Comparing Predictive Performance Of Near Infrared Spectroscopy At A Field, Regional, National And Continental 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 is a crucial step for variable rate application in precision agriculture. The objective of the present study was to compare the prediction performance of vis-NIR spectroscopy at local, regional, national and continental scales using data mining techniques including spiking. Fresh soil samples collected from farms 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. The partial least squares regression (PLSR), multivariate adaptive regression splines (MARS) and support vector machines (SVM), with leave-one-out cross-validation were used to establish calibration models of total nitrogen (TN), total carbon (TC) and soil moisture content (MC). The results showed the lowest model performance to be obtained when the single field (local scale) data were used in the calibration models. The effect of spiking was significant and the best model performance was obtained when local samples collected from two fields in the UK were spiked with European soil samples (continental), followed by when the same samples were spiked with UK samples (national). Therefore, these results suggest that continental and national vis-NIR calibration models can be successfully used to predict TN, TC and MC. Therefore, selection of the optimal soil samples with the appropriate data mining technique should be considered when developing vis-NIR calibration models for a non-standard soil to cover a wide variation range.*

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 characterisation. It offers high spatial resolution sampling compared with that possible in conventional laboratory analysis (Shepherd and Walsh, 2002; Wetterlind et al., 2010). This technique also allows for on-line measurement with high soil-sampling resolution (Maleki et al. 2008, Kuang and Mouazen 2013). Precision agriculture aims to optimize management of within field variability for sustainable increase in land productivity. Variable-rate fertiliser application, which requires reliable soil information at a high spatial resolution, is required to achieve this goal (Wetterlind et al., 2010). Vis-NIR spectroscopy, under both mobile and non-mobile measurement, has been used successfully for modelling and mapping soil properties (i.e.,, Shibusawa et al., 2001, Kuang and Mouazen 2013, Kuang et al., 2015), and producing application maps for phosphorus (Maleki et al. 2008, Mouazen and Kuang 2016) and N-fertilizer application (Halcro et al., 2013).

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 data mining and spiking with other soil spectral library (Wetterlind et al. 2010, Kuang and Mouazen 2013). Regional, national or continental calibrations would be favourable in this respect, but the overall variation or the geographical scale for which calibrations are representative clearly influences their degree of precision (Sudduth and Hummel 1996). This will be especially evident when predicting variations on a smaller scale (Brown, 2007). Combining global and local samples by adding a few local ones to a more general soil library and recalibrating (spiking) is proposed by Brown (2007) as another way to increase the accuracy of predictions, as opposed to using only local calibrations (about 206 or 418 samples). Sankey et al. (2008) also reported improved prediction results for clay content, soil organic carbon (SOC) and inorganic carbon, using the same global calibration set spiked with local samples (52–234 samples) from three highly variable landscape study sites (~10–30,000 ha) in Montana, US, compared with global or local calibrations alone. However, to our knowledge, few studies combining samples of local calibration sets (spiking) with a regional, national and continental calibration set, with local samples at farm scale (e.g. Guerrero et al., 2010, Kuang and Mouazen, 2013).

Partial least square regression (PLSR) is the most commonly used technique for spectral analysis. When dealing with a highly heterogeneous sample set, in which the parameters measured may vary considerably, the precision of linear-regression techniques tends to decrease due to the non-linear nature of the relationship between spectral data and the dependent variable. Data-mining techniques, such as multivariate adaptive regression spines (MARS) and support-vector machines (SVM), can be used to improve the accuracy of the calibration models (Mouazen et al., 2010; Biligil et al., 2011; Nawar et al., 2015).

In the present study, we focus on farm scale calibration, for small area farms of ~100 ha, compared to the modelling case studies mentioned above. Presumably, these farms should be of smaller variability, and is limited to agricultural soils. The aim was to compare the predictive performance of the vis-NIR spectroscopy at local, regional, national and continental scales, using PLSR and two multivariate data-mining techniques, namely, MARS and SVM. The calibrations were made using on-line collected soil spectra for predicting within-field variation in TN, TC and moisture content.

