High resolution measurement of soil organic carbon and total nitrogen with laboratory imaging spectroscopy

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ABSTRACT

Soil is a critical component of global biogeochemical cycles, and there is an increasing need for cost effective tools to measure soil carbon stocks and determine soil nitrogen contents. Reflectance spectroscopy can deliver large volumes of soil carbon data. However, as soil carbon concentrations can be spatially heterogeneous, imaging spectroscopy presents the best potential to provide high resolution measurements and accurately characterize soil carbon heterogeneity. For this study, discrete, intact and unground soil samples were collected and analyzed using a SisuROCK automated hyperspectral imaging system in a laboratory setting, focused on the shortwave infrared portion of the electromagnetic spectrum. Samples were also analyzed for soil organic carbon and total nitrogen concentrations by dry combustion to prepare a training data set. Predictive models were built using continuous wavelet processing along with partial least squares regression and CUBIST models. Spatial variation of carbon and nitrogen was determined using Moran's i and comparisons of spatial variations among soil types and horizons were made using a spatial generalized least squares model. Overall, soil organic carbon was more aggregated in Chernozemic soils and in B and C horizons compared to A horizons. Nitrogen in turn showed more aggregation for all soil types and horizons compared to soil organic carbon. Results indicated that imaging spectroscopy can be successfully used to measure and characterize the spatial variability of soil carbon and nitrogen at the soil aggregate scale.

1. Introduction

Soil organic carbon (SOC) is a critical component of the global carbon cycle as soil contains 4.5 times the amount of carbon present in aboveground biomass (Jobbágy and Jackson, 2000), and soils can act as a source or sink for carbon. Quantifying SOC is essential for understanding how much carbon will be released from areas where soils will become a source for carbon and to understand how much carbon can be stored in soils acting as carbon sinks. In addition to SOC, nitrogen plays an essential role in biogeochemical cycles with nitrogen limitation widespread in terrestrial ecosystems (Vitousek and Howarth, 1991). There is a need for more rapid and cost-effective methods to quantitatively measure and characterize SOC and total nitrogen (TN). The increasing need for soil data has been referred to as a soil data crisis (McBratney et al., 2006).

Reflectance spectroscopy has the potential to solve this crisis, as it is a rapid and non-destructive analysis that can be utilized both in the laboratory and in the field. There is an extensive literature on the use of point measurement reflectance spectroscopy in many regions of the world to quantify SOC (Bartholomeus et al., 2008; Ben-Dor and Banin, 1990, 1995; Chang et al., 2001; Ge et al., 2014; Gomez et al., 2008; McBratney et al., 2006; McCarty et al., 2002; Rossel and Behrens, 2010) and total nitrogen (TN) (Chang et al., 2001; Chang and Laird, 2002; Morellos et al., 2016; St. Luce et al., 2014). While some work has been done analyzing SOC and TN with point reflectance spectroscopy in Canada (Martin et al., 2002; Xie et al., 2011), the literature is not as extensive.

Previous research has established that machine learning models can outperform partial least squares regression when used to build predictive models to measure soil properties from reflectance spectra (Doetterl et al., 2013; Nawar et al., 2016; Rossel and Behrens, 2010; Sorenson et al., 2017b). Additionally, an alternative signal processing method, continuous wavelet transforms, has improved results derived from the analysis of reflectance spectra compared to conventional signal processing techniques such as Savitsky-Golay smoothing, derivatives and multiplicative scatter correction (Rossel and Behrens, 2010; Viscarra Rossel and Lark, 2009). Combining wavelet analysis with machine learning models has been successful in producing SOC and TN

Table 1
Soil taxonomic classification and properties for the samples used to build predictive models.

Soil classification (Canadian) (Soil Classification Working Group, 1998)	Soil classification (WRB) (IUSS Working Group WRB, 2014)	Horizon	Number of samples	Soil organic carbon (g kg^{-1})	Total nitrogen (g kg^{-1})
Orthic Gray Luvisol	Albic Luvisol	A	5	4.8–16.4	0.6–1.3
		B	10	2.4–7.6	0.4–0.9
		C	10	2.3–6.2	0.2–0.6
Dark Gray Luvisol	Albic Luvisol	A	28	2.7–26.3	0.4–2.3
Gleyed Dark Gray Luvisol	Gleyed Luvisol	A	3	4.4–20.1	0.5–1.7
		B	3	3.2–9.0	0.4–0.6
Humic Luvic Gleysol	Planosol	A	4	4.5–43.3	1.7–3.4
		B	5	4.4–29.8	0.7–2.2
		C	1	22.9	
Orthic Luvic Gleysol	Planosol	A	2	2.9–5.0	0.5–0.6
		B	5	1.9–6.5	0.4–0.9
		C	5	2.1–6.2	0.3–0.9
Eutric Brunisol	Eutric Cambisol	A	5	5.8–37.1	0.5–2.0
		B	2	2.9–3.7	0.3–0.4
		C	4	0.9–2.1	0.1–0.2
Gleyed Black Chernozem	Gleyic Chernozem	A	1	35.2	3.1
		B	3	8.2–19.8	0.5–0.6
Orthic Black Chernozem	Chernozem	A	51	11.2–64.2	1.0–6.3
		B	4	11.2–31.9	0.8–1.2
Rego Black Chernozem	Chernozem	A	3	29–52.6	2.7–5.0
Orthic Gleysol	Eutric Gleysol	B	1	7.1	0.5
		C	5	3.5–8.4	0.3–0.5
Orthic Humic Gleysol	Mollic Gleysol	A	29	9.2–75.9	0.8–7.6
		B	1	0.61	0.6
		C	2	2.5–3.2	0.4
Rego Gleysol	Gleysol	C	3	6.8–20.2	0.6–2.0
Rego Humic Gleysol	Mollic Gleysol	A	6	55.6–75.6	5.2–7.4

