2>0.89) for sand, clay, pH, total C and N, exchangeable Ca, Mg and effective CEC; but not for silt, available P and exchangeable K and Al (R^2<0.82). Minimum sample sizes required to accurately estimate the mean of each soil property in each village were calculated. With regard to locations, fewer samples were needed in the new resettlement area than in the other two areas (e.g. 66 versus 133-473 samples for estimating soil C at 10% error, respectively); regarding parameters, less samples were needed for estimating pH and sand (i.e. 3-52 versus 27-504 samples for the remaining properties, at same error margin). Spatial analyses of soil properties in each village were assessed by constructing standardized isotropic semivariograms, which were usually well described by spherical models. Spatial autocorrelation of most variables was displayed over ranges of 250-695 m. Nugget-to-sill ratios showed that, in general, spatial dependence of soil properties was: new resettlement > old resettlement > communal area; which was potentially attributed to both intrinsic (e.g.

texture) and extrinsic (e.g. management) factors. As a new approach, geostatistical analysis was performed using MIRS data directly, after principal component analyses, where the first three components explained 70% of the overall variability. Semivariograms based on these components showed that spatial dependence per village was similar to overall dependence identified from individual soil properties in each area. In fact, the first component (explaining 49% of variation) related well with all soil properties of reference samples (absolute correlation values of 0.55-0.96). This showed that MIRS data could be directly linked to geostatistics for a broad and quick evaluation of soil spatial variability. It is concluded that integrating MIRS with geostatistical analyses is a cost-effective promising approach, i.e. for soil fertility and carbon sequestration assessments, mapping and monitoring at landscape level.

Key words

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1. Introduction

Soil properties are inherently variable in nature mainly due to pedogenetical factors (e.g. parental material, vegetation, climate), but heterogeneity can be also induced by farmers' management (Dercon et al., 2003; Giller et al., 2006; Samake et al., 2005; Wei et al., 2008; Yemefack et al., 2005). Soil spatial variability can occur over multiple spatial scales, ranging from micro-level (millimeters), to plot level (meters), up to the landscape (kilometers) (Garten Jr. et al., 2007). Thus, soil spatial variability is a function of the different driving factors and spatial scale (in terms of size and resolution), but also of the specific soil property (or process) under evaluation and the spatial domain (location), among others factors (Lin et al., 2005). Recognizing spatial patterns in soils is important as this knowledge can be used for enhancing natural resource management (e.g. Borůvka et al., 2007; Liu et al., 2004; Wang et al., 2009), predicting soil properties at unsampled locations (e.g. Liu et al., 2009; Wei et al., 2008) and improving sampling designs in future agro-ecological studies (e.g. Rossi et al., 2009; Yan and Cai, 2008). In fact, the identification of spatial patterns is the first step to understanding processes in natural and/or managed systems, which are usually characterized by spatial structures due to spatial autocorrelation: i.e. where closer observations are more likely to be similar than by random chance (Fortin et al., 2002). Conventional statistical analyses are not appropriate to identify spatial patterns, as these analyses require the assumption of independence among samples, which is violated when auto-correlated (spatially dependent) data are present (Fortin et al., 2002; Liebhold and Gurevitch, 2002). Thus, since 1950s, alternative methods, so-called spatial statistics, have been developed for dealing with spatial autocorrelation (Fortin et al., 2002). Today several methods for spatial analyses exist (e.g. Geostatistics, Mantel tests, Moran's I, Fractal analyses), while the reasons for the different studies carried out to date on spatial assessments are also diverse (e.g. hypotheses testing, spatial estimation, uncertainty assessment, stochastic simulation, modeling) (Goovaerts, 1999; Liebhold and Gurevitch, 2002). However, a common characteristic is that all methods intent to capture and quantify in one way or another underlying spatial patterns of a specific spatial domain (Liebhold and Gurevitch, 2002; Olea, 2006).

Geostatistics is one of the most used and powerful approaches for evaluating spatial variability of natural resources such as soils (Sauer et al., 2006). However, construction of stable semivariograms (the main tool on which geostatistics is based) requires considerable amount of geo-referenced data (Davidson and Csillag, 2003). Infrared spectroscopy (IRS) has been suggested as a viable option to facilitate access to the extensive soil data required (Cécillon et al., 2009; Shepherd and Walsh, 2007). IRS is able to detect the different molecular vibrations due to the stretching and binding of the different compounds of a sample when illuminated by an infrared beam in the near, NIRS (0.7-2.5 μm), or mid, MIRS (2.5-25 μm) ranges. The result of the measurements is summarized in one spectrum (e.g. wavelength versus absorbance), which is later related by multivariate calibration to known concentration values of the properties of interest (e.g. carbon content, texture) from reference samples. Thus, a mathematical model is created and used later for the prediction of concentration values of these properties in other samples from which IRS data is also available (Conzen, 2003). IRS measurements are therefore not destructive, take few minutes, and one spectra can be related to multiple physical, chemical and biological soil properties (Janik et al., 1998; McBratney et al., 2006). Hence the technique is more rapid and cheaper than conventional laboratory analysis, especially when a large number of samples must be analyzed (Viscarra-Rossel et al., 2006). IRS has the additional advantage that spectral information can be used as an integrative measure of soil quality, and therefore employed as a screening tool of soil conditions (Shepherd and Walsh, 2007). The few existing initiatives in this regard are, however, limited to NIRS. For example, a visible-NIRS (VNIRS) soil fertility index based on ten common soil properties has been developed and applied in Madagascar (Vågen et al., 2006); ordinal logistic regression and classification trees were used to discriminate soil ecological conditions by using biogeochemical data and VNIRS in the USA (Cohen et al., 2006); and in Kenya, Awiti et al. (2008) developed an odds logistic model based on principal components from NIRS for soil fertility classification. Nevertheless, despite its multiple applications, to date IRS has not been widely used, especially for wide-scale purposes and in developing countries (Shepherd and Walsh, 2007).

African regions are usually characterized by food insecurity and poverty, which have been extensively attributed to low soil fertility and soil mining (Sanchez and Leakey, 1997; Vitousek et al., 2009). Therefore, to boost land productivity in the continent, there is an increasing need to develop and apply reliable indicators of land quality at different spatial scales (Cobo et al., 2010). In fact, Shepherd and Walsh (2007) proposed that the successful "combination of infrared spectroscopy and geographic positioning systems will provide one of the most powerful modern tools for agricultural and environmental monitoring and analysis" in the next decade. The present study aims to contribute to this goal, and follows up a study from Cobo et al. (2009), in which three villages as typical cases of three settlement schemes in north-east Zimbabwe (communal area, old resettlement and new resettlement) were evaluated to determine specific cropping strategies, soil fertility investments and land management practices at each site. The assessment, however, was done at plot and farm level, and did not take into account spatial structures of soil properties. Hence, the same three villages of Cobo et al. (2009) were systematically sampled, soils characterized by MIRS, and data subsequently analyzed using conventional statistics and geostatistics tools. The main objectives of this study were: i) to evaluate advantages and disadvantages of using MIRS and geostatistics in the assessment of spatial variability of soils, ii) to test if MIRS can be directly integrated with geostatistics for landscape analyses, and iii) to present recommendations for guiding future sampling designs.

2. Materials and methods

2.1 Description of study sites

The study sites consisted of three villages, selected as typical cases of three small-holder settlement schemes, in the districts of Bindura and Shamva, north-east Zimbabwe (Table 1). The first village, Kanyera, is located in a communal area, covers 730 ha, and is mainly characterized with loamy sand soils of low fertility. The second village, Chomutomora, is located in an old resettlement area (from 1987), covers 780 ha and mostly presents sandy loam soils of low quality. The third village, Hereford farm, is located in a new resettlement area (from 2002), covers 1360 ha and is predominantly characterized by clay soils of relatively higher fertility. All villages are located in natural region II, which covers a region with altitudes of 1000 to 1800 m a.s.l. and unimodal rainfall (April to October) with 750–1000 mm per annum (FAO, 2006). Maize (*Zea maiz* L.) is the main crop planted in the three areas, and farmers have free access to communal grazing areas and woodlands. A full description of the sites' selection and characteristics is provided in Cobo et al. (2009).

2.2. Soil sampling design

A non-aligned block sampling design was used in the three villages to capture both small and large variation over large areas (Urban, 2002). It started with the delineation of the villages' boundaries by using a hand-held GPS. Coordinates were later overlaid in ArcView (www.esri.com) to a Landsat TM image of the zone acquired on 12 June 2006. A buffer of 30 m inside each village boundary was created and later a grid of 750 x 750 m was drawn for each village in ILWIS (www.ilwis.org) (Figure 1a). Next, each main cell of 750 x 750 m was divided in 25 sub-cells of 150 x 150 m, which were subsequently divided once again in 25 micro-cells of 30 x 30 m. All grids were later transferred to ArcView, where 3 sub-cells from each main cell and 3 micro-cells from each sub-cell were randomly selected. This yielded a cluster of 9 micro-cells per main cell (Figure 1b). Finally, the centroids of each selected micro-cells were estimated and included into the GPS to locate these points in the field (Figure 1c). However, as some points were found in unsuitable places for sampling (e.g. road, water way, household) they were re-located (if possible) to alternate locations within cropping fields, grasslands or woodlands, mostly inside a radius of 30 m. In the same way, in cropping fields maize was preferentially chosen for future comparison purposes. At Hereford farm, a part of the woodlands in the southern border was considered to be sacred by the villagers, hence this sector was excluded. 432 points were successfully sampled in the three villages: 159 points in cropping fields (105 in maize, 32 in fallow and 22 in other crops), 163 in woodlands and 110 in grasslands. Maximum sampling distance between points was 5.2 (communal area), 3.8 (old resettlement) and 4.6 km (new resettlement); while minimum sampling distance was 30 m (for all three villages). Sample collection was carried out at the end of the 2006-7 cropping season.

Each sampling point consisted of a radial-arm containing four sampling plots: one central and other three located at 12.2 m in directions north, south-west and south-east (Figure 1d), which were designed to represent the internal characteristics and variations in each 30 x 30 m micro-cell (K. Shepherd & T. Vågen, personal communication, 2006). Once plots were established, they were fully characterized by using the FAO land cover classification system (FAO, 2005). Soils were sampled (0-20 cm depth) in each plot and all soil samples per point (4 plots) were thoroughly mixed to account for short-range (<30 m) spatial variability, and a composite sub-sample (~250 g) was taken from the field. Composite soil sub-samples were air-dried, sieved (<2 mm) and a sub-sub-sample sent to Germany for laboratory analyses.

