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Prediction of soil TN and TC at a farm-scale using VIS-NIR spectroscopy

Haiqing Yang[1,*,a], Boyan Kuang[2,b], Abdul M. Mouazen[2,c]

[1] College of Information Engineering, Zhejiang University of Technology, Hangzhou 310032, P.R.China

[2] Department of Environmental Science and Technology, School of Applied Sciences, Cranfield University, Bedfordshire MK43 0AL, United Kingdom

* Corresponding author, [a]email: yanghq@zjut.edu.cn,

[b]email: b.kuang@cranfield.ac.uk, [c]email: a.mouazen@cranfield.ac.uk

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Abstract. Building cost-effective models is of academic and practical value for fast measurement of soil properties, especially at a farm-scale. The aim of this study is to build quantitative models for soil total nitrogen (TN) and total carbon (TC) using visible and near infrared (VIS-NIR) spectroscopy. Dried samples (n=122) collected from an experimental farm, at Silsoe, Bedfordshire, United Kingdom, were scanned from 350 to 2500 nm at 1-nm intervals. Samples were divided into a calibration set (75%) and an independent validation set (25%). A partial least squares regression (PLSR) with leave-one-out cross validation was carried out based on different spectral ranges. Result shows that the best predictions (R^2>0.90 and RPD>3.3) are achieved for TN using the VIS range (400-700nm) and for TC using the VIS-NIR range (400-2500nm). It is concluded that VIS-NIR spectroscopy coupled with PLSR can be adopted for the prediction of soil TN and TC at a farm-scale.

Introduction

There is an increasing interest in the development of rapid and cost-effective methods for the measurement of soil nitrogen (N) and carbon (C), due to the growing concerns about the increase in atmospheric N and C content, which could be limited through soil N and C sequestration. However, due to spatial variability and non-linear temporal dynamics, accurate estimation of soil N and C requires measurements on numerous samples. Due to the fact that standard procedures for the measurement of soil N and C are time-consuming and expensive [1], attention is being given to possible alternatives such as near-infrared diffuse reflectance spectroscopy (NIR-DRS). The technique mainly measures overtones and combination bands of fundamental vibrations of O-H, N-H, and C-H bonds in the mid-infrared region.

The factors affecting the accuracy of soil property measurement originate from soil heterogeneity [2], moisture content [3], soil texture [4,5], soil color [6], model size [7], sample pretreatment [8,9], data preprocessing [10,11], and calibration procedures [12]. The effect of different spectral ranges for the prediction of soil properties has been examined [13-15]. For example, Mouazen *et al*. compared the performance of two commercially-available spectrophotometers with different wavelength ranges for the measurement of selected soil attributes including total carbon (TC) and total nitrogen (TN)[13]. They found that the best accuracy is obtained when using a full wavelength range of 451-2459 nm, as compared to a short wavelength range of 401-1770 nm. Islam *et al*. compared the ability of reflectance spectroscopy in the UV (250-400 nm), VIS (400-700 nm) and NIR (700-2500nm) to predict several soil properties including organic carbon (OC)[14]. Viscarra Rossel *et al*. analyzed the capability of using VIS (400-700 nm), NIR (700-2500 nm), MIR (2500-25,000 nm) and combined VIS-NIR-MIR

for simultaneous assessment of soil OC and other properties[15]. They found the cross-validated prediction of soil OC based on the VIS and NIR range of similar accuracy (R2-adj of 0.60), but less accurate than the MIR and combined VIS-NIR-MIR models (R2-adj > 0.72).