2. Material and Methods

2.1. On-line soil measurement and collection of soil samples

A total of 122 and 149 soil samples were collected during the on-line measurement respectively form Hessleskew and Hagg farms, Yorkshire, UK. The on-line measurement system designed and developed by Mouazen (2006) was used to measure both fields. It consists of a subsoiler, which

penetrates the soil to the required depth, making a trench, whose bottom is smoothened by the downwards forces acting on the subsoiler. The subsoiler was retrofitted with the optical unit and attached to a frame. This was mounted onto the three point linkage of the tractor (Mouazen et al., 2005). An AgroSpec mobile, fibre type, vis–NIR spectrophotometer (Tec5 Technology for Spectroscopy, Germany) with a measurement range of 305–2200 nm was used to measure soil spectra in diffuse reflectance mode. A deferential global positioning system (DGPS) (EZ-Guide 250, Trimble, USA) was used to record the position of on-line measured spectra with sub-meter accuracy.

2.2. Laboratory chemical and spectral measurements

Each sample was divided into two parts; one part was dried for 24 h at 105 ºC and the other part was left fresh (wet). The dried soil sample was analyses of total carbon (TC), total nitrogen (TN) by TrusSpecCNS spectrometer (LECO Corporation, St Joseph, MI, USA) using the Dumas combustion method. Soil MC was determined by oven drying of the soil samples at 105 ºC for 24 h.

The fresh part of soil sample was placed in a glass container and mixed well. Three Petri dishes with 2 cm in diameter and 2 cm deep were used for three replicate measurements. Each soil sample 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 has been used in the online measurements. The sampling interval of the instrument was 1 nm. A total of ten scans were collected from each replicate, and these were averaged into one spectrum for each sample.

2.3. Data pretreatment

The same pretreatment of spectral data was carried out for all soil properties investigated by using the R packages (ChemoSpec and 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 & Naes, 1989) with a second-order polynomial approximation. Finally, the Savitzky-Golay smoothing was carried out to remove noise from spectra.

2.4. Spectral dataset with different scale

The spectral dataset for each single field (local scale) were produced, and those of the two fields were merged into one dataset, which was designated as regional scale dataset in this study. Spiking were used to introduce variability of each field data into a general calibration dataset consisted of 500 soil samples, collected from five European countries (Czech republic, Germany, Sweden, Denmark, and UK) with total soil samples of 200, 120, 130, 140, and 70, respectively. Two spiking strategies were followed in this study. These included spiking of each field dataset samples with those previously collecting from UK fields (national scale), and spiking with those collected from different farms in Europe forming European scale dataset.

2.5. Development of calibration models

The four calibration sets were subjected to PLS, MARS and SVM regression analyses with the leave-one-out cross validation using R software (R Core Team, 2013), which resulted in four groups of PLS, MARS and SVM models for each soil property. For all four Models, dataset of the target field was been divided into 75% for cross validation, and 25% for prediction using both laboratory and on-line collected soil spectra.

The prediction performance of calibration models developed were assessed using R2, RMSE and RPD parameters. Chang et al. (2001) grouped the RPD value, which is defined as ratio of standard deviation of the measured values to standard error of prediction values into three classes: category A (RPD > 2) are models that accurately predict a given property; category B (1.4 < RPD < 2) are models that have limited prediction ability; and category C (RPD < 1.4) are models with no prediction

ability.

3. Results

3.1 Soil data

The results of the descriptive statistical analyses for soil parameters are shown in Table 1. For Hessleskew Farm, the TN was low, with the mean and maximum values of 0.19% and 0.34%, respectively (Table 1). The maximum TC content was 3.67%, whereas the MC ranged between 14.94% and 22.26%. In the Hagg Farm, the TN was also low, with a maximum of 0.35%, and the TC content was even smaller than in Hessleskew, ranging between 1.34% and 3.18%. The MC was higher than in Hessleskew, with a maximum value of 24.64% (Table 1).