2.3. Conventional and MIRS analyses of soil samples

Soil texture, pH, total carbon (C) and nitrogen (N), available phosphorus (P_{av}), exchangeable potassium (K), calcium (Ca), magnesium (Mg) and aluminum (Al), and effective cation exchange capacity (CEC) were analyzed on 25% (texture) to 38% (other soil properties) of all collected samples (referred in this study as “reference samples”) for the calibration and validation of the MIRS models. Soil texture was determined by Bouyucos (Anderson and

Ingram, 1993), pH by $CaCl_2$ (Anderson and Ingram, 1993), total C and N by combustion using an auto-analyzer (EL, Elementar Analysensysteme, Germany), P_{av} by the molybdenum blue complex reaction method of Bray and Kurtz (1945) and exchangeable cations and effective CEC by extraction with ammonium chloride (Schöning and Brümmer, 2008).

All 432 soil samples were analyzed by Diffuse Reflectance Infrared Fourier Transform (DRIFT) -MIRS. Five grams of ball-milled soil samples were scanned in a TENSOR-27 FT-IR spectrometer (Bruker Optik GmbH, Germany) coupled to a DRIFT-Praying Mantis chamber (Harrick Scientific Products Inc., New York, US). Spectra were obtained at least in triplicate, from 600 to 4,000 wavenumber cm^{-1}, with a resolution of 4 cm^{-1} and 16 scans/sample, and expressed in absorbance units [log(1/Reflectance)]. Potassium bromide (KBr) for IR spectroscopy (assay ≥99.5%), kept always dry in a desiccator, was used as a background. All spectral replicates per sample were averaged and later subjected to multivariate calibration by using partial least square (PLS) regression, which relates the processed spectra (e.g. Figure 2) to the related concentration values from the reference samples. Through a random split selection of the reference samples, half of the samples were used for calibration, while the other half left for validation. Chemometric models were constructed with the “Optimization” function of the OPUS-QUANT2 package (Bruker Optik GmbH, Germany). Calibration regions were set to exclude the background CO_2 region (2300-2400 cm^{-1}) and the edge of the detection limits of the spectrometer (<700 and >3900 cm^{-1}) to reduce noise. Prediction accuracy of selected MIRS models was evaluated by the residual prediction deviation (RPD) value, the coefficient of determination (R^2) and the root mean square error of the prediction (RMSEP). Once suitable chemometric models were selected, models were applied to every spectrum replicate of non reference samples for the prediction of unknown concentration values for each possible soil property; and results of all replicates per sample were finally averaged. All spectral manipulation and development of chemometric models were carried out in OPUS, version 6.5 (Bruker Optik GmbH, Germany).

2.4. Conventional statistical analyses

Descriptive statistics were calculated to explore the distribution of each soil property under evaluation and as a critical step before geostatistical analyses (Olea, 2006). This comprised the calculation of univariate statistical moments (e.g. mean, median, range), construction of scatter plots, box plots, frequency tables and normality tests, as well as the identification of true outliers and their exclusion if necessary, as even a few outliers can produce very unstable results (Makkawi, 2004). We usually considered as outliers those points with values higher or lower than three standard deviations from the mean (Liu et al., 2009). The coefficient of variation (CV) was calculated as an index for assessing overall variability (Gallardo and Paramá, 2007). The non-parametric tests of Kruskal-Wallis and Mann-Whitney (a Kruskall-Wallis version for only two levels) were chosen for testing the equality of medians among villages following the method of Bekele and Hudnall (2006). All classical statistical analyses were performed in SAS version 9.2 (SAS Institute Inc).

2.5. Minimum sample size estimations

The minimum number of samples required for estimating the mean of the different evaluated soil properties in each village, at different probabilities of its true value (error), with a 95% of confidence, was estimated by using equation 1:

$$n = [(t_\alpha * s)/d]^2 \qquad \text{(equation 1)}$$

where n is the sample size, t is the value of t Student (at α=0.05 and n-1 degrees of freedom, i.e. 1.96), s is the standard deviation, and d is the margin of error (Garten Jr. et al., 2007; Rossi et al., 2009; Yan and Cai, 2008).

2.6. Geo-statistical analyses of estimated soil properties

The spatial dependence of soil properties, as determined by the combination of conventional laboratory analyses and MIRS, was assessed in each area by using geostatistical analyses, via the semivariogram, which measures the average dissimilarity of data as a function of distance (Goovaerts, 1999) as illustrated in equation 2:

$$\gamma(h) = 1/2N(h) \sum_i \sum_{i+h} [z(i)-z(i+h)]^2 \qquad \text{(equation 2)}$$

where γ is the semivariance for N data pairs separated by a distance lag h; and z the variable under consideration at positions i and $i+h$. As construction of semivariograms assumes a Gaussian distribution (Olea, 2006; Reimann and Filzmoser, 2000), variables were transformed if necessary to approximate normality and to stabilize variance (Goovaerts, 1999). Data were also detrended by fitting low-order polynomials according to the exhibited trend (if existent) to accounting for any systematic variation (i.e. global trend) and hence fulfilling the assumption of stationarity (Bekele and Hudnall, 2006; Sauer et al., 2006). Thus, after detrending, respective residuals were used to construct standardized isotropic semivariograms for each soil property in each village. Hence, anisotropy (effect of direction in the intensity of spatial dependence) was not taken into account, as this analysis required a higher number of samples for the construction of stable semivariograms in each direction. When number of samples is limited an ommnidirectional (isotropic) characterization of spatial dependence is more recommendable (Davidson and Csillag, 2003). The standardization was achieved by dividing the semivariance data by the sample variance, and this allowed a fair comparison among variables and sites (Pozdnyakova et al., 2005). The half of the maximum sampling distance in each village was chosen as the active lag distance for the construction of all semivariograms, and more than 100 pairs per each lag distance class interval were included in the calculations.

Once semivariograms were constructed, theoretical semivariogram models were fitted to the data. This was done by selecting the model with the lowest residual sum of squares and highest R^2 (e.g. Liu et al., 2009; Wang et al., 2009; Wei et al., 2008). As the spherical model characterized well most of the cases, this model was selected to fit all data (with the exception when a linear trend was found). Having the same model further facilitates comparisons among variables and villages (Cambardella et al., 1994; Davidson and Csillag, 2003; Gallardo and Paramá, 2007). The spherical model is defined in equation 3 (Liu et al., 2004; Pozdnyakova et al., 2005) as:

$$\gamma(h) = \begin{cases} Co + C\,[\,1.5\,(h/a) - 0.5(h/a)^3\,] & 0 < h \leq a \\ Co + C & h > a \end{cases} \qquad \text{(equation 3)}$$

where γ is the semivariance, h the distance, Co is the nugget, $Co+C$ is the sill, and a is the range. These parameters were used to describe and compare spatial structures of soil properties in each village. ArcGIS version 9 (ESRI) and procedures Univariate, Means and Variogram of SAS version 9.2 were used for exploratory data and trend analyses; while Proc GLM of SAS was used for data detrending. Construction of semivariograms and model fitting were performed in GS^+ version 9 (Gamma Design Software, USA).

2.7. Geo-statistical analyses of MIRS data

To determine the feasibility of using MIRS data as direct input for the determination of spatial variation of soils, all spectra were baseline corrected (Rubberband correction method, 64 baseline points) and derived (1^{st} order derivative, Savitzky-Golay algorithm, 9 smoothing points) in OPUS. Data were later exported to SAS, where the CO_2 regions and the edges of the spectra were excluded, as explained for the multivariate calibration. Next, spectral data were reduced by re-sampling at 12 cm^{-1} and selected wavenumbers (i.e. variables) subjected to Spearman correlation analyses among each other, where highly autocorrelated variables (i.e. $r > 0.99$) were manually excluded, to reduce computational demands. Data were later standardized to zero mean and unit variance, and analyzed by principal component analyses (Borůvka et al., 2007; Yemefack et al., 2005). The three first components were retained, rotated (varimax option) and respective scores assigned to each soil sample. Score components were thus used as input variables for the constructions of semivariograms per each village, by following the same methodology previously explained for the conventional soil parameters. Spearman correlation analyses were finally performed between the principal components and chemical data from reference samples.

3. Results

3.1. MIRS models and prediction

A good representation across the different concentration ranges for most of the soil properties was obtained by the selection of the samples, as shown in Figure 3. Calibration and validation models also showed that predictability potential of MIRS varied with the specific soil property under evaluation and location, as indicated by the different model fit and performance indicators (Figure 3, Table 2). For example, in agricultural applications RPD values higher than 5 indicate that predictions models are excellent; RPD values greater than 3 are considered acceptable; while values less than 3 indicate poor prediction power (Pirie et al., 2005). Besides, R^2 values near 1 typically indicate good models (Conzen, 2003), in particular when bias is minimal and regression line follows the 1:1 line. Hence, excellent models ($5<\text{RPD}\leq6.8$, $0.96\leq R^2\leq0.98$) were obtained for sand, clay, C, N, Ca and CEC; acceptable models ($3<\text{RPD}<5$, $0.89<R^2<0.92$) were obtained for pH and Mg; while unsuitable models ($\text{RPD}<3$, $R^2\leq0.82$) were obtained for silt, P_{av}, K and Al. Poor validation for these last variables (especially P_{av}, K and Al) was the result of a deficient calibration, as indicated by their model fit (Figure 3) and parameters (Table 2). Mid-infrared spectroscopy models for these variables were thus not used for prediction, and hence these data were dropped from any further analyses. Silt fraction, however, could be calculated from the other two fractions (silt = 100 – sand - clay). Therefore, by using the selected MIRS models shown in Table 2 for the prediction of soil parameters in non-reference samples, the entire dataset of sand, silt, clay, pH, C, N, Ca, Mg and CEC could be completed.