Although VIS-NIR diffuse reflectance spectroscopy has the advantage of being nondestructive, chemical free and repeatable, equipment cost is an important factor governing the spread of this technique in precision farming. Costs are high (a) because the large number of samples have to be analyzed per field, (b) because VIS-NIR spectra analysis currently requires the use of two different photoelectric detectors (typically a Si-array and an InGaAs diode-array), and (c) because the spectral resolution links with high sampling frequency. Thus, simpler and cheaper technology based on a few of wavelengths would reduce the cost of equipment significantly. Viscarra Rossel *et al*. compared different color space models [16] and used a digital camera to measure soil OC [17]. Sudduth and Hummel compared the spectra in the range of 1640-2640 nm at 40-nm data spacing interval and those in the range of 1670-2630 nm at 60-nm data spacing interval for determining the optimum number of scans for soil OC prediction in 30 Illinois soil samples [18]. To our knowledge, however, no reports have been published on the effect of wavelength reduction on the prediction accuracy for soil N and C. Furthermore, nor on an optimization process for wavelength reduction.

The objectives of this study is to investigate the effect of different VIS-NIR spectral ranges on the performance of prediction models developed for the measurement of soil total nitrogen (TN) and total carbon (TC). The influence of spectral range reduction on the accuracy of these models was also examined, with an aim of optimizing the spectral range without losing accuracy in model performance.

Materials and Methods

Soil Samples. Samples were collected from the top 10-20 cm of the soil layer from multiple fields on an experimental farm, at Silsoe, Bedfordshire, United Kingdom. A total of 122 samples with variable proportions of sand, slit and clay, colors and chemical attributes were used in this study. Soil samples were air-dried, crushed and sieved to pass a 2-mm mesh. Plant residues and stones were removed. The sieved samples were then air-dried again at 40℃ for 48h. About 50 mg in each sample was used for the measurement of TN and TC by a TrusSpecCNS spectrometer (LECO Corporation, St. Joseph, MI, USA) using the Dumas combustion method.

Spectrophotometer and Spectral Acquisition. About 5g in each sample was loaded into a static ring cup and measured using a LabSpec 2500 spectrophotometer (Analytical Spectral Devices Inc. Boulder, CO, USA) with spectral range of 350-2500nm at 1-nm sampling interval. Before each sample measurement, 25 reference scans were taken on a ceramic standard supplied with the instrument. Ten photometric scans were conducted for each sample, followed by another ten scans of the refilled sample cup. The twenty scan results were then combined and averaged on each sample.

Spectral Pretreatment and Data Analysis. The spectra were treated with the Unscrambler software (CAMO Inc., Oslo, Norway). Spectra preprocessing included moving average smoothing (MA), multiplicative scatter correction (MSC), standard normal variate (SNV), 1st- and 2nd- order de-trending, 1st- and 2nd- derivatives and three types of spectral normalization.

After spectral preprocessing, the entire data set were divided into a calibration set (75%) and an independent validation set (25%). The calibration spectra were subjected to a partial least squares regression (PLSR) with leave-one-out cross validation. The optimal number of latent variables (LVs) was determined by minimizing the predicted residual error sum of squares (PRESS). In order to examine the effect of using different spectral ranges on the performance of PLS models, the following six spectral ranges were tested: VIS (400 - 700 nm), SWNIR (700 - 1100 nm), LWNIR (1100 - 2500 nm), NIR (700 - 2500 nm), the combination of VIS and SWNIR (VIS-SWNIR, 400 - 2500 nm) and the entire VIS-NIR (400 - 2500 nm). The performance of the calibration model was assessed using the coefficient of determination (R^2) and root-mean-square error (RMSE) for calculated vs. reference

compositions in calibration and cross validation. The coefficient of determination (R^2) and root-mean-square error of the prediction (RMSEP) were used for the evaluation of prediction performance of the established PLS models based on the independent validation set. Also, the prediction accuracy of each PLS model was evaluated using the residual predictive deviation (RPD), which is the ratio of standard deviation of reference values to SEP of the independent validation set. Generally, a good model would have high values of R2 and RPD, and low values of RMSE for calibration and cross-validation and of RMSEP for independent validation.

Results and Discussion

Laboratory Analysis of Soil Properties. Table 1 shows the sample statistics of calibration, cross-validation and independent validation of samples considered in this study. The two NIR-spectrally active soil properties of TN and TC have similar statistical reference values with a coefficient of variation (CV) range of 0.26-0.29 and high inter-correlation (r) of 0.97.

