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Predictive performance of mobile vis-near infrared spectroscopy for key soil properties at different geographical scales by using spiking and data mining techniques

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Abstract

The development of accurate visible and near infrared (vis-NIR) spectroscopy calibration models for selected soil properties based on mobile measurements is essential for site specific soil management at fine sampling scale. The objective of the present study was to compare the mobile and laboratory prediction performance of vis-NIR spectroscopy for total nitrogen (TN), total carbon (TC) and soil moisture content (MC) of field soil samples based on single field (SFD), two-field dataset (TFD), UK national dataset (UND) and European continental dataset (ECD) calibration models developed with linear and nonlinear data mining techniques including spiking. Fresh soil samples collected from fields in the UK, Czech Republic, Germany, Denmark and the Netherlands were scanned with a fibre-type vis-NIR spectrophotometer (tec5 Technology for Spectroscopy, Germany), with a spectral range of 305-2200 nm. After dividing spectra into calibration (75%) and validation (25%) sets, spectra in the calibration set were subjected to three multivariate calibration models, including the partial least squares regression (PLSR), multivariate adaptive regression splines (MARS) and support vector machines (SVM), with leave-one-out cross-validation to establish calibration models of TN, TC and MC. Results showed that the best model performance in cross-validation was obtained with MARS methods

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for the majority of dataset scales used, whereas the lowest model performance was obtained with the SFD. The effect of spiking was significant and the best model performance in general term was obtained when local samples collected from two target fields in the UK were spiked with the ECD, with coefficients of determination (R^2) values of 0.96, 0.98 and 0.93, root mean square error (RMSE) of 0.01, 0.1 and 1.75, and ratio of performance to interquartile distance (RPIQ) of 7.46, 6.57 and 3.98, for TC, TN and MC, respectively. Therefore, these results suggest that ECD vis-NIR MARS calibration models can be successfully used to predict TN, TC and MC under both laboratory and mobile measurement conditions.

Keywords: Diffuse reflectance spectroscopy, Spectral library, Soil properties, Data mining, Spiking.

Introduction

Visible and near-infrared (vis-NIR) diffuse reflectance spectroscopy has attracted increasing interest among soil scientists in recent times, and has been proposed as a possible method of soil analysis. It provides higher soil sampling density for mapping purposes compared with conventional laboratory analysis (Shepherd and Walsh, 2002; Wetterlind et al., 2010). This technique also allows for in field (in situ) non mobile (Viscarra Rossel and Chen, 2011; Brodský et al., 2013) and mobile measurement with high soil-sampling resolution (Maleki et al., 2008; Kuang and Mouazen, 2013). Literature show that Vis-NIR spectroscopy has been used successfully for modelling and mapping of soil properties, under both mobile and non-mobile measurement conditions, (i.e., Shibusawa et al., 2001; Mouazen et al., 2005; Kuang and Mouazen, 2013; Kuang et al., 2015). However, compared to laboratory spectral measurements that is done under controlled conditions, mobile spectroscopy analyses are affected by

environmental factors such as ambient light, soil moisture content, soil structure, temperature, contamination by stones and excessive residues (Mouazen et al., 2007; Stenberg et al., 2010). One way to overcome these negative influences is by adopting effective spectral data preprocessing and advanced data mining techniques when developing calibration models for mobile spectroscopy.

Precision agriculture aims at optimizing management of within field variability for sustainable increase in land productivity (Bongiovanni and Lowenberg-Deboer, 2004). Variable-rate fertilizer application, which requires reliable soil information at a high spatial resolution, is required to achieve this goal (Wetterlind et al., 2010; Mouazen and Kuang, 2016). Successful implementation of the mobile vis-NIR spectroscopy was reported for sensor based and map-based variable rate phosphorus fertilization (Maleki et al., 2008; Mouazen and Kuang, 2016) and variable rate N-fertilizer application (Halcro et al., 2013). However, accurate recommendation maps for variable rate applications will depend on accurate prediction of soil properties with vis-NIR spectroscopy, which can be achieved by minimizing error in reference and spectra measurements, minimizing influences of ambient conditions and finally by adopting effective spectra pre-processing and advanced data mining techniques.

In order to gain the full advantage of the use of vis-NIR, different techniques have been applied to the development of calibration models, such as spiking of samples from target site or dataset into existing spectral library (Brown, 2007; Sankey et al., 2008; Wetterlind et al., 2010; Kuang and Mouazen, 2011, 2013; Guerrero et al., 2014). The geographical scale of soil samples collected was reported to have influence on model performance (Sudduth and Hummel 1996). This will be especially evident when predicting variations on a small scale (Brown, 2007). Combining global and local samples by adding a few local ones to a more general soil library

73 (spiking) and recalibrating was proposed by Brown (2007) as another way to increase the
74 accuracy of soil organic carbon (SOC) prediction, as opposed to local-sample calibrations.
75 Sankey et al. (2008) also reported improved prediction results for clay content, SOC and
76 inorganic carbon, using the same global calibration set spiked with local samples from three
77 highly variable landscape study sites in Montana, US, compared with global or local calibrations
78 alone. Kuang and Mouazen (2013) used spiking technique with different dataset ratios for mobile
79 vis-NIR modelling at European field scale. They achieved good results using partial least square
80 regression (PLSR) models for soil moisture content (MC), SOC, and total nitrogen (TN) with
81 residual prediction deviation (RPD) (calculated as standard deviation of measured soil properties
82 divided by root mean square error of prediction) of 2.76 to 3.96, 1.88 to 2.38, and 1.96 to 2.52,
83 respectively. Limited works have been reported on the combined effect of spiking and samples
84 scale on model predictive performance in soil analysis (Sankey et al., 2008; Guerrero et al.,
85 2010; Wetterlind and Stenberg, 2010; Guerrero et al., 2014), particularly for mobile collected
86 vis-NIR spectral data, where no reports could be found in the literature.