Table 1. Descriptive statistics of the soil total carbon (TC), total nitrogen (TN) and moisture content (MC) for Hessleskew and Hagg farms.

	Min	1st Qu.	Median	Mean	3rd Qu.	Max	St.dev
Hessleskew	**(n=122)**						
TN (%)	0.19	0.23	0.25	0.25	0.26	0.34	0.023
TC (%)	1.72	1.94	2.05	2.121	2.22	3.67	0.308
MC (%)	14.93	18.23	18.97	18.9	19.71	22.26	1.23
Hagg	**(n=149)**						
TN (%)	0.13	0.19	0.21	0.21	0.24	0.35	0.04
TC (%)	1.34	1.68	1.9	1.921	2.08	3.18	0.31
MC (%)	11.53	15.92	17.29	17.29	18.54	24.64	2.06

3.2. Performance of calibration models at different scales

The calibration methods considered in this study provide different prediction accuracies of TN, TC and MC. Tables 2 and 3 summarise the cross-validation, laboratory and on-line prediction results of TN, TC and MC for different modelling scales. Figures 1 and 2 show better results are achieved with the MARS models for all modelling scales. For the cross validation, the best results were obtained with MARS using the continental dataset with R2 = 0.96, RMSE = 0.01%, and RPD = 5.26 for Hagg field (Table 3 and Fig. 2), and R2 = 0.96, RMSE = 0.01%, and RPD = 4.73 for Hessleskew field (Table 2 and Fig. 1) The least acceptable results were produced for TN by PLSR using the local dataset of Hessleskew field (R2 = 0.56, RMSE = 0.01%, and RPD = 1.52, shown in Table 2 and Fig. 1). SVM showed a good performance for predicting TN for all scales datasets, outperforming PLS (RPD values for all SVM models were above 1.4). In addition, SVM showed a good performance in modelling TN, and all the calibration models had an RPD above 1.4. The worst results for SVM were achieved using the local scale in Hessleskew field for TN (R2=0.64, RMSE=0.01% and RPD = 1.67).

Table 2. Hessleskew field results in cross-validation, laboratory and on-line predictions using local, regional, spiked national and spiked continental samples based on PLSR, MARS and SVM calibration models.