3.2. Exploratory data analysis and differences among villages

Exploratory data analyses in the entire dataset indicated that most soil properties presented skewed and kurtic distributions (data not shown). For example, texture fractions showed clearly a bimodal distribution, which suggested the presence of different populations, as it was in fact the case (i.e. different villages presenting different textural classes). Descriptive statistics and histograms were therefore also obtained by village. In this case, although texture fractions often approximated normality, the other soil properties still exhibited non-normal distributions (data not shown). Non-normality is usually the rule and not the exception when dealing with geostatistical and environmental data (Reimann and Filzmoser, 2000). This is why the median (instead of the mean) and non-parametric approaches were preferably used for classical statistical analyses, in spite of data transformation of skewed variables usually helped to approximate normality.

Overall variability of soil properties in each area was evaluated by its coefficient of variation. According to Wei et al. (2008), a CV less than 10% indicates that variability of a considered property is low; while a CV higher than 90% indicates high variation. Thus, calculated CVs in the entire dataset (Figure 4A) showed that Ca, Mg and CEC were the properties with the highest overall variability (>90%); while only pH presented a relative low variation (~10%). Other evaluated soil properties showed intermediate variability (CV=10-90%). When calculations were performed by village (Figure 4B-D), CVs of all soil properties reduced considerably, as expected. Data showed that Mg varied the most in the three villages, while pH (in all villages) and sand (in the communal and old resettlement area) presented the lowest variation. With the particular exception of sand and pH, variability of all soil properties in the new resettlement was lower than in the other two areas.

Differences in medians among villages for all soil properties were significant at $p<0.001$ (Figure 5). Differences were especially evident when the communal and old resettlement areas were compared to the new resettlement area, mainly due to divergent soil textural types (Table 1). In fact, the new resettlement area presented the lowest values for sand and the highest for the remaining properties. This is why a Mann-Whitney test was also performed to compare only between the communal and old resettlement area. This analysis showed highly significant differences ($p<0.001$) in medians between these two villages for all evaluated soil properties (Figure 5).

3.3. Minimum sample size requirements

Estimated minimum sample sizes, for all evaluated parameters, exhibited a negative exponential trend by increasing the margin of error (Figure 6). Taking soil C as an example, a minimum of 473 samples would be required in the communal area to estimate the mean at 5% of its true value; while a minimum of 118, 53, 30 and 19 samples would be necessary at margins errors of 10, 15, 20 and 25%, respectively. With the exception of sand and pH, the required number of samples was found to be lower in the new resettlement area than in the other villages. In general, a higher number of samples would be required for Mg, CEC and Ca, while relatively fewer samples would be necessary for pH, silt and sand.

3.4. Geostatistical analyses of generated soil data

Geostatistical analyses require data following Gaussian distribution. Thus, transformation of variables was necessary in most of the cases (see Table 3) and this generally allowed to approximate normality. However, for Mg in the communal and old resettlement areas any transformations used could shift the highly skewed distribution of this variable. This was attributed to the low concentrations measured (Figure 5), where a high proportion of samples had null values as they were below analytical detection limits. Approximations to normality in a situation like this is simply not possibly by any mean (Reimann and Filzmoser, 2000); therefore data for Mg must be interpreted with caution for these two areas.

To determine the grade of spatial dependence of each soil property, the nugget-to-sill ratio from all semivariograms was calculated. According to Cambardella et al. (1994), and since then further applied by many others (e.g. Huang et al., 2006; Rossi et al., 2009; Wang et al., 2009), if this ratio is lower than 25% the spatial dependence is considered strong; if the ratio is between 25-75% the dependence is considered moderate; and if this ratio is higher than 75% the dependence is considered weak. A similar approach was used here, but their moderate range of spatial dependence (25-75%), that in our opinion is quite wide, was subdivided, and the following classes of spatial dependency used: class I (very strong) <25%, class II (moderately strong) = 25-50%, class III (moderately weak) = 50-75%, class IIII (very weak) >75%, and class O (null) = 100%. Hence, spatial dependence of evaluated soil properties was mostly moderately strong to very strong in the new resettlement area; moderately weak to moderately strong in the old resettlement area; and null to moderately weak in the communal area (Figure 7, Table 3). In fact, in the communal area N and CEC showed null spatial dependency, while sand, clay and Mg exhibited a linear trend with an undefined spatial autocorrelation at the considered lag distance. From the other two areas only N in the old resettlement area exhibited lack of spatial dependence. All the rest of the cases could be very well represented by spherical models with variable parameters depending on the soil property and area under evaluation. For example, while the nugget-to-sill ratio for Ca was 74% in the communal area (moderately weak dependency), in the old and new resettlement areas this ratio reduced to 42 and 28% (moderately strong dependency), respectively. This contrasted with silt, as the nugget-to-sill ratio increased from 30 and 34% in the communal and old resettlement area, respectively, up to 67% in the new resettlement area. Ranges of the semivariograms for all soil properties and sites ranged from 250 m (silt in the communal area) to 695 m (clay in the new resettlement). With the exception of Ca, estimated ranges were lowest in the communal area and highest in the new resettlement.

3.5. Principal components and geo-statistical analyses of MIRS data

Forty nine percent (49%) of overall variability of MIRS data could be explained by the first principal component (PC1), while 11, 10, 6, 4 and 4% could be explained by PC2, PC3, PC4, PC5 and PC6 respectively. Therefore, only the first three components, accounting for 70% of overall variability, were retained. Scores of the first three components were next correlated to concentration values of reference samples. In general, PC1 related very well to texture fractions, C, N, Ca and Mg (absolute Spearman coefficient values of 0.55-0.96, Figure 8); while relationships between PC2 or PC3 with analyzed soil properties were weaker (0.39-0.69) or mostly non significant (0.01-0.27), respectively (data not shown).

Standardized semivariograms based on the principal components were usually represented very well by spherical models, with variable parameters according to the component and village. PC1, however, showed a linear trend in the communal area, indicating an undefined spatial dependence at the considered lag distance. In fact, semivariograms showed mainly that spatial dependence was usually moderately strong to very strong in the new resettlement area; moderate weak to moderately strong in the old resettlement area; and very weak to moderately weak in the communal area (Figure 9, Table 4). Ranges of these semivariograms were 399 m (in the communal area), 161-481 m in the old resettlement area, and 604-744 m in the new resettlement.

4. Discussion

4.1. MIRS and Geostatistics: a viable combination?

This study clearly illustrated that MIRS can be successfully used for complementing large soil datasets required for spatial assessments at landscape level. Furthermore, it suggested that spectral information from MIRS, after principal component analyses, could be directly integrated in geostatistical analyses without the need of a calibration/validation step. Effectively, MIRS proved its potential in predicting most of the soil properties under evaluation; although the technique was not effective for all properties. This was evident for silt, P_{av}, K and Al which presented inadequate MIRS models and therefore, predictions for these variables could not be carried out. Hence, semivariograms for silt, P_{av}, K and Al were not constructed due to insufficient data. Working with different soils in Vietnam, and by using the same MIRS methodology and equipment, Schmitter et al. (2010) found, conversely, acceptable models for silt and K; while their models for clay and CEC were inadequate (P. Schmitter, personal communication). Hence, applicability and efficacy of MIRS depends on the soil type and/or location, and illustrates why regional calibrations are still required for a successful prediction of soil properties (McBratney et al., 2006; Shepherd and Walsh, 2004). These issues limit a generic applicability of MIRS in the prediction of soil variables for agro-ecological assessments. Some advances in the development of global calibrations, however, have been achieved in the last few years (Brown et al., 2005; Cécillon et al., 2009), which should help to overcome this limitation in the near future. Alternative solutions could be the use of MIRS-based predictions models to estimate through pedotransfer functions those soil properties that cannot be predicted accurately by sole MIRS (McBratney et al., 2006), or the utilization of auxiliary predictors (i.e. simple and inexpensive conventional soil parameters, like pH and sand; or from complementary sensors, like NIRS) that can improve the prediction of other soil properties (Brown et al., 2005). Thus, all data could be later used in spatial analyses without restriction.

Semivariograms based on the soil dataset clearly showed that spatial autocorrelation of most soil properties in the villages followed the order: communal area < old resettlement < new resettlement. Variography analyses based on the principal components from MIRS data showed comparable spatial patterns (i.e., nugget to sill ratios and ranges of semivariograms, Figure 10). This implies important savings in terms of analytical costs and time, as it creates the possibility of a broad and quick assessment of soil spatial variability at landscape scale based only on MIRS, confirming previous suggestions by Shepherd and Walsh (2007) and complementing studies based on NIRS (i.e. by Awiti et al., 2008; Cohen et al., 2006; Vågen et al., 2006). A related approach to our study, but at plot level and by using NIRS, was carried out by Odlare et al. (2005). However, they found out that spatial dependence from principal components (based on spectral information) was not related to the spatial dependence from considered soil properties (i.e. C, clay and pH). Hence, although spatial variation based on NIRS could be identified, the authors did not know what the variation represented. Thus, to properly understand the meaning of the spatial structures from the principal components it is necessary to link the component scores to soil parameters of reference samples. In our case, this was possible for the first principal component (PC1), which was well related to textural fractions, C, N, Ca, Mg and CEC. Therefore, PC1 was clearly associated to soil fertility, and thus, derived spatial results could be used for distinguishing areas of different soil quality. However, for PC2 and PC3 simple relationships with measured variables were not evident. A reason for this may be related to the explained variance in each component, where PC1 accounted for 49% of the overall variability, while the other two components each explained a lower proportion (10-11%). The unexplained variance and lack of relationships for the other components would indicate that MIRS could be either generating noise or capturing additional characteristics of soils that this study did not take into account (e.g. carbonates, lime requirements, dissolved organic C, phosphatase and urease activity, among others). In fact, MIRS can be related to a wide range of physical, chemical and biological soil characteristics (for further details please refer to Shepherd and Walsh, 2007; and Viscarra-Rossel et al., 2006). All this would further suggest that MIRS may present great potential as an integrative measurement of soil status and, hence, could be a valuable tool for characterizing spatial variation of soils.