87 As a linear multivariate analysis, PLSR is the most commonly used technique for soil spectral
88 analysis (Conforti et al., 2013, 2015). However, the accuracy of linear-regression techniques in
89 spectroscopic analysis tends to decrease due to the non-linear nature of the relationship between
90 spectral data and the dependent variable (Araújo et al., 2014). Data-mining techniques, such as
91 artificial neural network (ANN) (Mouazen et al., 2010; Kuang et al., 2015), multivariate adaptive
92 regression splines (MARS) (Bilgili et al., 2010; Nawar et al., 2015) and support-vector machines
93 (SVM) (Morellos et al., 2016; Nawar et al. 2016), were reported to improve the accuracy of the
94 calibration models. As a nonlinear method based on the machine learning theory, SVM was
95 proposed by Vapnik (1998) to be capable of modelling linear and nonlinear relationships and

96 solving calibration problems with high performance (Suykens and Vandewalle, 1999). SVM has
97 been used successfully for modelling soil properties based on reflectance spectroscopy (e.g.
98 Viscarra Rossel and Behrens, 2010; Vohland et al., 2011; Peng et al., 2014; Nawar et al., 2016),
99 and has gained extensive application in soil spectroscopy, because of its advantages and high
100 performance (Viscarra Rossel and Behrens, 2010; Vohland et al., 2011). As nonparametric
101 method MARS estimates complex nonlinear relationships among independent and dependent
102 variables (Friedman, 1991), and has been effectively applied in different fields (Luoto and Hjort,
103 2005; Bilgili et al., 2010; Felicísimo et al., 2012; Samui, 2012) and generally exhibits higher
104 performance results for modelling soil properties (e.g. Shepherd and Walsh, 2002; Bilgili et al.,
105 2010; Nawar et al., 2016). However, these linear and non-linear modelling methods were not
106 compared in the literature for soil analyses at different geographical scales including spiking.
107 This is particularly true for modelling of mobile collected vis-NIR soil spectra.

108 The aim of this paper was to compare the predictive performance of the vis-NIR spectroscopy of
109 TN, TC and MC for field samples based on single field, two-field, national and continental
110 scales, using PLSR and two multivariate data-mining techniques, namely, SVM and MARS. The
111 calibrations were made using laboratory and mobile collected soil spectra for predicting within-
112 field variation in named soil properties.

113 **2. Materials and methods**

114 *2.1. Experimental sites*

115 The experimental wok was carried out in two fields in Yorkshire, UK. Hagg field is located at
116 Cawood, north Yorkshire with longitudes of -1.172° and -1.166° W, and latitudes of 53.936° and
117 53.941° N with total area of about 21 ha (Fig. 1). This field is characterised by fosters cooler

118 summer conditions with regular rainfall (average annual 600 mm), and the mean air temperatures
119 range from 1°C to 6°C in winter and from 8°C to 18°C in summer, allowing more consistent
120 crop growth. The field is cultivated with vegetables crops (leeks, cabbage, carrots and onions).
121 The soil type is a slightly acidic sandy loam with impeded drainage to the south and eastern
122 margins of the field. The soil organic matter (SOM) ranges between 0.7 and 1.95% at 0–30 cm
123 depth. Hessleskew field is located in Sancton, north Yorkshire between longitudes -0.590° and -
124 0.586° W, and latitudes 53.844° and 53.844° N and with total area of about 12 ha (Fig. 1).
125 Elevations in the area barely reach 212 m above sea level. The annual rainfall and air
126 temperature are in the same range of the Hagg field. The field is characterised by freely draining
127 with texture varies between clay loam to clay. The SOM ranges between 0.9 and 2.1%, and it is
128 cultivated with cereal crops in rotation.

129 *2.1. Mobile soil measurement and collection of soil samples*

130 The mobile measurement system designed and developed by Mouazen (2006) was used to
131 measure both fields. It consists of a subsoiler, which penetrates the soil to the required depth,
132 making a trench, whose bottom is smoothened by the downwards forces acting on the subsoiler
133 (Mouazen et al., 2005). The subsoiler was retrofitted with the optical unit and attached to a
134 frame. This was mounted onto the three point linkage of the tractor (Mouazen et al., 2005). An
135 AgroSpec mobile, fibre type, vis–NIR spectrophotometer (Tec5 Technology for Spectroscopy,
136 Germany) with a measurement range of 305–2200 nm was used to measure soil spectra in
137 diffuse reflectance mode. The sampling interval of the instrument was 1 nm. A deferential global
138 positioning system (DGPS) (EZ-Guide 250, Trimble, USA) was used to record the position of
139 mobile measured spectra with sub-meter accuracy. Each scan consisted of three spectra that were
140 averaged in one spectrum representing about 1.2 m travel distance. Outlier spectra were visually

141 detected and removed from further analyses. These outlier spectra represented 2.5 and 4% out of
142 12766 and 14276 soil spectra collected from Hessleskew and Hagg fields, respectively. During
143 the measurement at each line, 3 or 4 soil samples were collected from the bottom of the trench
144 and the sampling positions were carefully recorded with a DGPS. The locations of soil samples
145 were selected to cover the soil variation within both fields. A total of 122 and 149 soil samples
146 were collected during the mobile measurement form Hessleskew and Hagg fields, respectively
147 (Fig. 1). Measurements were carried out in 2015 and 2016 for the former and latter fields,
148 respectively, pulling the sensor at 12 m gap between adjacent transects (Fig. 1).

