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Penetrometer-mounted VisNIR spectroscopy: Application of EPO-PLS to *in situ* VisNIR spectra

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ABSTRACT

Visible near-infrared spectroscopy (VisNIR) has been used to measure many soil properties. Typically, VisNIR is used on air-dried and ground soils in the laboratory. Recent developments in VisNIR instrumentation have allowed for the collection of VisNIR spectra from *in situ* soils. In this study, we demonstrate the viability of an *in situ* VisNIR system. VisNIR spectra were collected using a penetrometer-mounted VisNIR probe. The penetrometer-mounted VisNIR system requires no field calibration or pre-drilling of access holes. This system has several advantages in that it: 1) allows for measurement of soil properties without sample collection, preparation, and laboratory analysis and 2) can provide rapid soil measurement at high-depth-resolutions (2 cm). We applied an external parameter orthogonalization (EPO) to the *in situ* spectra to remove the effects of soil moisture and other *in situ* effects from the spectra. We calibrated partial least-squares (PLS) models using spectra from an existing library of air-dried and ground spectra. PLS models were then used to predict clay content of the EPO-transformed *in situ* spectra. Model results showed good predictive ability for *in situ* spectra with RMSE, bias, and R^2 of 88 g kg^{-1}, -15 g kg^{-1}, and 0.76, respectively. A site-wise hold–out validation of EPO calibration demonstrated that EPO calibrations were robust to changes in soil characteristics and parent materials between study areas. These results show that by using the EPO-PLS method, *in situ* VisNIR is a viable tool for rapid, minimally invasive collection of soil data.

1. Introduction

Despite the continued demand for soil data in applications such as digital soil mapping and precision agriculture, these applications are still limited by the availability of reliable soil measurements. Data on soil properties are typically limited by the high cost of soil sample collection and laboratory analysis. Laboratory-based spectroscopy systems such as visible near-infrared spectroscopy (VisNIR) can reduce the cost of laboratory analysis by replacing, or supplementing, traditional analytical approaches. Laboratory-based VisNIR has been used for prediction of many soil properties including clay content (*e.g.* Chang et al., 2001; Shepherd and Walsh, 2002), organic and inorganic carbon content (*e.g.* Shepherd and Walsh, 2002; McCarty et al., 2002), cation exchange capacity (*e.g.* Chang et al., 2001; Shepherd and Walsh, 2002), and properties primarily related to clay content. Despite the success of laboratory-based VisNIR the method still requires collection and preparation of soil samples.

To reduce the need for sample collection, several researchers have been investigating the use of VisNIR for measurement on *in situ* soils. In the most elementary approaches, spectrometers are used to measure soils collected from sections of soil cores (Ge et al., 2014; Morgan et al., 2009; Waiser et al., 2007) or on soil profiles exposed during sampling pit-excavation (Viscarra Rossel et al., 2009). While these methods were successful, the methods still require collection or disturbance of the soil.

An alternative approach is to build an instrument that can be inserted into the soil where VisNIR spectra can be collected for the undisturbed *in situ* soils. Ben-Dor et al. (2008) developed such an instrument that could be inserted into bore-holes pre-drilled into the soil. Once inside the pre-excavated bore-hole, the instrument could collect VisNIR spectra. The basic idea behind this instrument was further refined by equipping soil penetrometers with optical instruments capable of measuring the VisNIR reflectance of soil *in situ* (Poggio et al., 2015; Chang et al., 2011). Penetrometer-mounted VisNIR probes can be inserted into the soil without excavation of a soil bore-hole. Penetrometer-mounted VisNIR probes can collect VisNIR spectra at high-depth-resolutions (*i.e.* 2 to 5 cm) with minimal soil disturbance. If successful, VisNIR-equipped penetrometers could greatly reduce the need for expensive traditional soil sampling and laboratory approaches.

Abbreviations: EPO, External parameter orthogonalization; PLS, Partial least squares; VisNIR, Visible, near infrared spectroscopy; RMSE, Root mean squared error.

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Typically, in VisNIR modeling, prediction models are calibrated using the collection of spectra measured from soils of known properties. These spectral collections, referred to as spectral libraries, can contain thousands to tens of thousands of soil spectra (Viscarra Rossel et al., 2016; Brown, 2007) and represent a substantial financial investment. The vast majority of reference spectra in spectral libraries are collected from soils that have been air-dried and ground. A major challenge for *in situ* VisNIR is that *in situ* spectra are altered by the effects of soil moisture, ambient temperatures, and soil structure (Bricklemyer and Brown, 2010). These effects, henceforth referred to as *in situ* effects, alter the spectra enough that models calibrated with existing spectral libraries (*i.e.* calibrated with spectra from air-dried and ground soils) cannot be used successfully on *in situ* spectra (Ge et al., 2014).

One approach for VisNIR modeling with *in situ* spectra is to generate new spectral libraries specifically for *in situ* spectra. While this approach has been implemented (Roudier et al., 2015; Morgan et al., 2009; Waiser et al., 2007), it costly and can still result in errors due to the effects of differential soil moisture (Waiser et al., 2007). An alternative approach is to remove the *in situ* effects from the spectra using a spectral projection (Ji et al., 2015; Ackerson et al., 2015; Ge et al., 2014; Minasny et al., 2011). In this study we used a projection called an external parameter orthogonalization (EPO). The EPO rotates spectra in such a way the *in situ* effects are removed from the spectra (Roger et al., 2003). EPO has been used to remove soil-moisture effects from ground soil samples (Minasny et al., 2011) and spectra from intact soil cores (Ackerson et al., 2015; Ge et al., 2014). By removing *in situ* effects from spectra using the EPO, models calibrated with an existing library of spectra from air-dried and ground soils can be used on spectra collected *in situ*.

