



Spectral fusion by Outer Product Analysis (OPA) to improve predictions of soil organic C

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ABSTRACT

Soil organic carbon (C) is an important indicator of agricultural and environmental quality. It improves soil fertility and helps to mitigate greenhouse gas emissions. Soil spectroscopy with either vis–NIR (350–2500 nm) or mid-IR (4000–400 cm⁻¹) spectra have been used successfully to predict organic C concentrations in soil. However, research to improve predictions of soil organic C by simply combining vis–NIR and mid-IR spectra to model them together has been unsuccessful. Here we use the Outer Product Analysis (OPA) to fuse vis–NIR and mid-IR spectra by bringing them into a common spectral domain. Using the fused data, we derived models to predict soil organic C and compared its predictions to those derived with vis–NIR and mid-IR models separately. We analyzed 1259 tropical soil samples from surface and subsurface layers across agricultural areas in Central Brazil. Soil organic C contents were determined by a modified Walkley-Black method, and vis–NIR and mid-IR reflectance spectra were obtained with a FieldSpec Pro and a Nicolet 6700 Fourier Transformed Infrared (FT-IR), respectively. Reflectances were log-transformed into absorbances. The mean content of soil organic C was 9.14 g kg⁻¹ (SD = 5.64 g kg⁻¹). The OPA algorithm was used to emphasize co-evolutions of each spectral domain into the same one by multiplying the absorbances from both sets of spectra to produce a matrix with all possible products between them. Support Vector Machine with linear kernel function was used for the spectroscopic modeling. Predictions of soil organic C using vis–NIR, mid-IR, and fused spectra were statistically compared by the Tukey's test using the coefficient of determination (R²), root mean squared error (RMSE), and ratio of performance to interquartile distance (RPIQ). Absorbances in vis–NIR and mid-IR were emphasized in the common spectral domain presenting stronger correlations with soil organic C than individual ranges. Soil organic C predictions with the OPA fused spectra were significantly better (R² = 0.81, RMSE = 2.42 g kg⁻¹, and RPIQ = 2.87) than those with vis–NIR (R² = 0.69, RMSE = 3.38 g kg⁻¹, and RPIQ = 2.08) or mid-IR spectra (R² = 0.77, RMSE = 2.90 g kg⁻¹, and RPIQ = 2.43). Fusing vis–NIR and mid-IR spectra by OPA improves predictions of soil organic C.

1. Introduction

Soil organic carbon (C) comes from vegetation of natural and agricultural systems, which convert atmospheric CO₂ into organic compounds that are synthesized into organic matter (Corsi et al., 2012; Köchy et al., 2015a). Variations in land use and agricultural management practices can cause changes of organic C storage (Ogle et al., 2005; Zinn et al., 2005; Dieckow et al., 2009; Leite et al., 2009; Assad et al., 2013; Köchy et al., 2015b). Organic C is an important soil quality and productivity indicator, since its content is related to nutrient release, soil reactivity (cation exchange and buffering capacity), particle

aggregation, and development of soil structure, reducing bulk density and increasing soil water holding capacity and availability for plants (Batjes, 2010). The presence of organic C in soil has been associated with mitigation of greenhouse gas emissions (O₃, CO₂, CH₄, and N₂O) (Batjes, 2010; Brown et al., 2010; Viscarra Rossel et al., 2014).

Soil sensing using reflectance spectroscopy in visible–near-infrared (vis–NIR: 350 to 2500 nm) and mid-infrared (mid-IR: 2500 to 25,000 nm or 4000 to 400 cm⁻¹) has been proposed as effective alternatives to conventional laboratory analysis for the prediction of organic C in soil (McCarty et al., 2002; Reeves III et al., 2006; Madari et al., 2005b). Reflectance spectroscopy is a non-destructive technique

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that is based on interactions between electromagnetic radiation and functional groups of organic and mineral compounds in soil. These interactions can cause electronic transitions in atoms and vibrations (fundamentals, overtones, combinations, etc.) of bonds in molecules. These techniques do not need chemical reagents or elaborate preparation, and they are faster and cheaper than conventional analyses so that the analysis of many soil samples is feasible (Viscarra Rossel et al., 2011). There are some reviews on the use of reflectance spectroscopy for soil total organic and inorganic C analyses (Reeves III, 2009; Stenberg et al., 2010; Bellon-Maurel and McBratney, 2011; Croft et al., 2012; Soriano-Disla et al., 2014; Viscarra Rossel et al., 2016).

Generally, models developed with mid-IR spectra provide better predictions of soil organic C compared to those developed with vis-NIR spectra (McCarty et al., 2002; Viscarra Rossel et al., 2006; Madari et al., 2005b; Terra et al., 2015). However, reliable and accurate measurements have also been achieved in vis-NIR (Vasques et al., 2010; Vohland et al., 2011; Stevens et al., 2013; Viscarra Rossel and Hicks, 2015).