149 **(Fig. 1)**

150 *2.2. Laboratory chemical and optical measurements*

151 Each sample was divided into two parts; one part was dried for 24 h at 105 ºC and the other part
152 was left fresh (wet). The dried soil sample was analyses for total carbon (TC) according to the
153 British Standard BS 7755 Section 3.8:1995 using combustion method, which is identical to ISO
154 10694:1995. Total nitrogen was determined by the Dumas method, where the soil samples are
155 heated to 900ºC in the presence of oxygen gas as described by British Standard BS EN 13654-
156 2:2001. Soil MC was determined by oven drying of the soil samples at 105 ºC for 24 h. The
157 precision of standard laboratory analyses for TN, TC, and MC indicated that uncertainties values
158 (mean values and standard deviations) were 0.35±0.025%, 3.8±0.26%, and 20±1.22%,
159 respectively.

160 The fresh part of soil sample was placed in a glass container and mixed well. Three Petri dishes
161 of 2 cm in diameter and 2 cm deep were used for three replicate measurements. Each soil sample
162 was then placed into these Petri dishes and pressed gently before levelling with a spatula to

ensure a smooth surface; and therefore maximum light reflection and a large signal-to-noise ratio (Mouazen et al., 2005). Soil samples were scanned by the same spectrometer used in the mobile measurements. A total of ten scans were collected from each replicate, and these were averaged into one spectrum for each sample.

2.3. Spectra pretreatment

The same pretreatment of soil spectral data was carried out for all soil properties investigated using R packages (prospectr; https://cran.r-project.org/web/packages/prospectr). First, noise was removed at both edges of each spectrum and the spectra were cut to 370–1979 nm. Then, the number of wavelengths was reduced by averaging five successive wavelengths. Maximum normalization was followed, which is typically used to get all data to approximately the same scale, or to get a more even distribution of the variances and the average values. Spectra were then subjected to Savitzky–Golay first derivation (Martens and Naes, 1989) with a second-order polynomial approximation. Finally, the Savitzky-Golay smoothing was carried out to remove noise from spectra and to decrease the detrimental effect on the signal-to-noise ratio that conventional finite-difference derivatives would have. Spectra modification due to the different pretreatments followed in this study is shown in Fig. 2.

(Fig. 2.)

2.4. Spectral dataset with different scale

The following four different data sets were considered:

1- Single-field dataset (SFD; n=122 for Hessleskew and 149 for Hagg), where samples from one field either Hessleskew or Hagg fields were used.

2- Two-field dataset (TFD; n=271), where samples from both fields were merged into one

185 dataset;

186 3- UK national dataset (UND; n=89), where samples collected from four fields in the UK were
187 used; and

188 4- European continental dataset (ECD; n=529), where samples from sixteen fields collected from
189 five European countries were used. These included samples from Germany (two fields),
190 Denmark (five fields), the Netherlands (one field), Czech Republic (four fields) and the UK (four
191 fields), where 151, 147, 43, 99, and 89 samples were collected, respectively (Kuang and
192 Mouazen, 2011, 2013).

193 Spiking was used to introduce the local variability of the two experimental fields into the
194 existing data sets (e.g., UND and ECD). A total of 85 and 110 samples were spiked from the
195 Hessleskew and Hagg fields, respectively, into the UND and ECD. After spiking, the total
196 number of samples for UND and ECD used to develop calibration models were 174 and 614, and
197 199 and 639, for Hessleskew and Hagg fields, respectively. A principal component analysis
198 (PCA), was performed on 724 samples of the ECD including the two experimental fields of the
199 current studies to explore similarity between different groups of soil samples.

200 *2.5. Development of calibration models*

201 The four datasets discussed above were subjected to PLS, MARS and SVM analyses with the
202 leave-one-out cross validation using R software (R Core Team, 2013), which resulted in four
203 groups of models for each modelling technique for each soil property, e.g., for SFD, TFD, UND
204 and ECD. Before running the analysis the entire dataset of each target field (Hesseleskew or
205 Hagg) was divided into 75% for calibration, and 25% for prediction. This was done for both the
206 laboratory and mobile collected soil spectra. The 75% soil samples were also spiked into the

UND and ECD. The same prediction samples (25%) were used for both laboratory and mobile validation of obtained results of the four models for each soil property.