4.2 Analyses of spatial patterns

Nearly all experimental semivariograms of soil properties were very well described by the spherical model, with a reachable sill, which clearly indicates the presence of spatial autocorrelation. However, some of the semivariograms in the communal area (for sand, clay, Mg and PC1), could only be described by a linear model with an undefined spatial dependence. If there is no reachable sill this could indicate that spatial dependence may exist beyond the considered lag distance (Huang et al., 2006). Semivariograms for N and CEC in the communal area, and N in the old resettlement showed instead pure nugget effect. Pure nugget effect can represent either extreme homogeneity (all points have similar values) or extreme heterogeneity (values are very different, in a random way). However, pure nugget effect do not compulsory reveal spatial independence, as spatial structure may be present but at lower resolution than our minimum sample distance (that in our case was 30 m) (Davidson and Csillag, 2003). In any case, a high nugget effect would imply higher uncertainty when further interpolation is necessary (e.g. by using Kriging). In such circumstances, calculating the mean value from sampled locations would be sufficient for interpolation, as no spatial structure could be detected at the scale of observation. Finding no spatial dependence for some soil parameters is not an unusual result, as its magnitude (from strong to null dependency) can vary as a function of the soil property and location, among others factors (Garten Jr. et al., 2007).

As indicated before, spatial dependence (either based on soil properties or just on MIR spectral data) was in general lowest in the communal area and highest in the new resettlement. Although the reasons for these differences can not be completely determined, since our experimental design did not allow a proper separation of causal factors, direct and indirect evidence would suggest some potential drivers that nevertheless need to be investigated in future studies. For example, it is generally accepted (Cambardella et al., 1994;

Liu et al., 2004; Liu et al., 2009; Rüth and Lennartz, 2008) that a strong spatial dependency of soil properties is controlled by intrinsic factors, like texture and mineralogy; while a weak dependence is attributed to extrinsic factors, like farmers' management (e.g. fertilizer applications). Thus, in terms of intrinsic factors, spatial dependence seems to follow the particular textural classes and inherent soil quality of each area. In terms of extrinsic factors, findings from Cobo et al. (2009) would support this as investment in soil fertility and land management of cropping fields was higher in the communal area than in the two resettlement areas. Moreover, according to the history of each settlement (Cobo et al., 2009) the grade of disturbance of natural resources is in the order: communal area > old resettlement > new resettlement, which would also affect correspondingly the spatial variability of soil properties. The coefficient of variation of evaluated soil properties seems to support this, as (with the exception of pH and sand) usually the highest CVs were obtained in the communal area, while the lowest values were found in the new resettlement. However, despite this global trend, no clear relationships were found between the CVs and their respective spatial variability parameters, which indicates once more that only part of the variation could be explained. Similar observations between CVs and spatial variability parameters have been also reported by Gallardo and Paramá (2007).

4.3. Relevance of findings for future sampling designs

Knowledge of sample sizes for each soil property and village presented in this study could be used as guide for better planning sampling designs at landscape scale in areas of similar conditions, as it helps to estimate approximate minimum number of samples that must be taken in each location for achieving a predetermined level of precision. These data, however, do not indicate how samples should be distributed in space. Derived ranges from variography analyses complement very well this information. They indicate the adequate sample distances among points for obtaining spatially-independent samples (i.e. that distance that exceeds the ranges of the semivariograms), as better results are obtained when samples are not autocorrelated (Rossi et al., 2009). However, when a high level of precision is required, collection of spatially-independent samples may be problematic, especially for those properties exhibiting high ranges, due to the potential difficulty of arranging a high number of samples at the required (i.e. long) separation distances. For example, for C assessments, if a 5% of error is selected, a minimum of 264 samples should be distributed at >577 m of separation among each other in the new resettlement, which is simply not possible if we consider the same spatial domain. However, at 10% of error, only 66 samples are needed, thus their distribution in the same area is feasible. In the case of sand, clay, N, Mg and CEC for the communal area, and N for the old resettlement, samples could be placed at random instead, as these properties showed pure nugget effect. Data for pH, on the other hand, should be cautiously interpreted, as it is already in a logarithmic scale; hence, not surprisingly it showed the lowest CVs and minimum sample sizes. If the intention of the sampling is to characterize again the spatial variability within villages, results indicated that a sampling distance of 30 m is acceptable for the new resettlement; but lower distances may be necessary for the communal and old resettlement to be able to capture shorter-range variability which this study was not be able to detect. In any case, care is required if direct extrapolation of sampling sizes and ranges to other scales is carried out (e.g. at plot or national levels), as spatial dependence usually differ with the scale (Cambardella et al., 1994).

5. Conclusions

Results from this study clearly showed that required large soil datasets can be built by using MIRS for the prediction of several soil properties, and later successfully used in geostatistical analyses. However, it was also illustrated that not all soil properties exhibit a MIR spectral response, and those ones who were well predicted (i.e. sand, clay, pH, C, N, Ca, Mg and CEC) usually depend on the success of regional calibrations. As a new approach, results showed that MIRS data could be directly integrated, after principal component analyses, in geostatistic assessments without the necessity of calibration/validation steps. This approach is very useful when time and funds are limited, and when a coarse measure of soil spatial variability is required. However, principal components must be associated to soil functional characteristics to be able to explain the results, as was demonstrated with the soil properties considered in this study. Understanding variability of soils and its spatial patterns in these three contrasting areas brought out also important recommendations for future sampling designs and mapping. By combining information about minimum sample sizes, with corresponding reported ranges from the semivariograms, a better efficiency (in terms of time, costs and accuracy) during sampling exercises could be obtained. Hence, it is concluded that MIRS and geostatistics can be successfully integrated for spatial landscape analyses and monitoring. A similar approach would be very valuable in regional and global soil fertility assessments and mapping (e.g. Sanchez et al., 2009) and carbon sequestration campaigns (e.g. Goidts et al., 2009), where large soil sample sizes are required and uncertainty about sampling designs prevail.

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Table 1. Main characteristics of the villages under study

Village name	Settlement type	Settlement time	Location (District, Ward)	Dominant soil type[&]	Mean soil textural class	Village area (ha)
Kanyera	Communal area	1948	Shamva, 6	Chromic Luvisols	Loamy sand	730
Chomutomora	Old resettlement	1987	Shamva, 15	Chromic Luvisols	Sandy Loam	780
Hereford Farm	New resettlement	2002	Bindura, 8	Rhodic Ferrasols	Clay	1360

[&] According to FAO soil classification

Table 2. Optimization parameters and performance indicators of best MIRS models for each soil property under evaluation.

Property	n	Outliers removed	Preprocessing method[&]	Rank	Calibration			Validation			Prediction
					R^2	RMSEE	RPD	R^2	RMSEP	RPD	
Sand	110	1	1stDer+VN	7	0.98	3.7	6.7	0.98	3.3	6.8	Yes
Silt	110	1	1stDer+VN	6	0.85	3.1	2.6	0.82	3.6	2.4	No[#]
Clay	110	1	1stDer+SLS	3	0.97	3.0	6.1	0.97	2.6	6.2	Yes
pH	165	2	1stDer+SLS	9	0.93	0.20	3.8	0.89	0.24	3.1	Yes
C	165	1	1stDer+VN	14	0.99	0.14	10.1	0.98	0.19	6.4	Yes
N	165	2	1stDer+VN	9	0.98	0.01	6.6	0.96	0.02	5.2	Yes
P_{av}	165	0	SLS	6	0.47	5.5	1.4	0.49	6.2	1.4	No
K	165	0	None	5	0.48	1.9	1.4	0.56	1.4	1.5	No
Ca	165	1	COE	8	0.94	25.2	4.1	0.96	18.7	5.1	Yes
Mg	165	0	1stDer+MSC	8	0.96	14.8	5.2	0.92	18.0	3.4	Yes
Al	165	0	1stDer+SLS	12	0.69	0.70	1.8	0.66	0.61	1.8	No
CEC	165	0	1stDer+VN	9	0.98	22.8	7.6	0.98	24.4	6.6	Yes

[&] 1stDer: 1[st] derivative, COE: constant offset elimination, SLS: straight line subtraction, MSC: multiplicative scatter correction, VN: vector normalization. Considered spectral regions from the optimization process are not shown.

n: number of observations; Rank: number of factors used in the PLS regression; RMSEE: Root Mean Square Error of Estimation, RMSEP: Root Mean Square Error of the Prediction, RPD: Residual Prediction Deviation

[#] But could be calculated from the other two textural fractions

Table 3. Model parameters of standardized theoretical semivariograms of evaluated soil properties in the three villages under study. See Figure 7 for a visualization of respective experimental and theoretical semivariograms.

Property[$]	Outliers removed	Type of Model	R^2	*RSS*[@]	Nugget *Co*	Sill *Co+C*	Range *a* (in m)	*Co* / *(Co+C)*[#]	Class[&]
Communal area (n=120)									
Sand	0	Linear	0.26	6.79E-00	0.86	1.05	∞	82.1	IIII
Silt	0	Spherical	0.49	9.35E-01	0.30	1.01	250	29.7	II
Clay [L]	0	Linear	0.25	2.33E-02	0.89	1.09	∞	81.1	IIII
pH [L]	0	Spherical	0.21	5.64E-04	0.62	0.97	451	63.6	III
C [A]	0	Spherical	0.14	5.53E-05	0.56	1.01	400	56.0	III
N [A]	2	-	-	-	1.0	1.0	∞	100	O
Ca [S]	0	Spherical	0.29	1.08E-02	0.72	0.98	527	73.6	III
Mg [A]	0	Linear	0.25	1.67E-04	0.86	1.04	∞	82.8	IIII
CEC [L]	0	-	-	-	1.0	1.0	∞	100	O
Old resettlement area (n=132)									
Sand	0	Spherical	0.63	8.58E-00	0.49	0.94	441	51.6	III
Silt [L]	0	Spherical	0.67	5.34E-03	0.36	1.06	426	34.2	II
Clay [L]	0	Spherical	0.59	1.01E-02	0.48	0.95	415	50.4	III
pH [S]	0	Spherical	0.64	1.34E-03	0.51	1.07	484	48.1	II
C [L]	0	Spherical	0.52	7.20E-03	0.69	1.06	532	65.2	III
N [A]	1	-	-	-	1.0	1.0	∞	100	O
Ca [S]	0	Spherical	0.72	3.39E-02	0.45	1.08	483	41.6	II
Mg [A]	0	Spherical	0.56	3.18E-04	0.54	1.09	459	49.8	II
CEC [L]	0	Spherical	0.63	1.31E-02	0.61	1.02	386	60.0	III
New resettlement area (n=180)									
Sand [S]	0	Spherical	0.71	5.11E-02	0.42	1.06	506	39.4	II
Silt	0	Spherical	0.60	8.60E-01	0.69	1.03	671	67.3	III
Clay	0	Spherical	0.76	6.80E-00	0.46	1.05	695	43.7	II
pH [L]	0	Spherical	0.65	1.57E-03	0.39	1.08	638	36.2	II
C [L]	0	Spherical	0.75	1.11E-02	0.23	1.05	577	21.4	I
N [A]	0	Spherical	0.77	6.70E-06	0.23	1.04	517	22.1	I
Ca [S]	0	Spherical	0.64	2.51E-01	0.31	1.10	649	28.1	II
Mg [S]	0	Spherical	0.71	1.98E-01	0.17	1.05	522	15.8	I
CEC [A]	0	Spherical	0.70	4.91E-03	0.25	1.08	604	23.3	I

[$]: If carried out, the type of transformation is indicated ([L] = logarithm, [S] = square root, [A] = arcsin, n: number of observations; [@]: Residual Sum of Squares, [#]: Nugget-to-sill ratio (%), [&]: Spatial dependency class: I = very strong, II = moderately strong, III = moderately weak, IIII = very weak, O = null.

