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Effects of external factors on soil reflectance measured on-the-go and assessment of potential spectral correction through orthogonalisation and standardisation procedures

M.H.D. Franceschini[a,b], J.A.M. Demattê[a,*], L. Kooistra[b], H. Bartholomeus[b], R. Rizzo[a], C.T. Fongaro[a], J.P. Molin[c]

[a] Department of Soil Science, 'Luiz de Queiroz' College of Agriculture, University of São Paulo (ESALQ/USP), Av. Pádua Dias, 11, CEP 13418-260, Piracicaba SP, Brazil
[b] Laboratory of Geo-Information Science and Remote Sensing, Wageningen University and Research, Droevendaalsesteeg 3, 6708 PB Wageningen, The Netherlands
[c] Department of Biosystems Engineering, 'Luiz de Queiroz' College of Agriculture, University of São Paulo (ESALQ/USP), Av. Pádua Dias, 11, CEP 13418-900, Piracicaba SP, Brazil

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ABSTRACT

Reflectance spectroscopy is an alternative to describe soil properties, with potential to reduce costs and environmental impacts of conventional practices related to this activity. Acquisition of soil spectra on-the-go has several advantages over 'in-situ' static approaches, like deriving information with high spatial density. However, issues concerning on-the-go spectral measurements exist, mainly due to sensor movement and heterogeneous soil condition in the field. Procedures to mitigate these drawbacks, like external parameter orthogonalization (EPO) and direct standardization (DS), have mainly been applied so far to static spectral readings. In this study, EPO, DS and orthogonal signal correction (OSC) are tested in the context of on-the-go spectra acquisition for prediction of soil properties related to liming (i.e., pH in $CaCl_2$, pH in SMP buffer, concentration of organic matter, calcium and magnesium, potential acidity, sum of basis, cation exchange capacity and its saturation by basis, lime requirement and moisture content). A detailed dataset (300 soil samples coupled with laboratory and field spectral measurements) was acquired in two sites in Brazil with contrasting soil attributes (site 1 with 'clayey texture' – Ferralsol; site 2 with 'sandy texture' – Alisol), and variability of soil properties was increased in these sites through application of different limestone rates in experimental plots. Spectral correction procedures slightly improved the accuracy of lime requirement predictions, with reduction of root mean squared error (RMSE) from 1.43 to 1.17 t ha^{-1}, for study site 1 after applying OSC, and from 0.59 to 0.44 t ha^{-1}, for study site 2 after DS was implemented. However, models based on laboratory data still performed considerably better with RMSE of 0.99 and 0.43 t ha^{-1} for site 1 and 2, respectively. 'Global' (i.e., one general correction model for a given field) or 'specific' models (i.e., several correction models, derived according to clusters obtained through fuzzy k-means applied to OSC components) performed considerably worse in comparison with other studies. Probably occurrence of external factors affecting the spectral information was not constant in the mapped fields. Also, different external factors may have affected the spectra at the same time and efficiency of the correction procedures decreased. Considering the high sensitivity of predictions based on field data to the approach used to interpolate the spectra and the poor performance of the correction methods applied in this context, more investigation is needed to improve predictions based on spectral data acquired on-the-go. Homogeneous spatial distribution of factors not related to the properties of interest, or at least in a degree allowing correction by the methods tested here, may not happen when current measurement systems are used. Despite that, spatial patterns described by wet-chemical analysis could be represented, at certain extent, through predicted values of lime requirement (LR), derived from field spectra. For instance, predictions after spectral correction resulted in autocorrelation patterns and map of LR comparable with those observed using conventional methods, for the site 1. These results, coupled with a semiquantitative potential of predictions based on field data after spectral correction, indicate that on-the-go measurements have potential for soil properties characterization, although full quantitative potential will require further advances in sensing solutions and chemometric methods applied in this context.

* Corresponding author.
E-mail address: jamdemat@usp.br (J.A.M. Demattê).

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1. Introduction

Description of soil spatial variability in suitable scale to assist farmers in crop management is crucial to increase efficiency and mitigate impacts of agricultural activities. Conventional methods used to estimate soil properties, i.e. soil sampling and wet-chemical analysis, are intrinsically costly and time-consuming (Bartholomeus et al., 2011; Ben-Dor and Demattê, 2015). Therefore, alternative approaches to characterize variability of soil attributes have received increasing attention over the past years. One of them is reflectance spectroscopy in the visible, near-infrared, and shortwave infrared (Vis-NIR-SWIR), which can be used to estimate soil properties while reducing operational costs and environmental impacts related to soil mapping (Adamchuk et al., 2004; Bricklemyer and Brown, 2010).

The interaction between incident light and soil is affected by its organic and mineral composition, as well as by its physical properties (Ben-Dor and Demattê, 2015). In this context, radiation scattering is mainly related to iron-bearing and clay minerals, concentration of organic matter, soil moisture content and particle size distribution. Therefore, estimating soil properties based on reflectance depends on some spectrally active soil components. Although predicting concentration of plant nutrients in the soil is certainly of interest for agricultural practices due to their direct impact on crop production, most of these components are not expected to have straightforward relation with soil reflectance (Stenberg et al., 2010). The same applies to soil pH and lime requirement, their successful estimation using spectroscopic approaches are frequently reported as possible due to correlation with other soil attributes that are spectrally active. For instance, correlation with organic and mineral components are often pointed as possible mechanisms allowing to describe variability of pH and lime requirement since these properties are related to soil cation exchange and buffering capacity (Marín-González et al., 2013; Tekin et al., 2013).