PLSR is a popular multivariate regression method that has a good capacity for estimating attributes resulting from the spectral characteristics of the soil (Vasques et al., 2008; Song et al., 2013; Yu et al., 2016). To determine the optimal number of latent factors, leave-one-out cross-validation (LOOCV) was used (Efron and Tibshirani, 1993) to prevent over- or under-fitting the data, which may produce models with poor performance. The root mean squared error of cross validation (RMSECV) of the predictions and the coefficient of determination (R^2) were ascertained to identify the optimal cross-validated calibration model. Generally, a model with the highest cross-validated R^2 value and lowest RMSECV value was selected.

SVM is a kernel-based learning method originated from statistical learning theory (Vapnik 1995). Kernel-based learning methods use an implicit mapping of the input data into a high dimensional feature space defined by a kernel function (Karatzoglou and Feinerer, 2010). The ε-SVM-Regression (ε-SVMR) uses training data to obtain a model represented as a so-called ε-insensitive loss function, which maps independent data with maximum ε deviation from dependent training data. Error within the predetermined distance ε from the true value is ignored, error greater than ε is penalised (Vohland et al. 2011). In consequence, the model reduces the complexity of the training data to a significant subset of so-called support vectors. In the current study, the SVM models were developed using libsvm algorithm with ε-SVM and radial basis function (RBF) kernel using e1071 package in R (Meyer et al., 2015). The optimal parameters of SVM (cost, epsilon, gam(γ) and sig2(σ2)) were adopted to regulate the models. For each combination of cost, gam(γ) and sig2(σ2) parameters, the root mean square error of cross-validation (RMSECV) was calculated, and the optimum parameters were selected to produce

smaller RMSECV. The leave-one-out cross validation (LOOCV) was used for the validation process.

MARS is data mining technique developed by Friedman (1991). MARS was applied as a regression method in several disciplines (Shepherd and Walsh, 2002; Bilgili et al., 2010; Nawar et al., 2015) and was generally reported to show better performance than others traditional statistical methods for soil analysis based on vis-NIR spectra (Nawar et al., 2016). The MARS analysis uses basis functions to model the predictor and response variables (Hastie et al., 2009). To construct the basis functions, MARS splits the data into sub-regions (splines) with different interval ending knots where the regression coefficients change and fits the data in each sub-region by using a set of adaptive piecewise linear regressions. These basis functions are subsequently used as new predictor variables for modelling purposes. Each basis function may contain nonlinear and variable interaction factors of the second and third order as well as linear combinations. To measure lack of fit, avoid over-fitting, and improve prediction, the redundant basis functions are removed one at a time using a backward stepwise procedure. Additional basis functions in the model provide greater flexibility but also add complexity. However, MARS attempts to minimise model complexity by selecting the optimal model based on the lowest generalised cross-validation value.

In order to evaluate the model performance for the prediction of named soil properties three statistical parameters were used: R^2, root mean square error (RMSE) and the ratio of the performance to interquartile distance (RPIQ) (Bellon-Maurel et al., 2010) defined as fellow:

$$RPIQ = \frac{IQ}{RMSE}$$

where IQ is the difference between the third and first quartiles (IQ = Q3-Q1).

Arbitrary groups have been used for simplification of interpretation: (1) excellent models (RPIQ >2.5), (2) very good models (2.5 > RPIQ > 2.0), (3) good model (2.0 > RPIQ > 1.7), fair (RPIQ 1.7 > RPIQ > 1.4), and very poor model (RPIQ<1.4). This classification was adopted in this study to compare between different models in cross-validation and in laboratory and mobile prediction.

3. Results

3.1 Laboratory measured soil properties and spectral datasets

The results of the descriptive statistical analyses for soil parameters are shown in Table 1. For Hessleskew field, the TN is low, with a mean value of 0.25%, whereas the mean values of TC and MC ranges from 2.121% to 18.9%, respectively. In the Hagg field, the TN is also low, with a mean value of 19.21%. TC is smaller than that of Hessleskew field, ranging between 1.34% and 3.18%, whereas MC was higher than that in Hessleskew, ranging between 11.53% and 24.64% (Table 1). The small range of laboratory analysis values of the studied soil properties indicates these fields are not the ideal case study fields. This small soil variability within both fields may be reduced the prediction capability of the established calibration models (Kuang and Mouazen, 2011).

(Table 1)

The PC similarity maps of principal component (PC) 1 and PC2 shows clear separation between different groups of samples collected from the five European countries. A clear overlap of the two study field spectra with those of the UND collected can be observed (Fig. 3), explain the effect of geographical origin on soil samples on vis-NIR spectroscopy analysis for soil properties.

(Fig. 3)

3.2. Performance of calibration models in cross-validation

The calibration methods considered in this study provide different prediction accuracies of TN, TC and MC. Tables 2 and 3 summarise the cross-validation results for calibration models developed with different datasets. Figures (4 and 5) illustrate the performance of prediction models in terms of RPIQ for Hessleskew and Hagg field, respectively. Cross-validation results indicate that MARS has over-performed SVM and PLSR for modelling three studied soil properties in cross-validation, followed, successively by SVM and PLSR, which is the least performing method. Among MARS models, the best results for TN is obtained with ECD with R^2 = 0.96, RMSECV = 0.01%, and RPIQ = 7.46 for Hagg field (Table 3), and R^2 = 0.96, RMSECV = 0.01%, and RPIQ = 7.41 for Hessleskew field (Table 2). The best results for TC are achieved using a MARS model developed with the ECD in both Hagg field (R^2 = 0.98, RMSECV = 0.10% and RPIQ = 6.57) and Hesselskew field (R^2 = 0.98, RMSECV = 0.06% and RPIQ = 4.87). Similar model performance to those of TN and TC is also observed for MC, with the best results in cross-validation were calculated for the MARS models developed with the TFD (not with ECD as for TN and TC) for the Hagg field (R^2 = 0.93, RMSE = 0.53% and RPIQ = 5.15) and Hessleskew field (R^2 = 0.92, RMSECV = 0.53% and RPIQ = 5.11).