Table 4. Model parameters of standardized theoretical semivariograms of the three first principal components from MIRS data of the three areas under study. See Figure 8 for a visualization of respective experimental and theoretical semivariograms.

Property[$]	Outliers removed	Type of Model	R^2	*RSS*[@]	Nugget *Co*	Sill *Co+C*	Range *a* (in m)	*Co/(Co+C)*[#]	Class[&]
Communal area (n=120)									
PC1 [L]	0	Linear	0.09	4.41E-03	0.94	1.03	∞	90.9	IIII
PC2	0	Spherical	0.15	3.93E-03	0.59	1.01	399	58.7	III
PC3 [L]	0	Spherical	0.41	6.41E-03	0.60	1.03	399	58.0	III
Old resettlement area (n=132)									
PC1	1	Spherical	0.62	4.44E-03	0.54	1.05	481	51.0	III
PC2 [L]	4	Spherical	0.60	1.60E-03	0.59	1.15	479	51.1	II
PC3 [L]	2	Spherical	0.40	3.73E-03	0.41	0.99	161	41.0	II
New resettlement area (n=180)									
PC1 [A]	1	Spherical	0.69	9.74E-06	0.20	1.10	606	18.3	I
PC2	10	Spherical	0.80	4.66E-05	0.45	1.10	744	41.0	II
PC3	0	Spherical	0.78	2.13E-01	0.05	1.11	604	4.6	I

[$]: If carried out, the type of transformation is indicated ([L] = logarithm, [A] = arcsin), n: number of observations; [@]: Residual Sum of Squares, [#]: Nugget-to-sill ratio (%), [&]: Spatial dependency class: I = very strong, II = moderately strong, III = moderately weak, IIII = very weak.

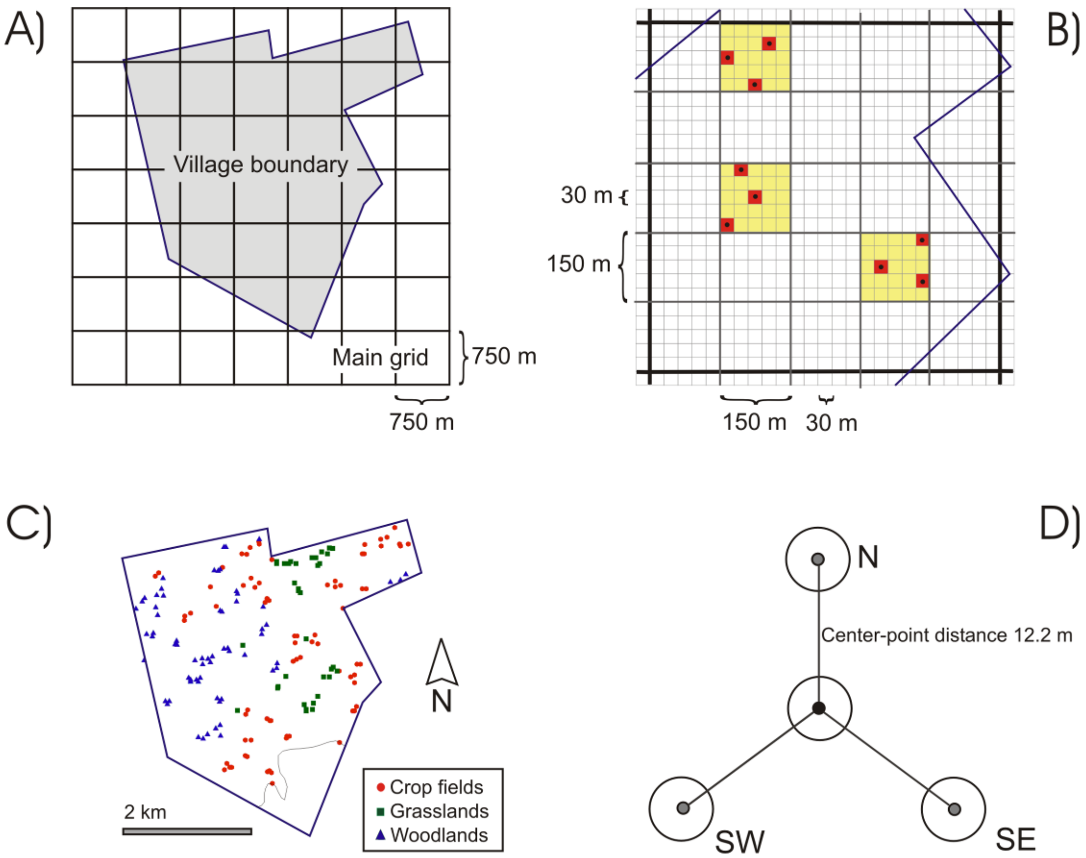

Figure 1. Soil sampling design. Hereford farm is used here as illustration: A) Representation of the overlay of a village boundary with main grid of 750 x 750 m; B) Zooming into a cell of 750 x 750 m where grids of 150 x 150 and 30 x 30 m, and selected sub-cells and micro-cells (with respective centroids), are shown; C) Final distribution of sampling points in the village; D) Schematic representation of the radial arm for each sampling point, where central circle indicates the centroid of each micro-cell (N: north, SW: south west; SE: south east).

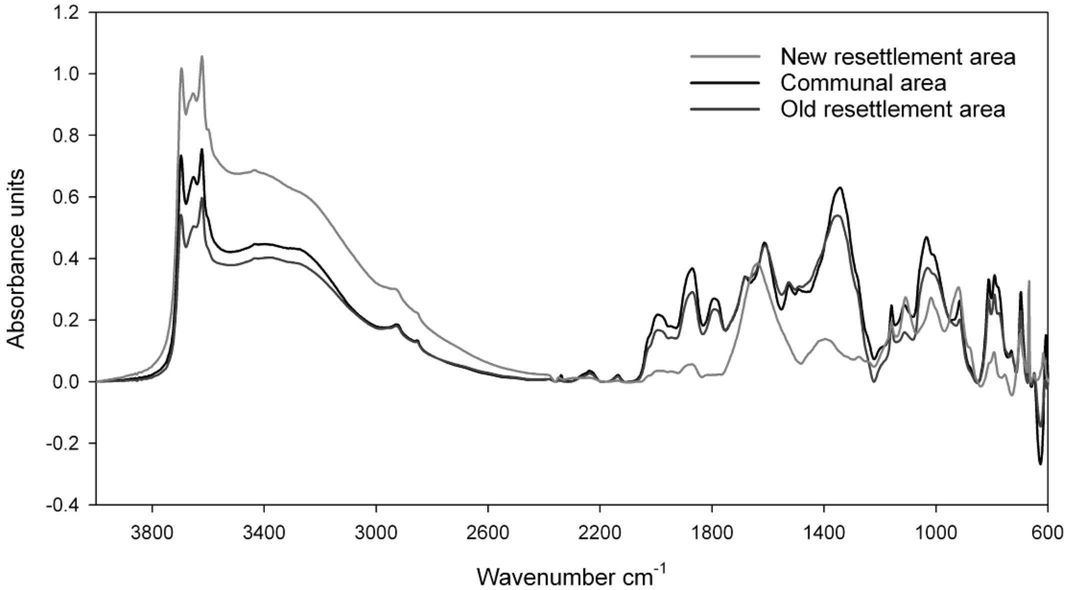

Figure 2. Examples of mid infrared spectra of soil samples from the three villages under study: i.e. the baseline-corrected spectrum of one sample per village having an average C content of 7, 11 and 29 g kg^{-1} for the communal area, and the old and new resettlement areas, respectively.

