



Predicting clay content on field-moist intact tropical soils using a dried, ground VisNIR library with external parameter orthogonalization



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ABSTRACT

The effect of variable soil moisture, which is found in natural field conditions, is the single most limiting aspect that limits proximal implementation of VisNIR spectroscopy for predicting soil properties using dried-ground spectral libraries. Though the external parameter orthogonalization algorithm (EPO) has shown promise in removing the effect of soil moisture on soil spectra of intact-field moist soils without having to know the soil moisture, EPO has not been widely tested and has not been tested on soils with highly weathered mineralogy (oxides and kaolinite). Thus, the objective of this work was to test the effectiveness of EPO on intact field moist soil spectra and a dried-ground spectral library from highly weathered soils located in Brazil and to use this diverse dataset to assess the sensitivity of the EPO-PLS parameterization and performance to changes in the structure of the calibration spectral dataset. A dried-ground spectral library of 1515 soils collected from Piracicaba and Sao Paulo State, Brazil was transformed using the EPO P-matrix from 80 surface and subsurface soils collected independently of the library and scanned at field-moist intact and at dried-ground condition. Results show that EPO can remove the effect of soil water from field-moist spectra for tropical soils with kaolinitic and ferritic mineralogies. Predicted clay content improved from 320 to 120 g kg⁻¹ for spectra before and after EPO, respectively. Bootstrapping analysis was performed to assess the sensitivity of the EPO-PLS procedure to changes in the structure of the calibration spectral dataset. All EPO-PLS parameterizations were constrained to a small set of values and small changes to EPO-PLS parameterization had little observed effect on model performance. Large spectral libraries, those developed at the national or continental level, will contain soils of varying mineralogy. While research has shown that EPO is effective on smectitic soils as well as on kaolinitic soils, it is still unclear to what extent mineralogy controls EPO effectiveness.

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1. Introduction

The availability of soil spatial information (*i.e.* soil maps) varies across the globe. For some countries, highly detailed soil maps have been published. For example, The Netherlands has published a national soil map at a scale of 1:50,000 (Hartemink and Sonneveld, 2013). However, in much of the world including South America and Africa, soil information is unknown or mapped at a scale that is unsuitable for management at the watershed or farm scale. For example, only 0.25% of the area of Brazil is mapped with a 1:100,000 scale (Mendonça-Santos & Dos Santos, 2006), which is still not suitable for soil management. Development and refinement of coarse-scale soil maps had been slow primarily due to the large expense associated with obtaining soil information (McBratney *et al.* 2003).

Abbreviations: EPO, external parameter orthogonalization; PLS, partial least squares; VisNIR, visible, near infrared spectroscopy; RMSE, root mean squared error; RPD, ratio of performance to deviation.

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Visible near-infrared (VisNIR) spectroscopy offers a viable tool for quantification of many soil properties (Chang *et al.*, 2001; Viscarra Rossel *et al.*, 2006). By replacing traditional laboratory analysis with VisNIR, the costs of soil survey and mapping can be reduced (Waiser *et al.*, 2007). The success of VisNIR has led to considerable investment in large spectral libraries (Brown *et al.*, 2006; Shepherd and Walsh, 2002) as well as portable VisNIR equipment for collection of *in-situ* spectra (Ben-Dor *et al.*, 2008; Brickleyer and Brown, 2010; Chang *et al.*, 2011; Christy, 2008; Mouazen *et al.*, 2007; Sudduth and Hummel, 1993; Viscarra Rossel *et al.*, 2009). *In situ* VisNIR has been used for successful prediction of clay content (Waiser *et al.* 2007) and soil organic carbon (Morgan *et al.*, 2009).