3.3. Performance of calibration models for laboratory prediction

The developed calibration models were validated using laboratory scanned spectra of the prediction sets. Tables 2 and 3 summarise the accuracy of the laboratory prediction for the studied soil properties at the different calibration scales. The cross-validation results show considerably better results than those obtained for laboratory predictions. Among the studied modelling techniques, MARS models generally provide the best results for the studied soil

296 properties. For TN, the best performance is obtained with MARS using the ECD dataset with R^2
297 = 0.87, RMSE = 0.03%, and RPIQ = 5.21 for Hessleskew field (Table 2; Fig. 4), and R^2 = 0.77,
298 RMSE = 0.03%, and RPIQ = 3.57 for Hagg field (Table 3; Fig. 5). PLSR-SFD based modelling
299 has resulted in the least appreciable results for TN in Hessleskew field (R^2 = 0.50, RMSE =
300 0.01%, and RPIQ = 1.21), followed by SVM with SFD (R^2 = 0.51, RMSE = 0.01%, and RPIQ =
301 1.41, as shown in Table 2). However, SVM showed better performances for predicting TN for
302 TFD, UND and ECD, compared to PLSR using the corresponding datasets. For Hagg field, the
303 worst results are obtained with PLSR-SFD based modelling (R^2 = 0.54, RMSE = 0.02%, and
304 RPIQ = 2.36, Table 3). Again SVM over-performed PLSR models, but under-performed MARS
305 models (Tables 2 and 3).
306 The best results for TC laboratory prediction are achieved using the MARS model based on the
307 ECD (R^2 = 0.88, RMSE = 0.19% and RPIQ = 5.94) for Hessleskew field, as well as for Hagg
308 field (R^2 = 0.85, RMSE = 0.46% and RPIQ = 4.34). The lowest prediction performance is
309 obtained with PLSR models particularly for the TFD in Hagg field and Hessleskew field with R^2,
310 RMSE, and RPIQ of 0.52 and 0.57, 0.24% and 0.23, and 1.95 and 1.98, respectively (Tables 2
311 and 3). SVM models show the same trend as for the cross-validation where it outperform PLSR
312 for all datasets in both fields, and the best results are obtained with TFD in Hagg field (R^2 = 0.89,
313 RMSE = 0.14% and RPIQ = 3.26) and with ECD in Hessleskew field (R^2 = 0.79, RMSE = 0.25%
314 and RPIQ = 3.19).
315 Results for MC show a similar trend to those of TN and TC, as the best performing prediction is
316 obtained with the MARS models based on the TFD (not with the ECD, as for TC and TN) in
317 both fields. The worst performing models are for PLSR with TFD in Hessleskew field (R^2 =
318 0.48, RMSE = 1.38% and RPIQ = 1.69) and ECD in Hagg field (R^2 = 0.57, RMSE = 1.72% and

RPIQ = 2.26). SVM generates acceptable results, with the best model accuracy obtained with ECD in Hagg field (R^2 = 0.77, RMSE = 1.72% and RPIQ = 3.0), and the lowest accuracy obtained with SFD in Hessleskew field (R^2 = 0.53, RMSE = 1.32% and RPIQ = 0.90) (Table 2). Similar trend to that of the cross-validation can be concluded for the laboratory prediction. For example, MARS has over-performed SVM and PLSR for the three studied soil properties followed, respectively by SVM and PLSR, which is the least performing method. The only exception is for MC, where depending on the dataset, SVM over-performed PLSR in two cases only out of four. Here, it is not necessary the case that the ECD models outperformed corresponding models developed with the other three datasets.

3.4. Performance of calibration models for mobile prediction

The mobile collected spectra were used to predict soil TN, TC and MC using the calibration models developed in advance, as explained above. The laboratory reference measurement values were compared with the mobile predicted concentration values at the same positions. Tables 2 and 3 summarise the accuracy of the mobile measurement for the studied soil properties at the different-scale datasets.

For TN, the best results are obtained with MARS, followed by SVM and PLSR, respectively, which is similar for the trends in cross-validation and laboratory prediction. The highest MARS model performance is resulted with the ECD dataset with R^2 = 0.79, RMSE = 0.02%, and RPIQ = 3.26 for Hessleskew field (Table 2; Fig. 4), and R^2 = 0.73, RMSE = 0.03%, and RPIQ = 3.16 for Hagg field (Table 3; Fig. 5). The least acceptable results are produced by SVM using SFD of Hessleskew field (R^2 = 0.48, RMSE = 0.02%, and RPIQ = 1.17), followed by PLSR-SFD for the Hagg field (R^2 = 0.49, RMSE = 0.03%, and RPIQ = 1.96, Table 3). However, SVM show a good

