Removing the effect of soil moisture from NIR diffuse reflectance spectra for prediction of soil carbon

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Abstract

Field measurement using NIR spectroscopy has become very popular for measuring soil properties. However NIR reflectance is quite sensitive to external environmental conditions, such as temperature, and soil moisture in particular. In field measurement, the soil moisture content can be highly variable. It is a challenge to find a method for predicting the properties of soil samples in the field that have variable moisture content. This paper attempts to develop a novel algorithm to remove the spectral effect of soil moisture for the calibration of soil carbon content. The algorithm projects all the soil spectra orthogonal to the space of variation. Here the unwanted variations of soil moisture can be effectively removed. We conducted experiments using soils at different moisture content, and the results show that it is feasible to remove the moisture effect from field spectra. This resulted in improved calibration of soil carbon content.

Keywords: orthogonal projection, partial least squares, soil carbon.

Introduction

Field measurement using Near Infrared Diffuse Reflectance Spectroscopy (NIR-DRS) spectroscopy has become very popular for measuring soil properties (Mouazen et al., 2007; Waiser et al., 2007). However NIR reflectance is sensitive to external environmental conditions, such as temperature, soil moisture, and structural conditions. While in the laboratory, soil can be scanned under standard air-dried conditions; in the field it is very difficult to control the water content. Studies have shown that with appropriate calibration NIR spectra can be used in the field (Kusumo et al., 2008). Sudduth and Hummel (1993) in a laboratory study showed NIR measurements on a wide range of soil moisture tensions. Although they found best organic C results with dry samples, reasonable estimates were obtained across the full range of tensions. Those authors suggested that including a wide range of water contents in the calibration set, could that take care of the issue of moisture variation.

This paper investigates the influence of soil moisture on the NIR-DRS signal and its effects on prediction of soil carbon. The ultimate objective is to remove the effect of moisture on the prediction of the soil carbon content.

Materials and methods

We used a library of 400 soil samples from southern NSW, Australia. The samples were taken from various soil horizons taken up to 1 m depth. They represent a range of soils with soil organic carbon (SOC) contents between 0.1 and 12%.

We used the AgriSpec™ instrument with a contact probe (Analytical Spectral Devices, Boulder, Colorado, USA) for collection of the Vis-NIR soil reflectance spectra. The samples were

illuminated by a halogen lamp (4.5 W) and the reflected light was transmitted to the spectrometer through a fibre optic bundle. A Spectralon (Labsphere Inc., North Sutton, N.H., USA) was used as a highest reflectance standard and employed to convert raw spectral data to reflectance. Each soil spectrum was obtained as the mean of 40 scans. Only data from wavelength of 500-2450 nm were used for analysis, they were transformed from reflectance to absorbance (log 1/Reflectance). The spectra wre then sampled to a resolution of 2 nm, smoothing were performed using the Savitsky-Golay algorithm with a window size of 11 and polynomial of order 2. We used a standardised normal variate to normalise the spectra.

To investigate the effect of the moisture on the accuracy of the prediction formula, we selected 20 samples randomly. The 20 samples were wetted to approximately field capacity. The soil samples were then scanned, and left to dry under laboratory condition. Every day (for 4 days), the 20 samples were weighed and then scanned. For each sample, each day, we have the amount of water and a spectrum.

To remove the effect of soil moisture we used a parameter orthogonalisation algorithm (Roger et al., 2003). The algorithm finds the areas in a spectrum which are affected by moisture and projects the spectra orthogonal to this variation. Here the unwanted variations of soil moisture can be effectively removed. This analysis describes the variation of the spectra in terms of a lower number of unobserved factors. It is related to principal component analysis (PCA), but PCA only performs a transformation to take into account all of the variability in the spectra. Meanwhile, the orthogonolisation takes into account the variability which is due to an external factor (i.e. moisture).

Results and discussion

We calibrated a PLS (4 factors) using air-dried soil samples, the formula was then used to predict SOC content from the spectra of the samples with different moisture contents. Figure 2a shows the prediction of the SOC using spectra at various moisture conditions. We can see that the prediction deteriorates significantly and also has a bias, a tendency to over-predict the SOC content with increasing moisture content.