To improve quantifications of soil organic C from spectra, some authors have tried combining both vis-NIR and mid-IR into a single vector and performing multiple calibration with the combined dataset (Knox et al., 2015), but results are unsuccessful. One approach that could be used to effectively fuse vis-NIR and mid-IR data for prediction of soil organic C is Outer Product Analysis (OPA) (Cécillon et al., 2012). OPA aims to combine two different signals (e.g. spectra) to obtain information about the relationships between them (Jaillais et al., 2005). OPA enables co-evolutions of spectral ranges from different domains (e.g. different sensors) calculating a mutual weighting of these two signals and bringing them to the same domain (Barros et al., 2008). Its main idea is to fuse two sets of spectra from different sensors for a same sample and analyze their mutual variations due to differences in the concentrations of this sample (e.g. soil organic C) (Veselá et al., 2007). For each sample, OPA builds a matrix containing all possible combinations of intensities (e.g. absorbance) from both types of spectra. This matrix is the result of the outer products between vectors whose values depend on the intensities of the original spectra (Maalouly et al., 2004; Barros et al., 2008). OPA is a chemometrics technique that has been mostly used in food sciences (Natale et al., 2002; Maalouly et al., 2004; Jaillais et al., 2005; Veselá et al., 2007; Barros et al., 2008; Borràs et al., 2015).

Our research is based on the hypothesis that fusing vis-NIR and mid-IR spectra by OPA can improve predictions of soil organic C compared to quantifications made separately by each spectral range. Thus, our aim is to compare predictions of soil organic C using vis-NIR, mid-IR, and OPA fused spectra.

2. Material and methods

2.1. Soil database

We used 1259 soil samples from surface and subsurface horizons of 458 profiles from a spectral library developed by Bellinaso et al. (2010) and Terra et al. (2015). The database contains soil analytical information, geographical location, and information on climate, geology, and relief. These samples are from areas of sugarcane production in São Paulo (SP), Minas Gerais (MG), Mato Grosso do Sul (MS), and Goiás (GO), Brazil (Fig. 1).

2.2. Soil analysis

Soil samples were oven-dried (at 45 °C for 48 h), weighted, milled, and sieved. The fine earth fraction (≤ 2 mm) was used in the soil organic C and vis-NIR analyses. Subsamples of approximately 5 g were milled further to particle size < 200 μm (approximately 80 mesh) for mid-IR analysis.

2.2.1. Soil organic C

Total content of soil organic C was determined according to a modification of the Walkley-Black method (Walkley and Black, 1934) where soil organic matter is oxidized with potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$) in the presence of sulfuric acid (H_2SO_4), and the heat released in the acid dilution is used to catalyze the redox reaction. After digestion, the remaining unreduced $\text{K}_2\text{Cr}_2\text{O}_7$ is titrated with ferrous ammonium sulfate. The methodological procedure for this analysis was followed as described by Camargo et al. (2009). Soil organic C was calculated by multiplying soil organic matter by 0.58 (Hesse, 1971).

2.2.2. vis-NIR spectroscopy

Reflectance spectra were recorded with the FieldSpec Pro spectroradiometer (Analytical Spectral Devices, Boulder, Colo.) under laboratory conditions. This instrument has a spectral resolution of 1 nm from 350 to 1100 nm and of 2 nm from 1100 to 2500 nm. Data acquisition and the geometry of the setup are described in Terra et al. (2015), and they follow protocols by Viscarra Rossel et al. (2016). Approximately 95 cm^3 of soil samples were placed inside Petri dishes and leveled to reduce surface roughness. Four measurements were obtained per sample by rotating dishes every 90° in order to obtain a better representativeness of surface area, and an average spectrum was calculated for each sample. A spectralon plate (barium sulfate) with 100% of reflectance was used as the reference sample, which we measured every 20 min or 20 samples.

2.2.3. mid-IR spectroscopy

Reflectance spectra were obtained with the Nicolet 6700 Fourier Transform Infrared (FT-IR) (Thermo Fisher Scientific Inc., Waltham, MA) equipped with an accessory for diffuse reflectance (Smart Diffuse Reflectance). Laser HeNe was used as lighting source positioned internally with calibration standard for each wavelength. The sensor has a KBr beam splitter enabling wide amplitude of energy incident on the sample (from 4000 to 400 cm^{-1}). Spectra were acquired with spectral resolution of 1.2 nm and 64 measurements per minute per spectrum. Approximately 1 cm^3 of soil sample was placed in a sample holder for the measurement. A background spectrum (reference plate) was obtained for sensor calibration before each measurement. A gold diffuse plate was used as reference to remove background radiation from sample spectrum.

2.3. Outer Product Analysis to fuse vis-NIR and mid-IR spectra

Before the spectral fusion by OPA, the vis-NIR and mid-IR spectra were transformed into apparent absorbance ($A = \log_{10}(1/R)$) and re-sampled to 25 nm and 10 nm, respectively. We used OPA algorithm to merge the absorbance spectra in order to emphasize co-evolutions of the different spectral ranges in the same domain (Barros et al., 2008). Fig. 2 presents a methodological description of OPA. For the same sample, all absorbances of the vis-NIR range (signal 1 with r dimensions) were multiplied by all absorbances of the mid-IR range (signal 2 with c dimensions) producing a $r \otimes c$ matrix (Eq. (1)) with all possible products between absorbances in both spectral domains (Fig. 2a). Absorbance intensities of the resulting matrix will be dependent on the intensities of the original spectra (Maalouly et al., 2004; Barros et al., 2008), and the final number of matrixes (n) will be dependent on the number of soil samples (m) (Jaillais et al., 2005).

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