Table 1 Sample statistics for calibration and independent validation sets

Item	Calibration set				Independent validation set				Intercorrelation	
	Mean	Range	SD[b]	CV[c]	Mean	Range	SD	CV	TN/%	TC/%
TN/%	0.20	0.09 - 0.31	0.06	0.29	0.20	0.12-0.30	0.06	0.28	1.00	0.97
TC/%	2.10	0.95 - 3.41	0.57	0.27	2.11	1.31-3.23	0.55	0.26		1.00

[b] standard deviation;
[c] coefficient of variation

PLSR Models. Table 2 lists the results of the best PLS models developed for the prediction of TN and TC based on different spectral ranges. To demonstrate how quantitative calibration and predictions were made for the soil properties in question, the TN is considered as an example. In general, PLSR models for TN provided excellent performance with R^2 of 0.83-0.91 and RMSECV of 0.018-0.024 % for the cross-validation of calibration set, and R^2 of 0.85-0.94, RMSEP of 0.014-0.021 % and RPD of 2.77-4.37 for the independent validation set. Although the performance of each model differs among different spectral ranges, PLSR models developed in the VIS-included ranges, i.e. VIS-NIR, VIS and VIS-SWNIR, perform better than those based on the VIS-excluded ranges (SWNIR, LWNIR and NIR). Statistically, the best model performance for the independent validation set was achieved for TN with RPD of 4.37 in the VIS range and for TC with RPD of 3.53 in the VIS-NIR range. This indicates that colour plays an important role in the prediction of TN and TC using VIS-NIR spectroscopy.

Table 2 Performance of best PLS models developed for the measurement of soil TN and TC using different spectral ranges

Spectral range[a]	TN/%				TC/%			
	LVs[b]	R^2_{val} (RMSECV)[c]	R^2_{pre} (RMSEP)[d]	RPD[e]	LVs	R^2_{val} (RMSECV)	R^2_{pre} (RMSEP)	RPD
VIS-NIR	3	0.89(0.019)	0.92(0.015)	3.63	**5**	**0.86(0.215)**	**0.92(0.156)**	**3.53**
VIS	**3**	**0.91(0.018)**	**0.94(0.014)**	**4.37**	4	0.87(0.209)	0.91(0.164)	3.32
VIS-SWNIR	5	0.88(0.020)	0.92(0.016)	3.83	5	0.86(0.212)	0.90(0.169)	3.23
SWNIR	3	0.83(0.024)	0.85(0.021)	2.77	3	0.81(0.250)	0.81(0.236)	2.33
LWNIR	5	0.87(0.021)	0.90(0.017)	3.38	4	0.84(0.226)	0.90(0.169)	3.24
NIR	4	0.90(0.018)	0.91(0.016)	3.58	5	0.86(0.217)	0.89(0.176)	3.10

[a] VIS-NIR(400-2500nm), VIS(400-700nm), VIS-SWNIR(400-1100nm), SWNIR(700-1100nm), LWNIR(1100-2500nm), NIR(700-2500nm);[b] latent variables; [c] calculated with cross-validation for calibration set; [d] calculated with independent validation set; [e] residual predictive deviation

Conclusions

In this study, soil samples at a farm-scale with five texture classes were analyzed using VIS-NIR spectroscopy and PLSR for the prediction of soil total nitrogen (TN) and total carbon (TC). Based on the results obtained from the analysis of PLS models, the following conclusions can be drawn:

1. PLS models for the prediction of TN and TC can be successfully developed, although the prediction capabilities of these models differ among different spectral ranges. The best predictions for TN and TC are obtained using the VIS range (400-700 nm) and the VIS-NIR range (400-2500 nm), respectively.
2. PLS models for soil TN and TC developed in the VIS-included ranges (VIS-NIR, VIS and VIS-SWNIR) perform better than those using VIS-excluded ranges (SWNIR, LWNIR and NIR). This confirms that soil color plays an important role in the prediction of these soil properties using VIS-NIR spectroscopy.

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