		Local			Regional			National			Continental		
		RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD
PLSR													
Cross-validation	TN	0.01	0.56	1.52	0.02	0.69	1.81	0.03	0.70	1.83	0.02	0.79	2.18
	TC	0.18	0.6	1.59	0.19	0.58	1.54	0.37	0.82	2.36	0.16	0.85	2.61
	MC	0.76	0.66	1.73	1.16	0.6	1.59	1.95	0.72	1.89	1.72	0.86	2.65
Lab Validation	TN	0.01	0.55	1.51	0.03	0.58	1.57	0.04	0.50	1.44	0.02	0.85	2.57
	TC	0.23	0.6	1.6	0.23	0.57	1.54	0.36	0.79	2.2	0.26	0.77	2.13
	MC	0.81	0.66	1.74	1.38	0.48	1.41	2.05	0.69	1.81	1.9	0.59	1.57
On-line Validation	TN	0.02	0.53	1.48	0.03	0.59	1.58	0.04	0.60	1.59	0.03	0.58	1.56
	TC	0.25	0.56	1.53	0.22	0.51	1.44	0.42	0.78	2.15	0.35	0.76	2.09
	MC	0.88	0.63	1.66	1.36	0.48	1.40	2.58	0.60	1.59	2.49	0.52	1.47
SVM													
Cross-validation	TN	0.01	0.64	1.67	0.02	0.72	1.90	0.02	0.88	2.86	0.02	0.80	2.22
	TC	0.16	0.66	1.71	0.17	0.64	1.166	0.17	0.92	3.58	0.15	0.86	2.68
	MC	0.72	0.69	1.81	1.11	0.64	1.66	1.17	0.90	3.23	1.68	0.86	2.71
Lab Validation	TN	0.01	0.51	1.44	0.02	0.75	2.02	0.03	0.61	1.61	0.02	0.85	2.57
	TC	0.25	0.53	1.48	0.21	0.64	1.69	0.23	0.74	2.00	0.25	0.78	2.13
	MC	0.9	0.59	1.58	1.32	0.53	1.48	1.45	0.64	1.69	1.97	0.56	1.52
On-line Validation	TN	0.02	0.48	1.41	0.02	0.64	1.70	0.02	0.61	1.64	0.03	0.52	1.47
	TC	0.27	0.48	1.41	0.20	0.60	1.60	0.28	0.74	2.00	0.35	0.76	2.09
	MC	0.98	0.53	1.48	1.32	0.50	1.44	1.92	0.56	1.53	2.34	0.58	1.56
MARS													
Cross-validation	TN	0.01	0.70	1.82	0.01	0.94	4.08	0.01	0.93	3.70	0.01	0.96	4.73
	TC	0.15	0.71	1.85	0.09	0.92	3.52	0.11	0.97	5.59	0.06	0.98	6.46
	MC	0.67	0.73	1.94	0.50	0.93	3.84	1.6	0.82	2.35	1.72	0.91	3.05
Lab Validation	TN	0.01	0.55	1.51	0.01	0.81	2.35	0.04	0.51	1.56	0.02	0.87	2.83
	TC	0.23	0.6	1.6	0.16	0.8	2.26	0.23	0.72	1.91	0.19	0.88	2.89
	MC	0.81	0.66	1.74	0.57	0.84	2.5	1.3	0.71	1.88	1.57	0.72	1.90
On-line Validation	TN	0.02	0.53	1.48	0.01	0.77	2.10	0.03	0.76	2.06	0.02	0.79	2.21
	TC	0.25	0.56	1.53	0.18	0.78	2.16	0.26	0.75	2.05	0.31	0.81	2.35
	MC	0.88	0.63	1.66	0.71	0.75	2.04	1.30	0.83	2.46	1.85	0.73	1.97

Table 3. Hagg field results in cross-validation, laboratory and on-line predictions using local, regional, spiked national and spiked continental samples based on PLSR, MARS and SVM calibration models.