EPO is not the only projection that has been used to remove water content effects from VisNIR spectra. Direct Standardization (DS) has also been used (Ji et al., 2015). The goal of this study was primarily to evaluate the penetrometer-equipped VisNIR system and a thorough comparison of the performance differences between DS and EPO is beyond the scope of this paper. For a more thorough discussion of DS and EPO readers are directed to Wijewardane et al. (2016) and Ji et al. (2015).

In this study we demonstrate the utility of a penetrometer-mounted VisNIR probe as a viable tool for measuring soil properties *in situ*. To do this, we collected two sets of VisNIR spectra. One set of spectra was collected from *in situ* soils using a penetrometer-mounted VisNIR probe. The second set of spectra was collected from the same soils in the air-dried and ground condition. Using this data we test: 1) if the EPO can remove the *in situ* effects from *in situ* spectra and 2) that after application of EPO, clay content of *in situ* spectra can be estimated with models calibrated using a spectral library of air-dried and ground spectra. We will compare the performance of predictions made from *in situ* spectra with the performance made using spectra from the same soils in the air-dried and ground condition.

2. Materials and methods

2.1. Instrumentation for collection of in situ VisNIR spectra

A penetrometer-mounted VisNIR probe was used to collect *in situ* VisNIR spectra. The probe is similar to that used by Poggio et al. (2015). The probe consists of a stainless steel outer case, 32 mm in diameter (Fig. 1). The probe is attached to a hollow 25-mm diameter steel tube 1.2 m in length. This tube is then attached to a hydraulic soil probe (Giddings Machine, Fort Collins, CO, USA) which is used to insert the probe into the soil. The tube is hollow to allow power supply cables and optical fibers to be routed inside the tube itself, thus connecting the probe to instruments and a power supply located at the soil surface.

Inside the stainless steel case is a lamp which generates the initial light source for the probe. This light is reflected *via* a mirror across a sapphire window mounted on the side-wall of the spectrometer (Fig. 1). The light then interacts with soil and is reflected back into the probe where it is intercepted by an optical fiber. The optical fiber, housed inside the hollow steel tube, connects the probe to the spectrometer located on the soil surface. The optical fiber transmits light reflected from the soil to the spectrometer. An ASD AgriSpec spectroradiometer (Analytical Spectral Devices Inc., Boulder, Colorado, USA) was used for collection of all spectra in this study.

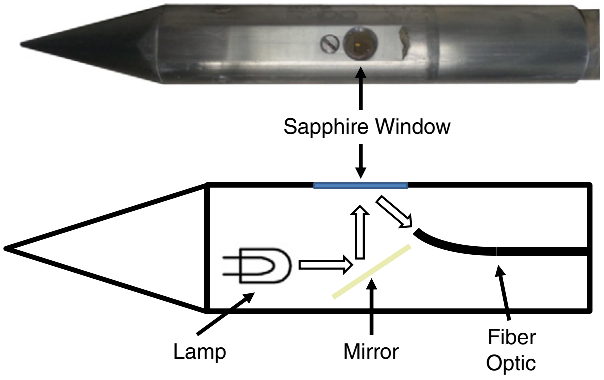

Fig. 1. Schematic of the penetrometer-mounted VisNIR probe. The upper photograph shows the probe exterior and the lower diagram shows the internal structure of the probe. White arrows represent the path of light inside the probe.

The optical fiber used in the penetrometer is five meters long, which is substantially longer than most fibers used for VisNIR. The longer fiber does result in minor signal loss; however, laboratory tests have indicated that the signal to noise ratio of the longer fiber is only increased by roughly 1.5%. Additionally, the signal processing used in this study, including the use of EPO, greatly minimizes any negative effects due to increased optical fiber length.

After initial setup, collection of VisNIR spectra using the penetrometer-mounted VisNIR probe is straight-forward. The probe is first calibrated by placing a spectralon panel against the sapphire window and by following typical VisNIR spectroradiometer calibration procedures (*i.e.* instrument optimization and standardization). Next, using the hydraulic soil probe, the instrument is inserted 5 cm into the soil and a spectra is collected. The probe is then inserted an additional 5 cm into the soil and a second spectra is collected. This procedure is repeated on 5-cm intervals until the probe has traveled the maximum distance of 120 cm.

2.2. Soil sampling

The penetrometer mounted VisNIR probe was tested at four sampling areas in Burleson and Brazos counties in the state of Texas, USA (Fig. 2). The sampling areas consist of a floodplain, a stream terrace, and two upland locations. These sampling locations were chosen because they offer a diverse range of parent materials and geologic ages. Soils on the floodplain and stream terrace were developed in alluvial materials dating from the Holocene and Pleistocene epochs, respectively. Soils from the upland areas were developed in coastal plain sediments of the Eocene-aged Yegua formation (Soil Survey Staff, 2002).

The soil moisture and temperature regimes of the sampling area are Usitic and Thermic, respectively. The clay minerology of the soils in the stream terrace and uplands is often smectitic, although soils located in the floodplain generally have mixed minerologies (*e.g.* mica, smectite, and kaolinite). In the floodplain, soils are mapped predominantly as Vertisols and Inceptisols. On the stream terrace and upland, soils are mapped as Alfisols, Vertisols, and their respective intergrades (Soil Survey Staff, 2002).

Within each sampling area, we chose several sampling locations, in a fashion that maximized the diversity of soil properties observed within each study site. At the stream terrace, where soils exhibited the largest range in physical and morphological properties, 20 locations, or soil