341 performance for predicting TN with TFD and less evident with UND, for both fields,
342 outperforming PLSR for both datasets.
343 Like for TN, the best results for TC are achieved using the MARS-ECD model for Hagg field
344 (R^2 = 0.81, RMSE = 0.29% and RPIQ = 4.33) and Hessleskew field (R^2 = 0.81, RMSE = 0.31%
345 and RPIQ = 3.57). The mobile perdition of PLSR models are of lower degree of accuracy
346 particularly for SFD of Hagg field with R^2, RMSE, and RPIQ of 0.50, 0.23%, and 1.97,
347 respectively, which is comparable to the results of SVM-SFD (Table 3). The best results for
348 SVM are obtained with ECD, which is a similar trend to that in the cross-validation modelling.
349 Generally MARS models provided considerably better performance in mobile prediction than
350 both SVM and PLSR, which performed almost equally. The one exception is when the UND is
351 used, with which both PLSR and SVM performed better than TC.
352 The mobile prediction of MC follows the same trend of the cross-validation, as the best results
353 are obtained with MARS for seven out of eight cases in both fields (Tables 2 and 3). The best
354 mobile prediction performance is resulted from the MARS-ECD modelling in Hessleskew field
355 (R^2 = 0.73, RMSE = 1.91% and RPIQD = 1.94) and MARS-UND in Hagg field (R^2 = 0.72,
356 RMSE = 1.91% and RPIQ = 2.58). The results of PLSR-TFD model of Hessleskew field are the
357 least accurate over all models (R^2 = 0.48, RMSE = 1.36% and RPIQ = 1.58). Depending on the
358 data set used, SVM generated slightly better results than PLSR with RPIQ values ranging
359 between 1.76 and 2.19 for Hagg field (Fig. 5), and 1.32 and 2.66 for the Hessleskew field (Fig.
360 4).
361 In the majority of models, MARS has over-performed SVM and PLSR for the three studied soil
362 properties in mobile prediction, followed, respectively by SVM and PLSR, which is the least

363 performing method. The only exception is for MC, where depending on the dataset, SVM over-
364 performed PLSR in three cases out of four.

365 **(Table 2)**

366 **(Table 3)**

367 *3.5. Analysis of uncertainty versus RMSE*

368 To investigate the accuracy and quality of results obtained with laboratory prediction, we
369 compared the RMSE with uncertainty calculated for standard laboratory chemical analyses (Figs.
370 6 and 7). The majority of models result in smaller RMSE than the uncertainty (0.35±0.025%,
371 3.8±0.26%, and 20±1.22% for TN, TC, and MC, respectively). This is indeed the case in for
372 Hessleskew field, particularly for TN and TC with MARS and SVM (Fig. 6), whereas RMSE
373 becomes larger than the uncertainty level for MC when the three modelling techniques are
374 applied for the UND and ECD datasets. Similarly in Hagg field, RMSE is larger than the
375 uncertainty level for not only MC but also TN and TC, for both the UND and ECD datasets (Fig.
376 7).

377 **(Fig. 4)**

378 **(Fig. 5)**

379

380 **4. Discussion**

381 *4.1. Comparison performance of modelling techniques*

382 This study compared the performance of the MARS, SVM and PLSR models for the prediction
383 of TC, TN and MC based on different datasets. The variations in RPIQ and RMSE values

obtained from models in cross-validation, laboratory and mobile prediction are shown in Tables 2 and 3. MARS models have over-performed SVM and PLSR for modelling the three studied soil properties in cross-validation, laboratory and mobile prediction. Examining the values of RPIQ in cross-validation, laboratory and online prediction, respectively, of MARS models allows confirming that the predictive performance of the MARS model in this study was high. This result is in line with results reported by Nawar et al. (2016) for non-mobile measurement, who found that MARS performed SVM and PLSR. Based on the adapted RPIQ groups, models in laboratory prediction show excellent accuracy for TN and TC, but only good for MC, whereas the accuracy of mobile prediction are excellent, very good and good for TN, TC and MC, respectively. Laboratory and mobile predictions of TN and TC are better than those obtained by other researchers for PLSR models (e.g. Kuang and Mouazen, 2011, 2013) (R^2 = 0.75–0.93 and 0.74–0.89; RMSE = 0.03–0.06% and 0.7–1.1%, for TN, and TC, respectively), while for MC the results of Kuang and Mouazen (2013) were better (RMSE = 0.32–0.74% and 0.36–0.84% for laboratory and online predictions, respectively. This is because the MARS modelling technique typically yields better results when a nonlinear relationship between reflectance and concentration exists, whereas the PLSR model fits only linear relationships (Brown et al., 2006; Mouazen et al., 2010; Viscarra Rossel and Behrens, 2010; Nawar et al., 2016).

Generally, after MARS SVM was the best performing method in cross-validation for the three studied soil properties. This was not always the case for laboratory and mobile prediction, where depending on the dataset PLSR overperformed SVM and even MARS (Tables 2 and 3). These results are supported by the findings of Viscarra Rossel and Behrens (2010), who showed that SVM provided more robust predictions of soil organic carbon than PLSR models. Similarly, and Nawar et al. (2016) also showed that the non-linear nature of SVM let to a better results than

PLSR. Morellos et al. (2016) also found SVM to overperform two linear methods, namely, PLSR and principal component regression for modelling OC, TN and MC. This is because SVM is a non-linear and flexible method, capable to model complex, non-linear and linear relationships between variables (Viscarra Rossel and Behrens 2010). However, in the current work we prove this to be the case for mobile prediction too.