		Local			Regional			National			Continental		
		RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD	RMSE (%)	R^2	RPD
PLSR													
Cross-validation	TN	0.02	0.62	1.62	0.02	0.64	1.68	0.03	0.72	1.91	0.02	0.75	2.02
	TC	0.20	0.61	1.6	0.24	0.52	1.45	0.37	0.82	2.36	0.3	0.85	2.55
	MC	1.16	0.63	1.65	1.06	0.69	1.8	1.95	0.72	1.89	1.87	0.82	2.33
Lab Validation	TN	0.02	0.54	1.50	0.02	0.61	1.62	0.04	0.50	1.44	0.03	0.55	1.50
	TC	0.22	0.58	1.56	0.24	0.52	1.46	0.36	0.79	2.20	0.36	0.82	2.40
	MC	1.19	0.60	1.61	1.07	0.68	1.79	2.05	0.69	1.81	1.72	0.57	1.55
On-line Validation	TN	0.03	0.49	1.42	0.03	0.59	1.58	0.04	0.57	1.55	0.03	0.65	1.71
	TC	0.23	0.51	1.44	0.23	0.50	1.43	0.42	0.78	2.15	0.39	0.80	2.25
	MC	1.43	0.51	1.44	1.41	0.52	1.46	2.58	0.60	1.59	2.36	0.58	1.57
SVM													
Cross-validation	TN	0.02	0.66	1.71	0.01	0.92	3.54	0.03	0.75	2.01	0.02	0.77	2.09
	TC	0.19	0.66	1.72	0.11	0.9	3.23	0.34	0.85	2.6	0.28	0.86	2.69
	MC	1.04	0.70	1.84	0.53	0.92	3.6	1.77	0.77	2.07	1.87	0.82	2.33
Lab Validation	TN	0.02	0.65	1.71	0.01	0.83	2.47	0.04	0.50	1.44	0.03	0.62	1.64
	TC	0.20	0.66	1.73	0.14	0.84	2.52	0.37	0.78	2.15	0.39	0.79	2.23
	MC	1.06	0.68	1.79	0.65	0.88	2.93	1.91	0.73	1.94	1.72	0.57	1.55
On-line Validation	TN	0.03	0.61	1.61	0.02	0.70	1.85	0.04	0.57	1.55	0.03	0.64	1.68
	TC	0.23	0.51	1.44	0.15	0.79	2.23	0.42	0.78	2.15	0.39	0.80	2.25
	MC	1.33	0.57	1.54	1.08	0.72	1.90	2.47	0.63	1.66	2.36	0.58	1.57
MARS													
Cross-validation	TN	0.02	0.74	1.97	0.01	0.92	3.53	0.02	0.78	2.13	0.01	0.96	5.26
	TC	0.17	0.72	1.89	0.10	0.91	3.41	0.31	0.88	2.84	0.10	0.98	7.30
	MC	0.96	0.75	2.00	0.54	0.92	3.56	1.65	0.80	2.23	1.75	0.93	3.57
Lab Validation	TN	0.02	0.65	1.71	0.01	0.84	2.56	0.04	0.50	1.44	0.03	0.77	2.08
	TC	0.20	0.66	1.73	0.13	0.84	2.56	0.37	0.78	2.15	0.46	0.85	2.36
	MC	1.00	0.72	1.91	0.69	0.87	2.77	1.97	0.71	1.88	1.93	0.76	2.06
On-line Validation	TN	0.03	0.61	1.61	0.02	0.72	1.92	0.04	0.56	1.52	0.02	0.74	1.98
	TC	0.21	0.60	1.61	0.15	0.80	2.28	0.42	0.74	1.98	0.29	0.81	2.37
	MC	1.23	0.63	1.67	1.15	0.68	1.79	2.33	0.70	1.85	1.90	0.73	1.94

The best results for TC were achieved using the MARS model and the continental dataset (R2=0.98, RMSE=0.01% and RPD = 7.30). The PLSR model for TC developed with the local local data set provided a lower degree of accuracy with R2, RMSE, and RPD of 0.6, 0.18%, and 1.52, respectively. The best results for MC were obtained for the MARS modelling with the continental dataset (R2=0.93, RMSE = 1.75% and RPD = 3.57) at Hagg Farm. SVM generated good results and the RPD ranged between 1.41 and 3.44. The best results for PLSR were achieved with the continental dataset at Hessleskew Farm with R2 of 0.86 and RMSE of 1.72% and RPD of 2.65.

4. Discussion

The best predictions were generally achieved for TC and MC, which are commonly accurately

predicted using NIR spectroscopy (Mouazen et al., 2005; Christy et al., 2008;

Kuang and Mouazen, 2103). This is attributed to the direct spectral responses of these soil properties in the NIR spectroscopy range (Stenberg et al., 2010; Kuang et al., 2012). As expected, MC is more accurately predicted due to significant O-H absorbance peaks at 950, 1450 and 1950 nm overtones typically dominating the NIR-spectra (Mouazen et al., 2007; Stenberg et al., 2010).

The predictions for TN presented here are roughly in accord with what could be expected according to the literature, with RMSE values well in line with earlier findings (although R2 values are among the lowest presented) (Viscarra Rossel et al., 2006, Kuang and Mouazen, 2103). This somewhat contradictory relationship is due to the very narrow variation of TN at the two sites (Table 1), resulting in low RPD values. This is especially the case with Hagg field. At Hessleskew field, the variation is slightly higher, while the RPD and R2 values are also slightly higher, despite RMSE values being higher. The difficulties in predicting TN are in line with the TN being predicted through secondary relationships to the vis-NIR (Stenberg et al., 2010, Kuang and Mouazen, 2103).