predictive models for point spectroscopy systems with Canadian soils (Sorenson et al., 2017b).

Imaging spectroscopy has the advantage over point measurements of providing high resolution continuous spatial measurements. Imaging spectroscopy studies in soil science have tended to focus on airborne or space borne applications (Gomez et al., 2008, 2012; Melendez-Pastor et al., 2010; Ouerghemmi et al., 2011) as compared to measurements at the soil sample or profile scale where higher spatial resolutions can be achieved (e.g.; < 1 mm in contract to > 1 m per pixel). These studies have mapped different soil properties using imaging spectroscopy including: clay, sand, silt, SOC, and inorganic carbon content. Imaging spectroscopy can also be utilized at the laboratory scale to measure variation within samples, as well as to obtain high vertical resolution data. Lastly, laboratory imaging spectroscopy has been used to characterize the spatial variability of SOC and TN for a soil profile in Germany (Steffens and Buddenbaum, 2013). There are no studies using imaging spectroscopy systems to measure SOC and TN in Canada, specifically using wavelet analysis to analyze intact and unground samples.

Soil organic matter varies spatially both horizontally and vertically, and conventional analytical methods have limited ability to measure SOC and TN in fine spatial resolution. Reflectance spectroscopy has been shown to be a valuable tool to measure SOC in high vertical spatial resolution (Doetterl et al., 2013). High vertical resolution measurements can illustrate how SOC changes with depth depending on, for instance, the underlying parent material, and how these changes may be affected by distinct parent materials. Approximately 50% of SOC is contained below 20 cm in boreal forest soils and 59% is below 20 cm in croplands (Jobbágy and Jackson, 2000). Subsoil organic matter corresponds to a substantial proportion of the global soil carbon pool, and its characterization is essential for accurate soil carbon budgets. Other work has found that approximately 63% of SOC and 64% of TN are contained below 30 cm (Wang et al., 2017). For these reasons, tools that can accurately and cost effectively measure SOC at depth are very valuable for developing soil carbon budgets.

As imaging spectroscopy contains spatial as well as spectral information, the spatial variability of several distinct soil attributes can be analyzed at a variety of spatial scales. Imaging spectroscopy has not been used to characterize the soil aggregate scale spatial structure of SOC and TN in Canadian soils, and to determine how spatial structure in SOC and TN may vary between soil types and horizons. Canadian soils tend to be distinct from other regions that have been a focus of reflectance spectroscopy research in that they have relatively high organic carbon contents, can be frequently water saturated and are relatively young due to recent glaciation. Based on the success of point spectra to measure SOC and TN, and the success of imaging spectroscopy to measure soil and geological properties, the first objective of this study was to determine if shortwave infrared imaging spectroscopy could be used to measure SOC and TN on intact and unground samples in the laboratory for a variety of Canadian soil samples. The second objective was to use the imaging spectroscopy results to characterize the spatial distribution of SOC and TN at the soil aggregate scale, and determine if the distribution of SOC and TN varies based on soil type and horizon at fine spatial scales.

2. Materials and methods

2.1. Sample collection and preparation

A total of 370 soil samples were collected in Alberta and Saskatchewan, Canada in August and September 2015 and May 2016 (Table 1). To capture a range of soil samples common across the Canadian Prairies, samples were collected from the main soil orders that occur in this region: Chernozems, Gleysols and Luvisols (Table 1). In total, 121 Chernozemic samples (58 A horizon samples, 48 B horizon samples and 17 C horizon samples), 137 Gleysolic samples (47 A horizons samples, 36 B horizon samples and 54 C horizon sample) and 96 Luvisolic samples (36 A horizon samples, 33 B horizon samples, and 27 C horizon samples) were collected. Additionally, 16 Brunisolic samples (5 A horizon samples, 5 B horizon samples, and 6 C horizon samples) were collected as they were encountered opportunistically during soil sampling. Less Brunisolic samples were collected because the focus of