Although spectroscopic techniques for soil properties estimation using laboratory measurements are relatively well established, approaches based on field data are less explored and often reported as substantially less accurate (Kuang et al., 2012). Lower accuracy of methods based on field readings can be attributed to several aspects, the so-called 'in situ' factors, like soil-to-sensor distance and inclination, illumination conditions, contamination by other targets, inconsistent soil presentation to the sensor, smearing, data averaged over a given travel distance and field natural heterogeneity concerning soil moisture and roughness (Mouazen et al., 2009; Bricklemyer and Brown, 2010; Kodaira and Shibusawa, 2013; Poggio et al., 2015; Ackerson et al., 2017; Nawar and Mouazen, 2017).

Acquiring data at higher density and investigating surface soil at adjustable depth are the main advantages of reflectance measurements taken on-the-go using systems pulled by tractor with measurement window in the bottom of a shank, as those proposed by Mouazen et al. (2005), Christy (2008) and Kodaira and Shibusawa (2013). Despite this fact, attempts to estimate soil properties using spectroscopy in the field with data acquired using static or on-the-go systems are still underrepresented in comparison with studies based on laboratory spectra, especially those targeting possible solutions to mitigate effects of soil heterogeneity and acquisition conditions on the prediction accuracy. Recently, Ackerson et al. (2017) applied the method called External Parameter Orthogonalization (EPO; Roger et al., 2003; Minasny et al., 2011) to remove effects of variation in soil water content, roughness, aggregation and temperature from static field measurements. These authors verified substantial improvement in the accuracy of clay content estimates after EPO was applied, using models derived from a spectral library corresponding to dried and sieved soil samples.

Before extending methodologies like these to datasets comprising on-the-go measurements it would be valuable to estimate how much of the effects from 'in situ' factors corresponding mainly to the sensor movement itself can be removed from the spectral information. Treatments like the EPO and direct standardization (DS; Wang et al., 1991; Ji et al., 2015), were applied so far to static field measurements. In this case, transfer samples measured in the laboratory, which are used to derivate correction models for field information, corresponded exactly to the same spatial support of field readings, i.e. measurements from laboratory and field were taken on the same samples. Besides, environment and acquisition set-up are more controllable when static systems are used instead of on-the-go approaches.

In this study, treatments aiming to remove the influence of 'in situ' factors from field spectra were tested using data acquired on-the-go and also non-processed samples measured in laboratory. Considering that procedures evaluated here aim to reduce disagreement between measurements taken in different conditions and that samples measured in laboratory were not dried or sieved before spectral measurements, it was expected that improvements in prediction accuracy due to spectral correction would be related to 'in situ' factors other than soil moisture, especially those concerning the sensor movement, e.g. changes in acquisition geometry, illumination and soil roughness. The methodologies applied were EPO, DS and Orthogonal Signal Correction (OSC; Wold et al., 1998). Although OSC has received less attention in previous studies it may have some advantages over other methods, since samples measured in the laboratory do not need necessarily to correspond to the same locations measured in the field and only information not related to the property of interest is removed from the spectral data (Woody et al., 2004).

Therefore, the main objectives of this study are: (1) estimate the potential of on-the-go spectroscopic techniques to predict soil properties related to soil lime requirement; (2) compare prediction accuracy of models derived from on-the-go spectral measurements with models based on laboratory data corresponding to 'non-processed' soil samples; (3) evaluate the efficiency of EPO, DS and OSC, usually applied to remove effects of 'in situ' factors from static field readings, in the context of on-the-go data acquisition, especially concerning other issues than soil moisture variability; (4) test if 'specific' models, developed after clustering the data according to orthogonal factors, can improve the correction performance, since clustered samples may have been subject to similar issues during acquisition; and (5) evaluate the description of spatial patterns through predicted values of lime requirement, based on comparison of interpolated maps and calculation of an spatial autocorrelation indicator (i.e., Moran's I index).

2. Materials and methods

2.1. Description of the study areas

Data was acquired in two areas (Fig. 1) in São Paulo state, Brazil: one near the city of 'Elias Fausto' (23°2′47″ S, 47°19′28.9″ W; Datum WGS84) and another near the city of 'Monte Mor' (22°58′5.8″ S, 47°16′28.4″ W; Datum WGS84). These sites have contrasting soil particles size distributions at the 0–20 cm depth. Analysis of a composite soil sample (10 random points; Bouyoucos, 1962) corresponding to site 1 (Ferralsol; IUSS Working Group, 2014), hereafter referred to as the clayey texture site, indicated 320.5, 545.1 and 134.4 g kg^{-1} of clay, sand and silt, respectively. On the other hand, for the site 2 (Alisol; IUSS Working Group, 2014), sandy texture site, analysis of a composite sample indicated 100.8, 806.0, and 93.2 g kg^{-1} of clay, sand and silt, respectively. Sugarcane was cultivated for four consecutive years on both sites before the establishment of the experiment, in 2012, and at the time the experiment took place both had undergone harvest before next cultivation.

2.2. Experimental design

In each site an area of 87 by 58 m was divided into 5 blocks, and 5 plots were established in each block (Fig. 1). Plots measured 10 by 15 m and were spaced 3 m apart, while blocks were spaced 2 m apart. One