The main difference between the local, regional, national and continental calibrations is a larger bias in the case of the latter, but, for many soil properties, R2 values were also reduced (Tables 2 and 3). However, these reductions in R2 values were not consistent and, in some cases (for example, TN at Hagg), the regional calibration models led to improved R2 values. At Hessleskew, fewer soil samples of 85 samples for cross validation and 37 for prediction may have affected model performance as compared to the Hagg farm.

Spiking local samples in the national and continental libraries almost always improved the prediction results compared with those obtained using the regional library, confirming the results presented by Brown (2007) and Sankey et al. (2008), also on the smaller, more homogenous scale used in the present study. The improvement was mainly expressed as a reduction in RMSE values, and only increase in terms of enhanced R2 values (Tables 2 and 3). This finding is in agreement with Brown 's (2007) findings which showed a great reduction in RMSE for predictions of soil organic matter (SOC) in upland soil samples from a catchment in Uganda, by adding local samples to a global library. Furthermore, it is consistence with the observations reported by Kuang and Mouazen (2013) that spiking local soil samples into continental datasets proved to be an efficient way to improve the prediction accuracy of predicting selected soil properties in a target field.

In the present study, spiked and recalibrated national and continental models did not result in substantially lower RMSE values compared with the results when using local calibrations alone. This corresponds to the small and variable differences for TN, TC and MC between the calibrations with the spiked national and continental libraries, and the local-only samples, which is in agreement with with observations found by Brown (2007). Moreover, these results are consistent with the observations for TN, OC, and MC made by Kuang and Mouazen (2013), who obtained substantially better predictions for some sites using the continental library spiked with local samples, compared with using only local samples. These authors confirmed that although higher R2 and RPD values can be obtained with spiked continental calibration models, also higher RMSE values are to be expected.