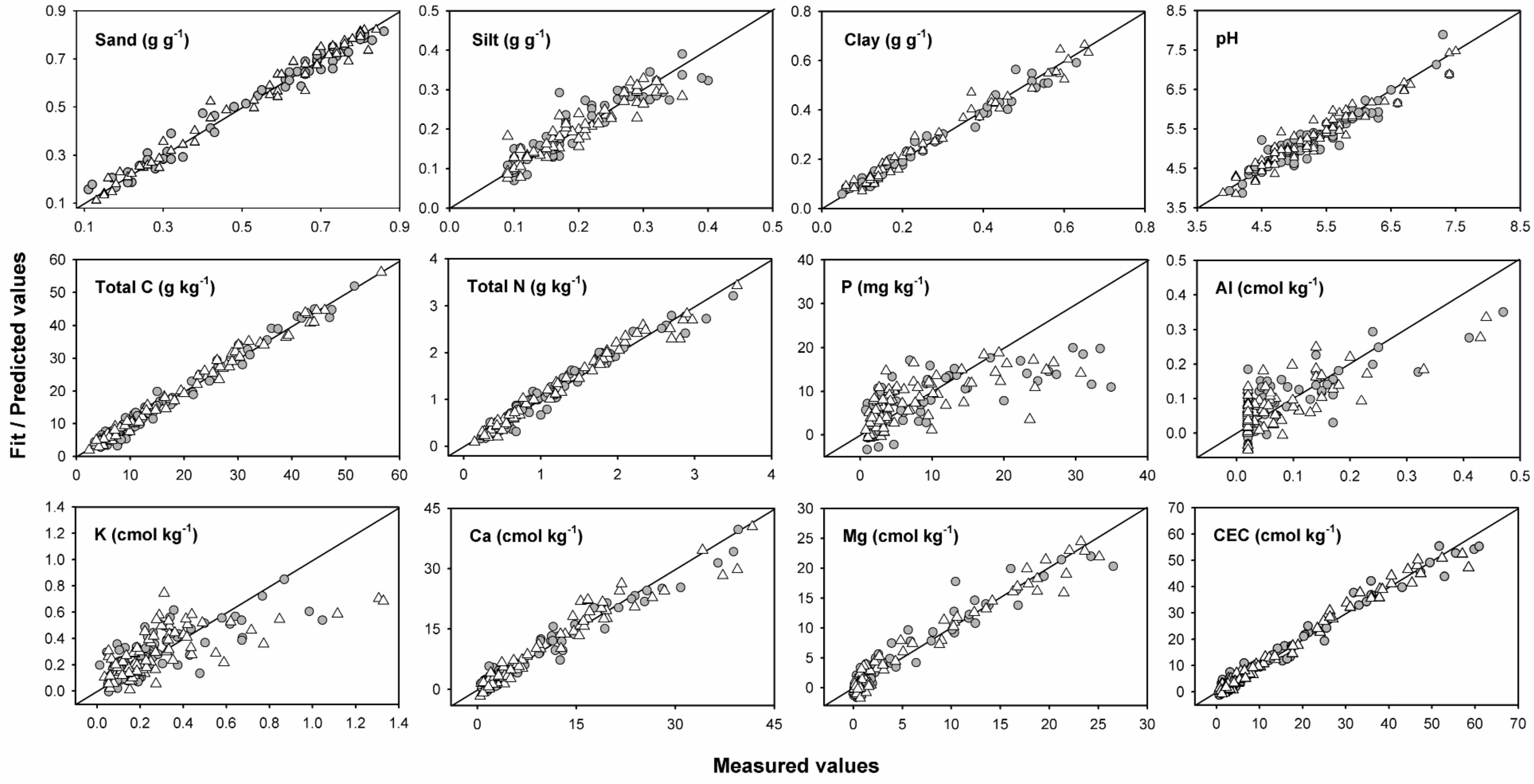

Figure 3. Calibration (triangles) and validation (circles) scatter plots of MIRS models from evaluated soil properties. For respective performance indicators refer to Table 2.

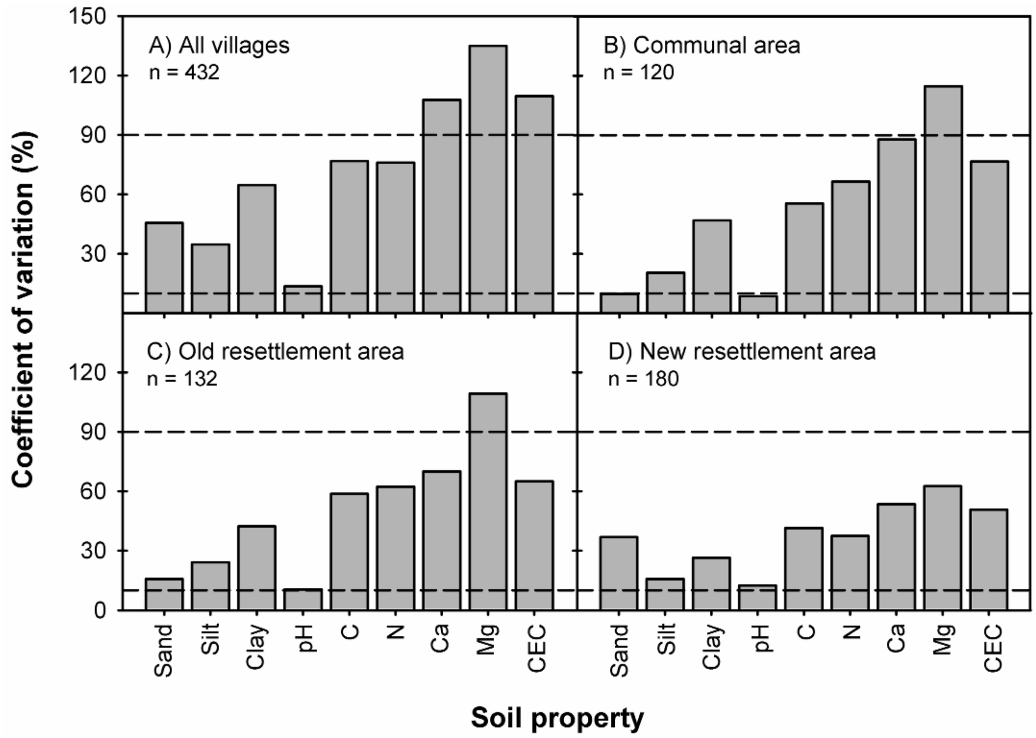

Figure 4. Coefficient of variation of soil properties in the entire dataset (A), and in each village under evaluation (B-D). Dashed lines indicate reference values of 10 and 90% for low and high variation, respectively.

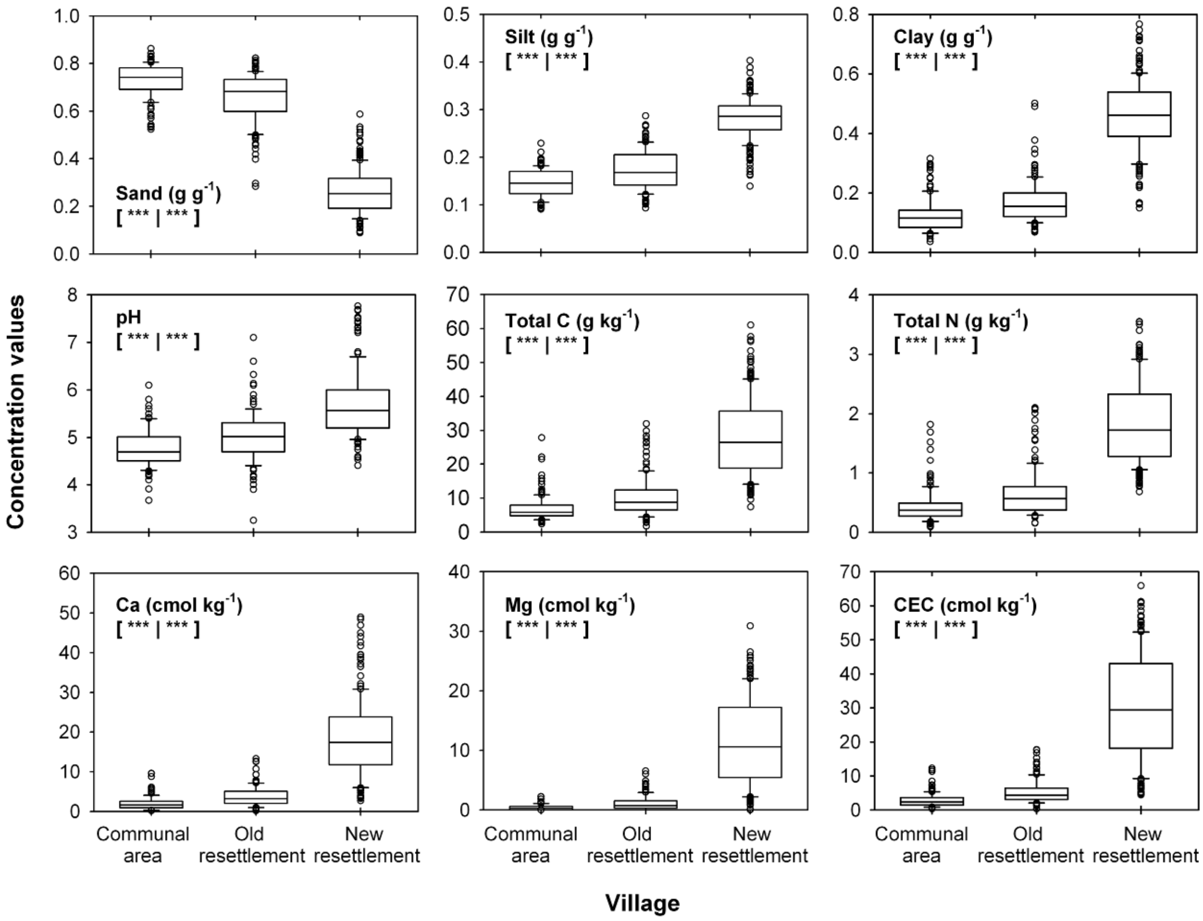

Figure 5. Box and whisker plots of soil properties in each village under evaluation, and associated statistical differences (*** : p<0.001) according to the [Kruskall-Wallis | Mann-Whitney] tests. Kruskall-Wallis compared medians (horizontal line inside boxes) of the three villages, while Mann-Whitney compared only the communal and old resettlement areas. Number of data as shown in Figure 4.