Multivariate modeling of many soil properties from VisNIR spectra is possible due to the interaction between soil water and the soil minerals (Demattê *et al.*, 2006). However, the non-linear effect of variable soil moisture in *in-situ* spectra interferes with VisNIR model predictions (Brickleyer and Brown, 2010; Minasny *et al.*, 2009). Due to the effects of soil water, spectral libraries collected on dry-ground soils are ineffective when applied to *in-situ* spectra. To correct for the effects of soil moisture, Minasny *et al.* (2011) applied the external parameter

orthogonalization (EPO) algorithm (Roger et al., 2003) to VisNIR spectra from moist soil. Their results showed that EPO could remove the effect of water content from VisNIR spectra allowing for successful predictions of soil organic carbon using partial least squares (PLS) models calibrated with air-dried spectra. The EPO-PLS method was also used for predicting clay content and soil organic carbon of intact and field-moist soil cores (Ge et al. 2014).

EPO removes the effect of soil water from spectra by projecting spectra into a portion of spectral space orthogonal to the effect of water content on the spectra. This projection is essentially a rotation in spectral space that reorients the spectra so that water content has no influence on the spectra. The projection is a rotation rather than a re-scaling; the success of the projection relies on correctly identifying the direction, in spectral space, of the soil water content effect rather than quantifying the magnitude of the effect. Because of this, no knowledge of the soil water content of individual samples is needed in order to use the EPO. Additionally, a single EPO projection can be applied to soils covering a wide range of soil water contents. It is well known that different soil minerals present unique VisNIR reflectance patterns (Demattê et al., 2004; Mulder et al., 2013). The uniqueness of these features stems, in part, from the fact that physical integrations between soil minerals and soil water are mineral dependent. When used to correct for the effects of soil moisture on VisNIR spectra, EPO-PLS relies on identifying the nature of the interactions between soil water and soil minerals. It is currently unclear to what extent mineralogy determines the effectiveness of EPO-PLS. Both Minasny et al. (2011) and Ge et al. (2014) showed that EPO could effectively remove the effects of soil water from VisNIR spectra of soils with predominantly smectitic mineralogy and minor components of 1:1 clays and mixed mineralogy. To be regarded as an effective tool, the effectiveness EPO-PLS needs to be demonstrated for soils where mineralogy is dominated by minerals other than smectites and silicate clays.

This research aims to show that EPO-PLS is an effective tool for VisNIR spectroscopy of tropical soils with mineralogy consisting of a mixture of kaolinite and iron–aluminum oxides. First, we demonstrate that EPO can effectively remove the effect of water content from field-moist spectra for tropical, mixed mineralogy soils. Additionally, we show that after EPO-projection, dry-ground spectral libraries can be used for PLS prediction of clay content from field-moist spectra.

One concern with EPO-PLS is that parameterization of the EPO projection may be unstable and sensitive to changes in the calibration dataset. Minasny et al. (2011) began to address this issue and showed that accuracy of EPO-PLS was sensitive to the size of the calibration dataset. They determined that a minimum of 60 spectra were needed for EPO-PLS parameterization. In this paper we elaborate on the work of Minasny et al. (2011) and investigate how variability in the EPO-PLS calibration dataset influences the parameterization and accuracy of EPO-PLS. To achieve this, we conducted a bootstrapping exercise to generate multiple realizations of an EPO calibration dataset. Using these bootstrapped datasets, we observed effects of dataset variability on EPO-PLS parameterization and performance.

2. Materials and methods

2.1. VisNIR datasets

A collection of 1515 soil samples from São Paulo state in Brazil (Dataset A), were collected from Piracicaba and Sao Paulo State, Brazil (longitude 47° 31' 00" W; latitude 22° 39' 00"S). Soils in this dataset are old and highly weathered containing soils classified as Ferrasols, Nitisols, Lixisols, and Arenosols (IUSS Working Group WRB, 2014). The time-scale required for development of Ferrasols is large. Estimates from Africa indicate that it takes about 75,000 years to develop 1 m of a Ferrasols (Aubert, 1960). The true age of Ferrasols is quite difficult to determine. Estimates place the age of Brazilian Ferrasols between 1 and 50 Ma (Buol, 2009; Richter and Markowitz, 2007). The climate of