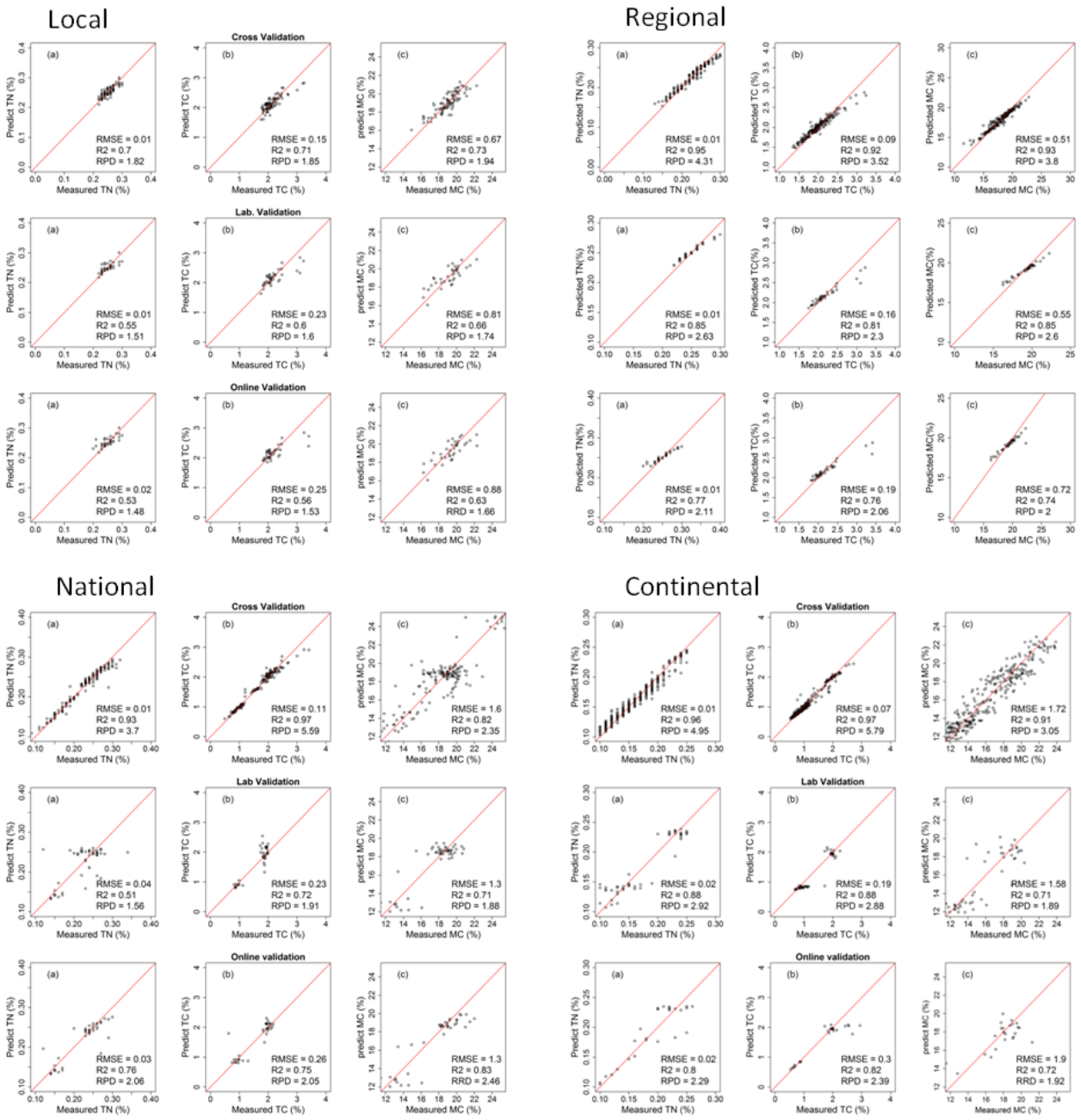

Fig 1. Scatter plots of near infrared (NIR)-predicted versus laboratory-analysed total nitrogen (TN), total carbon (TC) and moisture content (MC) in Hessleskew farm using the local calibration, regional, national and continental calibration based on MARS models