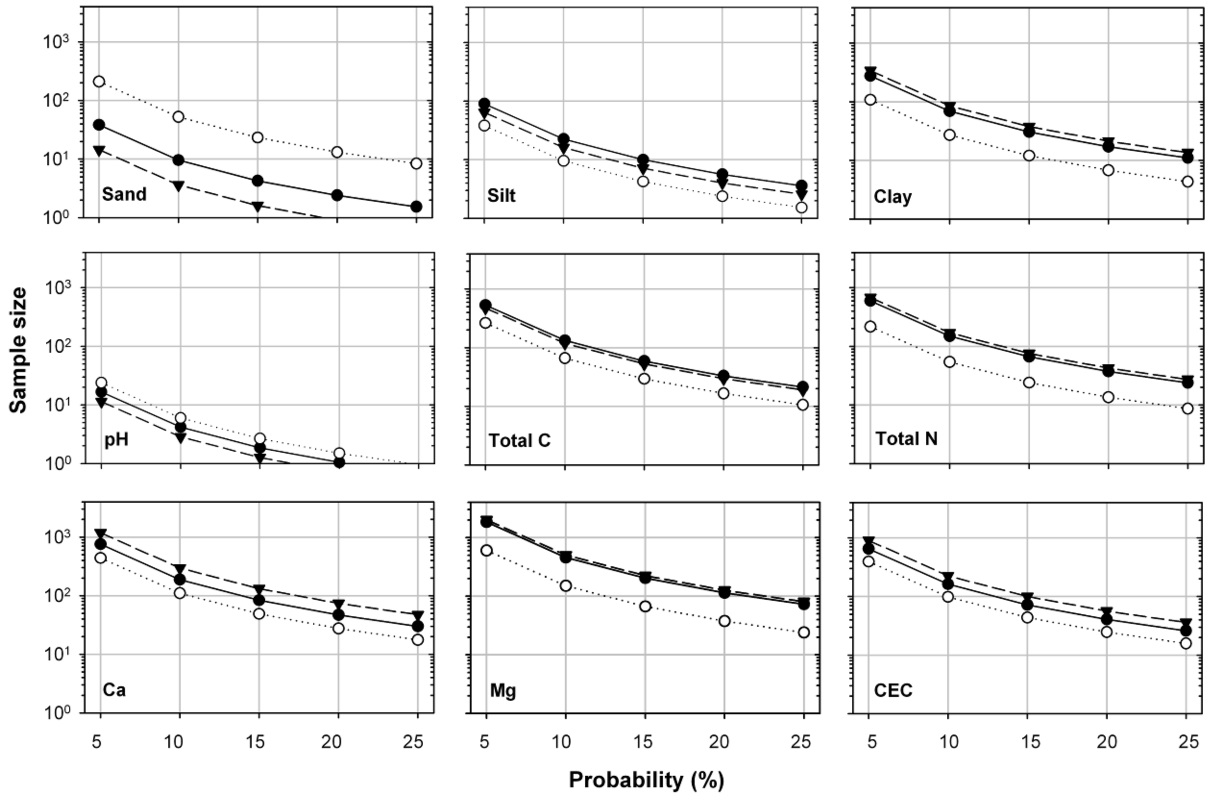

Figure 6. Minimum sample sizes required for estimating the mean of different evaluated soil properties at different probabilities of its true value (margin of error), with a 95% of confidence in: communal area (closed triangles), old resettlement (closed circles) and new resettlement (open circles). Notice that Y-axes are in logarithmic scale. Number of data for calculations and units as shown in Figure 4.

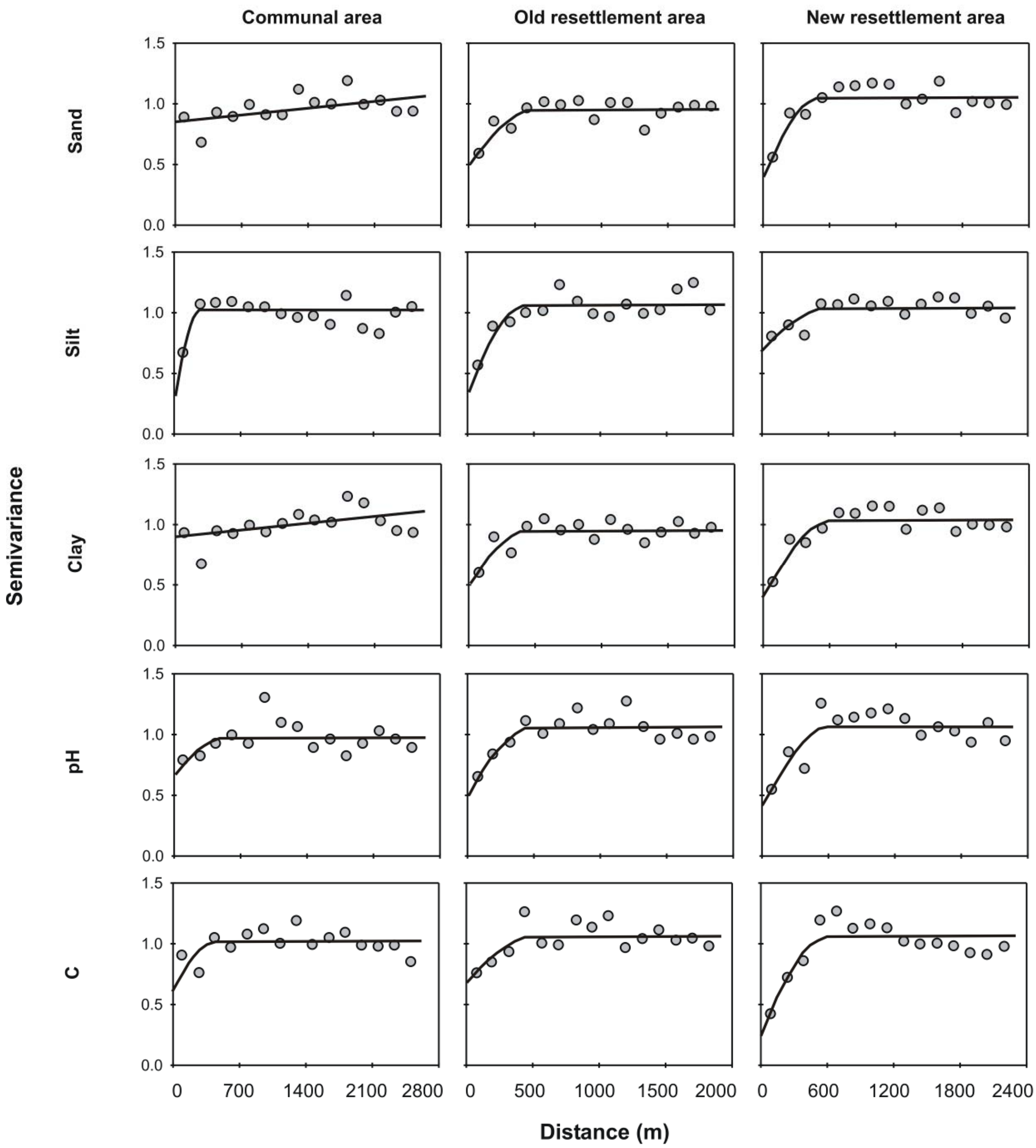

Figure 7. Standardized experimental (circles) and theoretical (line) semivariograms for evaluated soil properties in the three areas under study. For model parameters please refer to Table 3.