this area is a humid subtropical climate according to Köppen and Geiger, with dry winters and rainy summers (Peel et al., 2007). Annual average of temperature is 21.6 °C, and annual precipitation ranges from 1400 to 1600 mm. Parent materials from this area are broad and contain shales, sandstones, and basalts, all derived from the São Bento Group (Botucatu, Serra Geral and Pirambóia formations). The soils are highly weathered with mineralogy constituted by kaolinite and gibbsite, while few samples also have montmorillonite. The weathering indexes used to measure these soils are silt:clay ratio and Ki ($1.7\text{SiO}_2/\text{Al}_2\text{O}_3$). The Ki index indicates the soil weathering degree, where $\text{Ki} > 2$ indicates less weathered soils (2:1 silicate clays, vermiculite and montmorillonite); Ki between 2 and 0.75 indicates intermediate weathered soils (1:1 silicate clays, kaolinite); and $\text{Ki} \leq 0.75$ indicate highly weathered soils (gibbsitic and kaolinitic soils) (Empresa Brasileira de Pesquisa Agropecuária [Embrapa], 2013). In general, the soils in this library have silt:clay ratios less than 0.7, which indicates highly weathered soils (Empresa Brasileira de Pesquisa Agropecuária [Embrapa], 2013). As well, the Ki indexes are mostly less than 2.0. Approximately, 20% of the samples were collected in complete profiles, and the other 80% were collected with an auger in three depths (0–20, 40–60, 80–100 cm).

Spectra for the library (Dataset A) were obtained in the laboratory with an ASD FieldspecPro (Analytical Spectral Devices, Boulder CO) with a spectral range from 350 to 2500 nm. Scanning was completed using a fiber optic placed 8 cm above the sample. For lighting, two halogen lamps (50 W) placed 35 cm from the sample with a zenith angle of 35° were used. For each sample, three spectra consisting of 100 spectral acquisitions were collected. The three spectra were then averaged to yield the final spectra. Spectra for Dataset A were collected on soil that had been dried and ground to pass through a 2-mm sieve.

To test the EPO, intact field-moist soil samples from 58 locations within São Paulo State (Fig. 1), were collected. Site selection was based on locations that were likely to represent the soils within the area of Dataset A. Relief was used to determine sampling locations that would represent soils from the area of the library. Findings by Behrens et al. (2014) indicate that relief is effective for this type of site selection in this area. At each location, soil samples were collected with auger at two depths (0 to 20 and 80 to 100 cm). Soil samples were inserted into plastic bags and brought directly into laboratory. In total, the dataset consisted of 116 soil samples. Using the same spectrometer and geometry used to collect Dataset A, two sets of reflectance spectra were collected on these samples. The first set of spectra was collected immediately after samples were returned to the laboratory while the soils were in the field moist state. This set of spectra is assumed to be similar to the condition of spectra collected on *in-situ* soils. Soils were then air-dried and ground to pass through a 2-mm sieve after which spectra were again collected. This second set of spectra was collected under the same condition as Dataset A.

The collection of soils mentioned in the preceding paragraph, consisting of the 116 soil samples scanned in the field-moist and air-dry condition, was divided into two separate datasets. Using stratified random sampling by clay content, roughly 75% of soils from the EPO test dataset were assigned to Dataset B, which was used for estimation of the EPO. The remaining 25% of soils were assigned to Dataset C and used to assess the performance of the EPO. Stratified random sampling by clay content was used to ensure that Dataset B and Dataset C covered similar ranges of clay contents. During stratified random sampling, soils were selected by location so that surface and subsurface samples from each location were assigned to the same dataset insuring independence of the two datasets.

For all three datasets (A, B, and C), spectra were filtered using the Savitzky–Golay transformation with a second order filter and a window size of 11 nm (Savitzky and Golay, 1964). Spectra were then resampled at 10-nm intervals between 500 and 2450 nm. Resampling decreased the size of the spectra and removed portions of the spectra where the signal to noise ratio was poor (*i.e.* reflectance less than 500 nm and greater than 2450 nm). Finally, spectra were transformed to absorbance

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