Although the results of PLSR models showed the weakest performance among the three models in cross-validation, SVM and PLSR performed equally in the laboratory and mobile prediction depending on the data set. This was especially the case with the Hagg field. At the Hessleskew field, the variation in concentrations of studied soil properties was slightly higher (Table 1) than that in the Hagg field. This resulted in slightly higher not only RPIQ and R^2 values but also RMSE values, which is in line with findings of Kuang and Mouazen (2011).

The small prediction datasets used in the current work (37 and 39 for Hessleskew and Hagg fields, respectively), might have affected the prediction performance in the laboratory and mobile predictions, as a small data set size was reported to lead to various counterintuitive and unfamiliar side effects, which can significantly impact the validation results and lead to a very poor performance (Klement et al., 2008).

Model performance for TN and TC in cross-validation, laboratory and mobile prediction behaved differently from models for MC. It is interesting and rather odd to observe that TC and TN models to overperform MC model, which is not a typical finding in vis-NIR spectroscopy for soil analyses, as MC used to over-perform all other soil properties models (Kuang and Mouazen, 2013; Mouazen et al., 2010; Morellos et al., 2016). No other reason could be found for the odd MC prediction behaviours except that the current field were of stony soils that might contributed

to the error of MC laboratory measurement with the drying method.

Based on Figs. 6 and 7, we observed that relatively small values of RMSE for TN and TC, having large range of concentrations, indicate unbiased predictions. In addition, the majority of RMSE values lie within the uncertainties levels with an average deviation < 5% for TN and TC and 6.35% for MC. These deviations are much smaller for MARS compared to PLSR, indicating good prediction performance of MARS models for both the laboratory and mobile predictions.

(Fig. 6)

(Fig. 7)

4.2. Influence of geographical scale on Models' performance

The dataset (scale) has shown to have a considerable effluence on the performance of calibration and prediction of TN, TC, and MC. Spiking local samples in the UND and ECD libraries almost always improved the model performance, particularly in cross-validation, compared with those obtained using the SFD and TFD (Tables 2 and 3), which is in agreement with the results presented by Brown (2007) and Sankey et al. (2008), although the current work is based on a smaller scale datasets of a smaller variability. The improvement was mainly expressed as an increase in R^2 and RPIQ values, but a decrease in RMSE (Tables 2 and 3). This finding is in agreement with Brown (2007) findings, who reported a great reduction in RMSE for predictions of SOC in upland soil samples from a catchment in Uganda, by adding local samples to a global library. Furthermore, it is also in line with the findings of Kuang and Mouazen (2013) that spiking local soil samples into ECD datasets proved to be an efficient way to improve the prediction accuracy of target field samples.

Examining the RPIQ values obtained with different dataset suggest that spiking of laboratory scanned spectra into UND and ECD is a successful strategy to obtain accurate mobile predictions of soil properties. Figs. 4 and 5 and Tables (2 and 3) illustrate how spiking coupled with MARS have led to the highest mobile prediction performance compared to PLSR and SVM, particularly at ECD scale, for which RPIQ values were of good to very good values according to the adopted RPIQ groups. Compared to published results of spiking of a ECD with target field samples obtained with PLSR analyses (Kuang and Mouazen, 2013) for TN (RPD = 1.96–2.52), OC (RPD = 1.88–2.38), and MC (RPD = 2.76–3.96), comparable results with slight improvements were obtained in the current work for mobile MARS-ECD prediction, only for TN and TC. Compared with artificial neural network (ANN)-ECD (nonlinear) model performance for the mobile prediction of SOC reported by Kuang et al. (2015), slight improved results can be observed with MARS-ECD obtained in the current work (RPIQ for TC = 3.57 – 4.33), as RPD values reported by Kuang et al. (2015) were improved from 1.93 for PLSR analysis to 2.28, for ANN. Furthermore, the current results outperform those obtained by other researchers (Pietrzykowski and Chodak, 2014) for TN based on non-mobile measurement and PLSR analysis only (RPIQ = 2.34), and combined PLSR with genetic algorithm (RPIQ = 4.12; Ludwig et al., 2017). This is also true for TC based on PLSR (RPIQ = 31.3; Sarkhot et al., 2011) and SVM and PLSR (RPIQ = 2.03 and 2.59, respectively; Wijewardane et al., 2016). This is at least a step forward the current work have shown that there will be always an opportunity to improve the mobile prediction performance by adopting new data mining techniques (e.g., MARS in the current work). Considering the narrow variation range of soil properties in the two measured fields (Table 1), the concept of spiking a general dataset with samples from measured target field seems to be a successful calibration procedure for mobile vis–NIR measurement of soil TN, TC