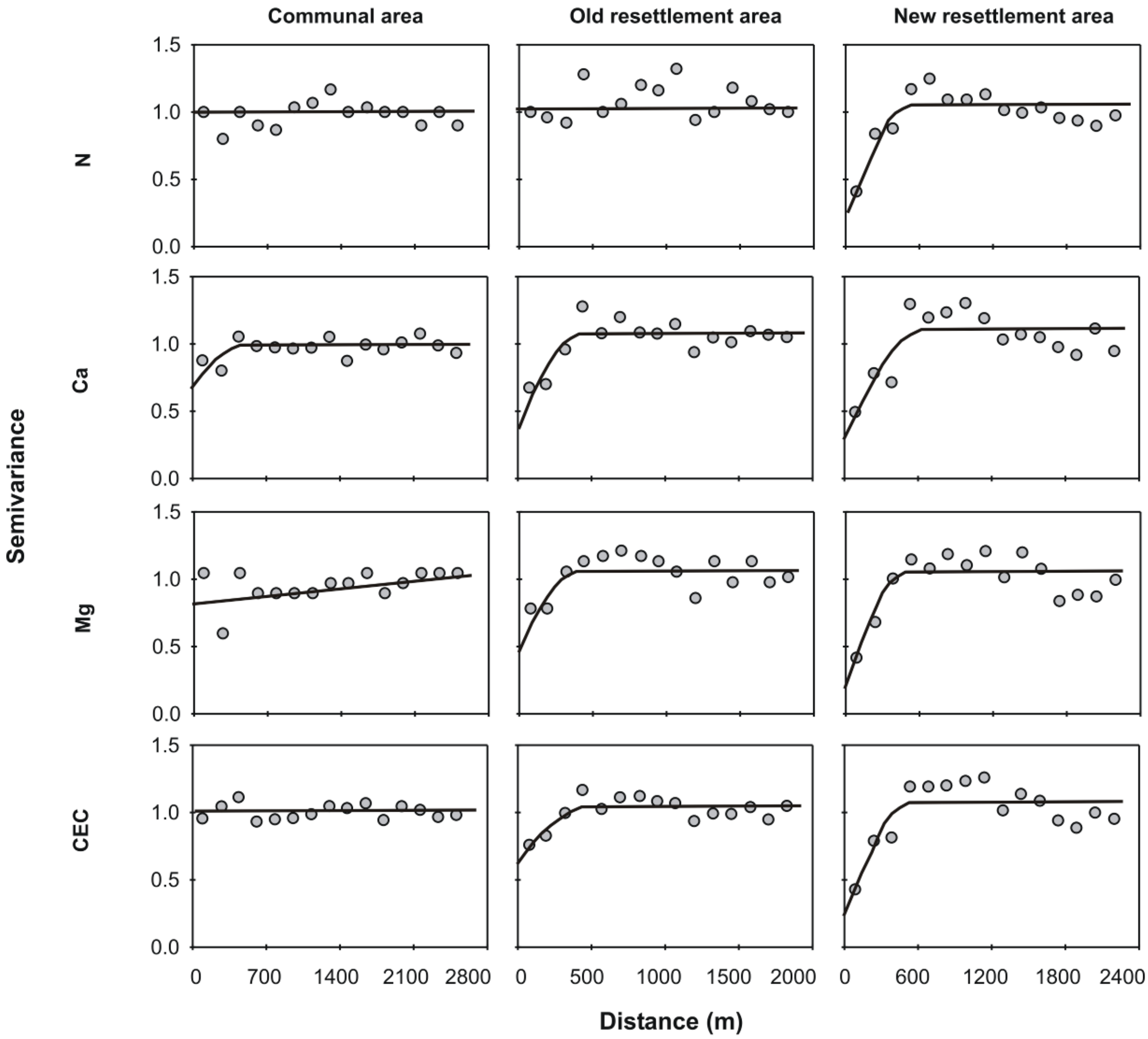

Figure 7. Continuation

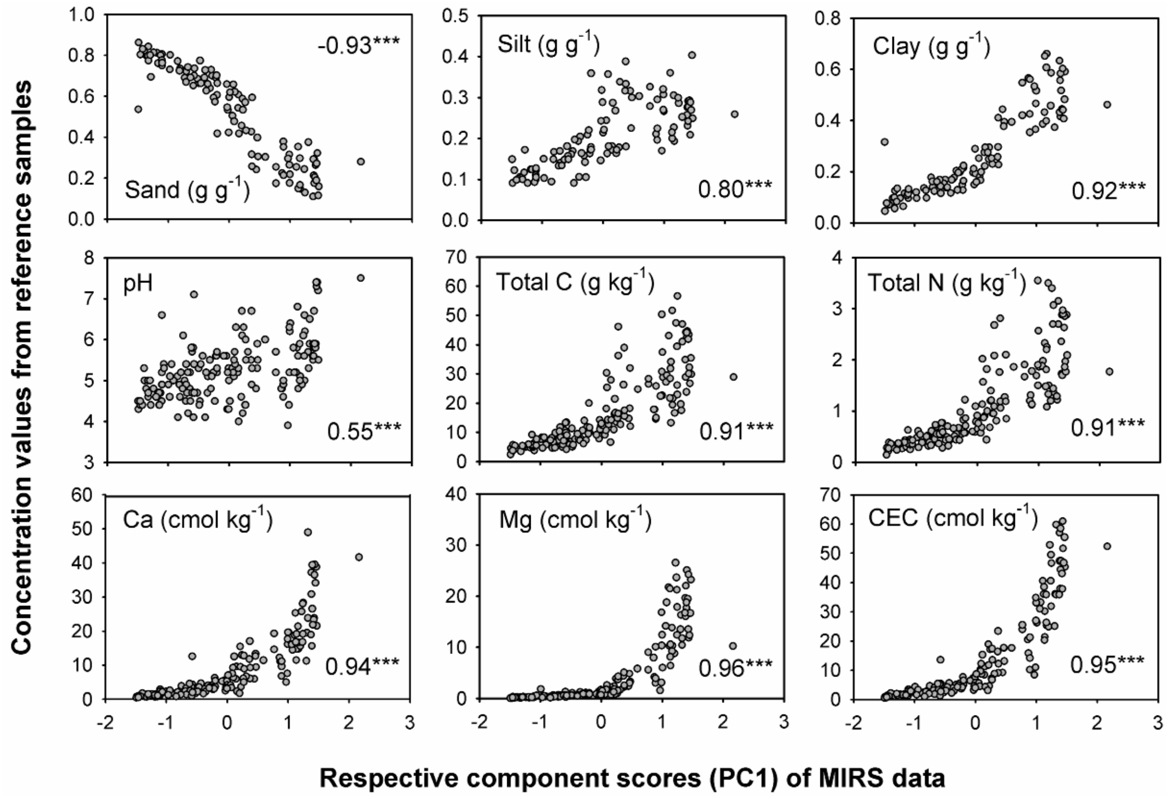

Figure 8. Scatter plots and Spearman correlation coefficients for the relationships between soil properties from reference samples (i.e. analyzed by conventional laboratory procedures) and respective component scores of the first principal component (PC1) based on MIRS data. ***: $p<0.001$.

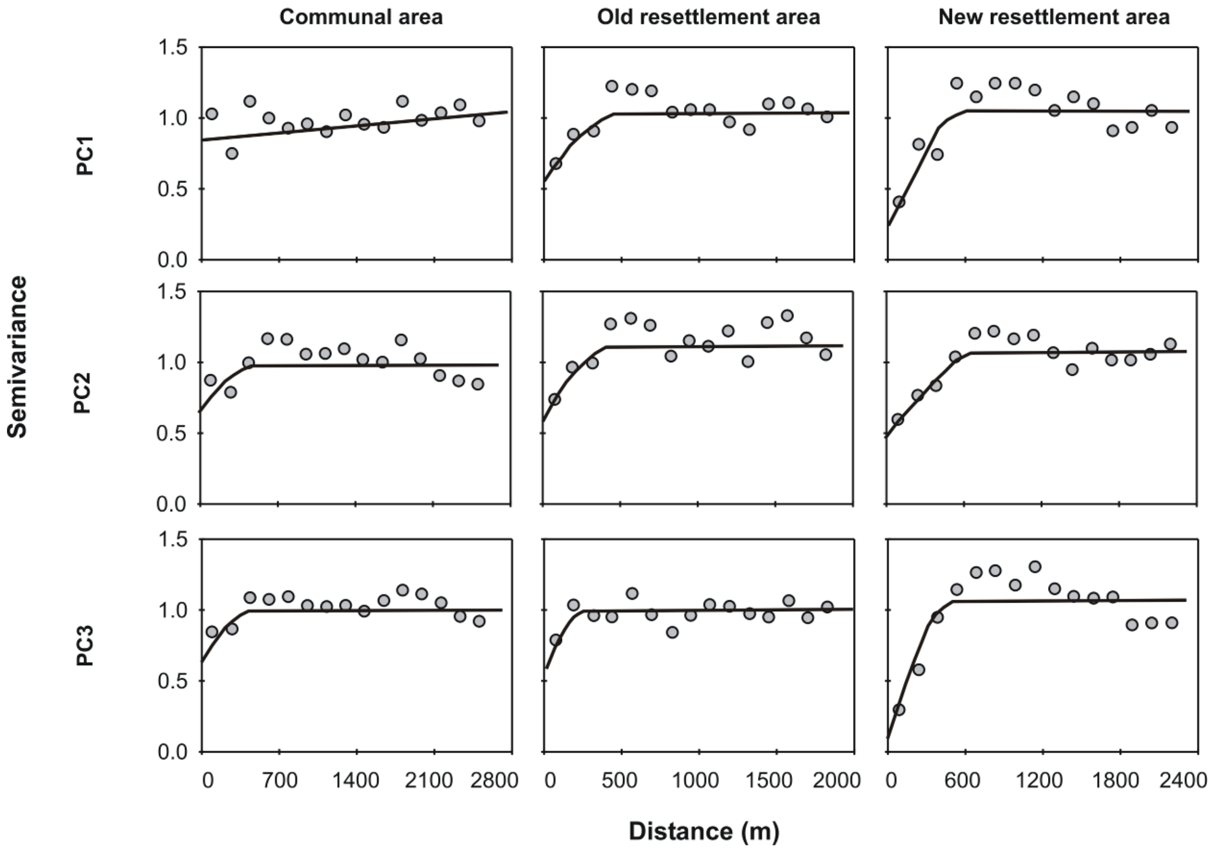

Figure 9. Standardized experimental (circles) and theoretical (line) semivariograms for the three first principal components based on MIRS data from all soil samples collected in the three areas under study. For model parameters please refer to Table 4.

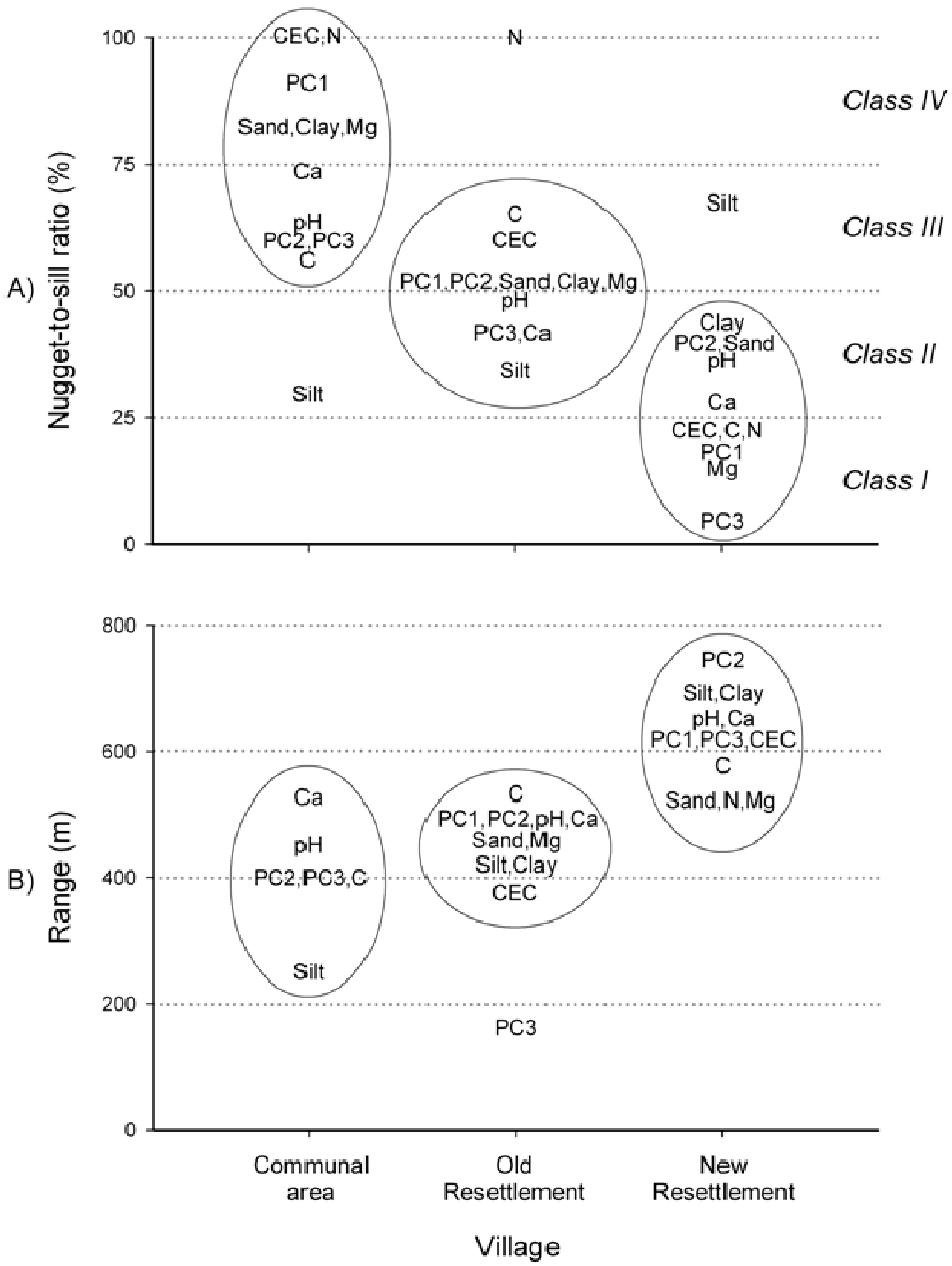

Figure 10. Comparison of A) nugget-to-sill ratios (and spatial dependency classes as defined in the text), and B) ranges, from semivariograms of the three studied settlement schemes based on MIRS-derived principal components (PC1-PC3) and evaluated soil properties. Circles exclude variables that deviate from the behavior of the main group. Variables with undefined ranges (see Tables 3 and 4) were not plotted.