We first tried to remove the effect of moisture by "spiking" the calibration data, i.e. including spectra from the wet samples (Viscarra Rossel et al., 2009). We included spectra from samples with different moisture contents (air-dried, 20%, 16%, 12%) as a calibration set. It was hypothesized that this will "trick" the PLS so that the calibration equation is not influenced by parts of the spectra which are affected by moisture. Figure 2b shows that prediction from a "spiked" calibration dataset. We can see that in this case although the spiking procedure improves the situation, it does not produce a good calibration and prediction.
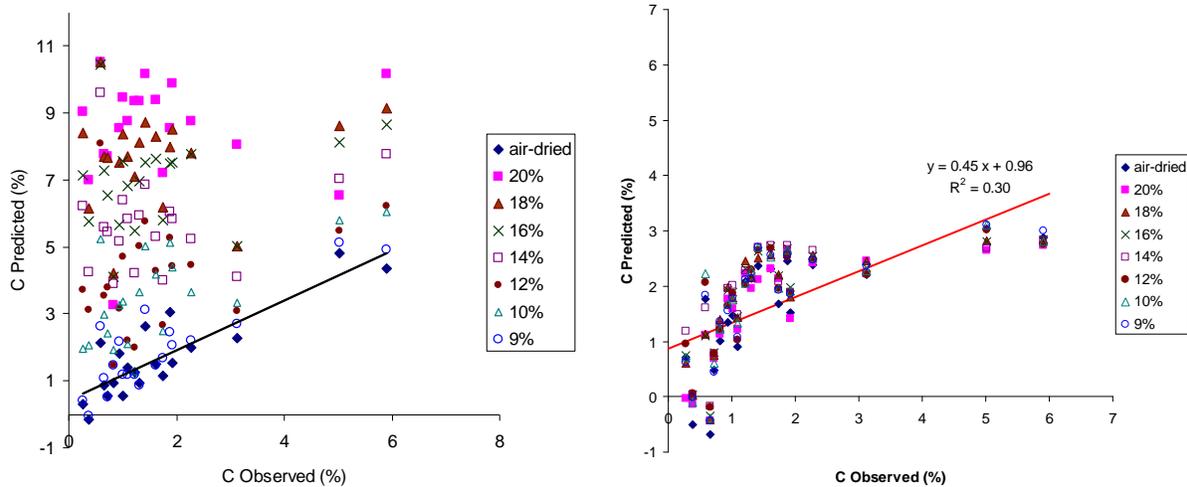
Figure 2. (a) Correlation between predicted C and measured C for samples with various moisture contents using PLS calibrated on air-dried samples. (b) Prediction of soil organic carbon content at different moisture content using a spiked calibration PLS.

Here we present the parameter orthogonalisation algorithm which builds a calibration in a spectral space which is not affected by water content, i.e. orthogonal to the moisture effect spectrum. The formulation is described as follows:

$$\mathbf{Z} = \mathbf{P}\,\mathbf{X}$$

where $\mathbf{X}$ is the original spectra, $\mathbf{P}$ is the transformation matrix, and $\mathbf{Z}$ is the new transformed spectra. The problem is to find matrix $\mathbf{P}$ which is orthogonal to the moisture effect. The new spectra $\mathbf{Z}$ then can be used to build a calibration function which is not affected by moisture.

We first established difference spectra which were used to build the transformation matrix $\mathbf{P}$. We then applied the transformation to the spectra of air-dried samples, to produce transformed spectra $\mathbf{Z_{ad}}$. These transformed spectra contain information where the effect of soil moisture has been removed. We build a PLS regression using just $\mathbf{Z}_{ad}$ as input to predict soil carbon content.

Spectra for different water content were transformed using $\mathbf{P}$, resulting in transformed spectra, e.g. $\mathbf{Z}_{20}$ for spectra at an average moisture content of 20%. The transformed spectra were then fed into the PLS model. The resulting prediction for the same samples at different water contents is shown in Figure 3. We can see that although the prediction is now barely affected by moisture content.

Conclusions

This is the first experiment that shows a feasible and robust method to predict soil organic carbon from NIR spectra independent of moisture content. This method will facilitate field methods for rapid measurement of soil carbon content. Further work is ongoing to validate this method for field NIR measurement.
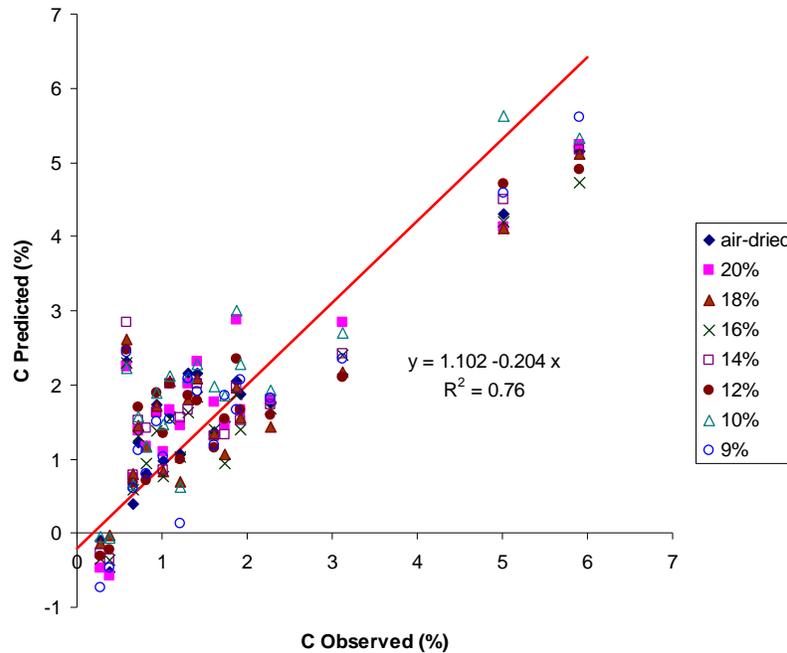
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Figure 3. Prediction of soil organic carbon content at different moisture content using an orthogonolised transformed calibration PLS.

Acknowledgements

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