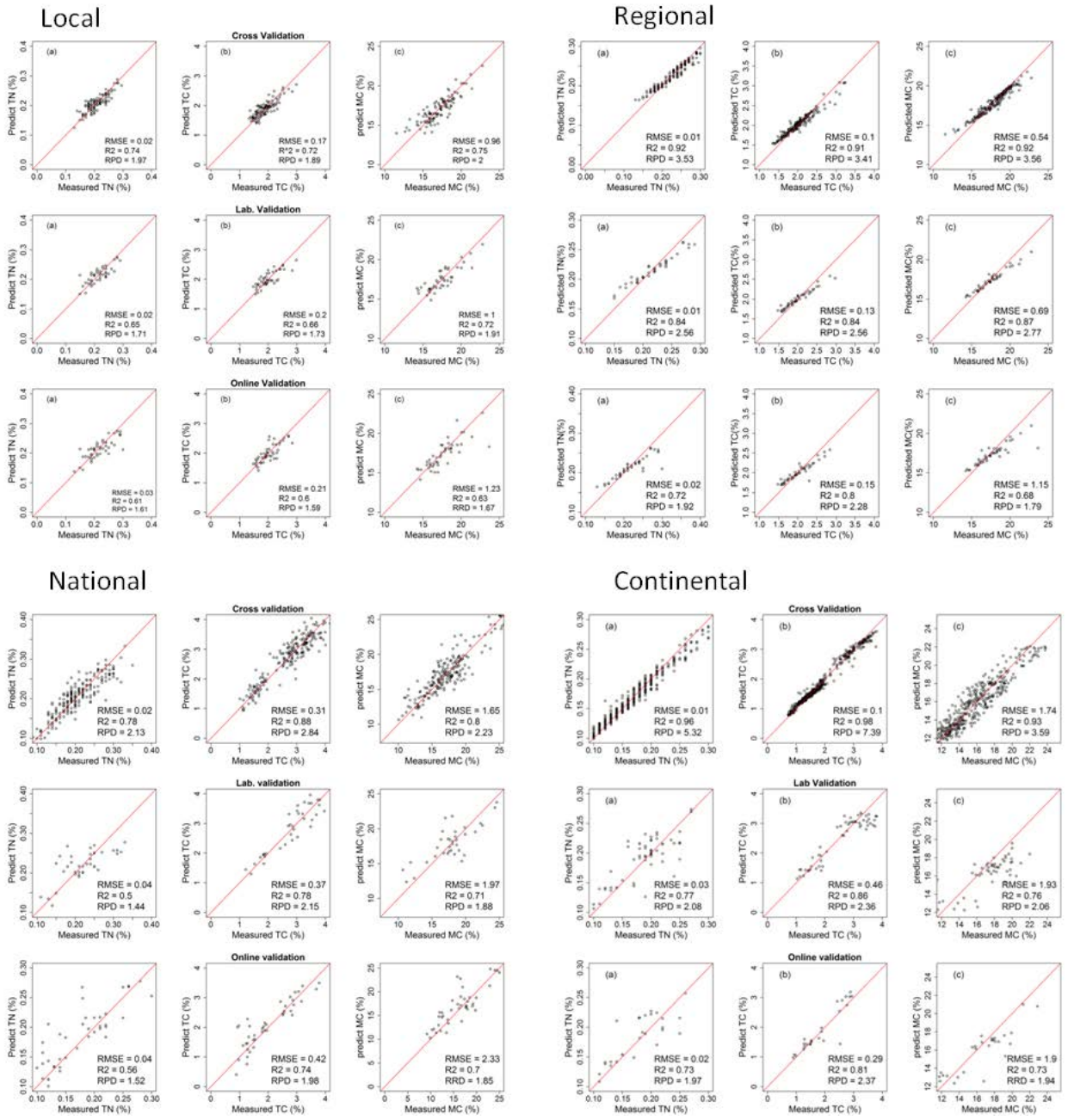

Fig 2. Scatter plots of near infrared (NIR)-predicted versus laboratory-analysed total nitrogen (TN), total carbon (TC) and moisture content (MC) in Hagg farm using the local calibration, regional, national and continental calibration based on MARS models.

5. Conclusions

In our study, the PLSR, SVM and MARS methods were used to compare the estimation of soil TN, TC and MC at different scales. Generally, the accuracy of the PLSR, SVM and MARS models varied in accordance with variations in the calibration scales. Results showed the majority of the non-linear calibration methods (particularly MARS) to outperform the linear PLSR in cross-validation modelling. However, PLSR provided acceptable accuracy for the prediction of the soil properties. The most

important finding was that results of cross-validation may well improve with increasing the scale of the data set from one field, to two fields, and finally spiking with large data set collected from several farms in Europe. However, the validation of model performance in prediction does not necessarily follow the same trend. Higher prediction results were observed for the individual and two-field data set as compared to the large EU data set. Another interesting finding was that the two-field data set resulted in skewness of predicted values towards the field with high concentration of a given soil property.

The continental calibrations seem to be the best option for predictions of the studied soil parameters at farm or field scale. The continental calibrations (585 samples) outperformed national (286 samples), regional (234 samples) and the local (122 and 149 for Hessleskew and Hagg, respectively) scales modelling for TN, TC and MC at both farms. The potential for good calibration was highest for TC and MC. There was a tendency for better predictions when spiking a continental dataset compared to spiking the national 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 national and continental libraries. Future research should focus on the potential for integration of data-mining techniques with spiked libraries forimproving 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.

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