473 and MC. The alternative concept to spiking would be to collect a sufficient number of soil
474 samples from a target site (e.g. SFD or TFD) and produce calibration models for mobile
475 prediction of soil properties as proposed by Mouazen et al. (2007). In this concept, one should be
476 lucky to encounter sufficient spatial variability in the target site, to enable establishing
477 calibration models (Guerrero et al., 2010; Wetterlind et al., 2010). This concept is definitely
478 more expensive than the spiking, as a much larger number of soil samples should be collected
479 from a site (> 5 sample per ha, or > 100 samples per field), compared to spiking, where
480 depending of the spatial variability only few samples (e.g., 1–2 sample per ha) would be
481 sufficient to account for the specific soil variability of the target site. Kuang and Mouazen (2012)
482 suggested that among different sample number datasets studied (e.g., 25, 50, 75 and 100
483 samples), the number of soil samples should be chosen according to the accuracy required,
484 although 50 soil samples was considered appropriate to establish calibration models of TN, SOC
485 and MC. This is correct assuming that considerable spatial variability exists in the dataset to
486 enable correlation between soil spectra and target soil properties to be established, which is not
487 the case for all fields where for some fields variability could be very small. Therefore, spiked
488 ECD calibration models with target field specific samples are successful prediction tools for
489 mobile vis–NIR spectroscopy sensing of the studied soil properties.

490 Similar to the mobile prediction, spiking of the ECD in particular seems to provide the best
491 prediction performance for laboratory scanned (non-mobile) soil spectra. Spiking local (target
492 site) soil samples into global or ECD models for non-mobile calibrations proved to be an
493 efficient approach to improve the prediction accuracy of a target field for some soil constituents
494 (Shepherd and Walsh, 2002; Janik et al., 2007; Waiser et al., 2007; Minasny et al., 2009;
495 Viscarra Rossel et al., 2009; Wetterlind and Stenberg, 2010; Guerrero et al., 2010; Kuang and

496 Mouazen, 2013).

497 In line with findings of Kuang and Mouazen (2011), it is believed that a fundamental factor that
498 leads to improved model performance (in both mobile and laboratory predications) is the wide
499 range of variability of TN, TC, MC which can be secured with the ECD. Stenberg et al. (2010)
500 reported that the model performance depends on to a large extent on variability encountered in
501 the dataset, including soil types, which is the case in the ECD of the current work. This may be
502 attributed to the fact that different soil types can have considerably different physical and
503 chemical characteristics influencing soil spectra, which is attributed to differences in the parent
504 materials. Thus, with large soil heterogeneity, regression can be more successful and this may
505 influence the model accuracy. The high performance for estimating the soil properties in the
506 current research obtained with MARS may be attributed to the wide range of variation of the
507 large-scale dataset (ECD), shown in Table 1.

508 In the present study, spiked UND and ECD models did not result in substantially lower RMSE
509 values compared with the results obtained with when using local calibrations alone (e.g., SFD
510 and TFD). This corresponds to the small and variable differences for TN, TC and MC between
511 the calibrations with the spiked UND and ECD libraries, and the local-only samples, which is in
512 agreement with observations found by Brown (2007). Moreover, these results were consistent
513 with the observations for TN, OC, and MC made by Kuang and Mouazen (2013), who obtained
514 substantially better predictions for some sites using the ECD library spiked with local samples,
515 compared with using only local samples. These authors confirmed that although higher R^2 and
516 RPD values can be obtained with spiked ECD calibration models, higher RMSE values should
517 be expected.

518

519 **5. Conclusions**

520 In this study, the partial least squares regression (PLSR), support vector machine (SVM) and
521 multivariate adaptive regression splines (MARS) methods were compared for the laboratory
522 (non-mobile) and mobile prediction of soil total nitrogen (TN), total carbon (TC) and moisture
523 content (MC) in two fields (e.g., Hessleskew and Hagg) using four different datasets of different
524 geographical scales. Generally, the accuracy of the PLSR, SVM and MARS models varied in
525 accordance with variations in the calibration scales. Results showed the majority of the non-
526 linear calibration methods (particularly MARS) to outperform the linear PLSR in cross-
527 validation modelling. However, PLSR provided acceptable accuracy for the prediction of the
528 studied soil properties. The most important finding was that in general results of cross-validation
529 to improve with increasing the scale of the data set from one field dataset (SFD), to two fields
530 (TFD), and finally spiking with large data set collected from some fields in the UK (UND), and
531 from several fields in Europe (ECD). However, the validation of model performance in
532 prediction does not necessarily follow the same trend. Higher prediction results were observed
533 for the individual and two-field data set as compared to the large EU data set. Another interesting
534 finding was that the two-field data set resulted in skewness of predicted values towards the field
535 with high concentration of a given soil property.

536 The ECD calibrations seem to be the best option for mobile predictions of the studied soil
537 parameters as compared to field or field scale. The ECD calibrations based on 529 samples
538 outperformed UND (89 samples), TFD (234 samples) and the SFD (122 and 149 for Hessleskew
539 and Hagg, respectively) models for TN, TC and MC at both fields. The potential for good
540 calibration was obtained particularly for TC and TN. There was a tendency for better predictions

when spiking the ECD dataset compared to spiking the UND dataset, particularly for TN and TC.

The predictive models for estimating TN, TC and MC may become more accurate through the selection of an optimal data set to spike with UND and ECD libraries. Future research should focus on the potential for integration of data-mining techniques with the optimal spiked libraries for improving the prediction accuracy at different scales. We believe that these estimation models should be subjected to further examination and optimisation prior to their broad application in soil TN, TC and MC modelling and mapping.

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Predictive performance of mobile vis-near infrared spectroscopy for key soil properties at different geographical scales by using spiking and data mining techniques

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