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Evaluation of soil structural quality using VIS–NIR spectra

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ABSTRACT

Application of visible (VIS) and near-infrared (NIR) spectroscopy for prediction of soil properties may offer a cost and time effective approach for evaluation of soil structural quality. Spectral data are often suitable for estimation of biochemical soil quality indicators such as soil organic carbon (SOC), total nitrogen and microbial biomass, while contradictory results have been reported for prediction of soil physical properties that are directly associated with soil structure. The aims of this study were to relate soil structural quality to overall indicators of soil quality, and to assess the efficiency of spectral data for the evaluation of soil structural quality. The study was conducted using 40 sites in Ireland under arable ($n = 20$) and grassland ($n = 20$) management systems. At each site five subplots were selected for soil sampling and twenty-one chemical, biological and physical properties were measured using standard methods as indicators of soil quality. The visual evaluation of soil structure (VESS) was performed to evaluate and classify soil structural quality. Soil properties that were significantly different ($P < 0.05$) between soil structural quality classes were considered for further analysis, and principal component analysis was used to determine the key indicators as a minimum data set (MDS). VIS and NIR spectra were then measured and partial least-squares regression used to predict soil quality indicators associated with soil structural quality. SOC, penetration resistance, magnesium (Mg), aggregate size distribution and CN ratio comprised the MDS. An excellent model was achieved for SOC (RPD > 4, $R^2 = 0.94$; RMSE = 0.42). A good model was obtained for Mg, CN (RPD from 2 to 2.5, $R^2 \geq 0.7$), and moderate capability for prediction of aggregate size distribution, and penetration resistance (RPD from 1.5 to 1.99, $R^2 \geq 0.64$). Soil structural quality classes were found to be associated with a number of biochemical and physical soil properties. Soil spectra produced acceptable models for predicting relevant soil structural indicators, and the mean soil spectra were different between soil structural classes. Therefore, a combination of spectroscopic and chemometric techniques can be applied as a practical, rapid, low cost and quantitative approach for evaluating soil structural quality under arable and grassland management systems in Ireland.

1. Introduction

Rapid, precise and quantitative assessment of soil quality is crucial for sustainable evaluation and monitoring the effects of management on soil resource under agricultural systems (Bone et al., 2012; Zhang et al., 2012). Inappropriate management can influence soil quality resulting in degradation and adverse effects on productivity (Batey and McKenzie, 2006; Munkholm et al., 2013). Evaluation of soil quality is usually a combination of physical and/or biochemical indicators as a minimum data set (Doran and Parkin, 1994; Qi et al., 2009). Therefore, choosing the appropriate indicators is the main step to an accurate assessment of soil quality (Aparicio and Costa, 2007; Doran and Jones, 1996). Principal component analysis (PCA) is commonly used to reduce data redundancy among properties for identifying a minimum data set (MDS) (Andrews et al., 2002; Govaerts et al., 2006; Li et al., 2007). Soil structural indicators are usually an important part of the minimum data set because structure plays a fundamental role in agricultural systems (Mueller et al., 2013; Roger-Estrade et al., 2010). Soil aggregate stability, which is an important indicator of soil structural quality, has a critical role in prevention of soil erosion and soil degradation (Barthès and Roose, 2002; Le

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Bissonnais et al., 2007) While more factors besides soil structure are usually employed for precise assessment of soil quality (Karlen et al., 1997), improvement in soil structure results in better soil quality associated with sustainable soil productivity (Andrews et al., 2004).

Visual methods have been successful for assessment of soil structural quality and can be reliably applied for the evaluation of soil structure in agricultural soils (Guimarães et al., 2013; Mueller et al., 2009, 2013; Shepherd, 2009). Of all visual approaches, the simpler methods such as the "visual evaluation of soil structure" (Ball et al., 2007; Guimarães et al., 2011) and the "visual soil assessment" (Shepherd, 2009) have been broadly used during the past few years. Visual Evaluation of Soil Structure (VESS), which was developed by Ball et al. (2007) based on the soil structure evaluation method (Peerlkamp, 1959), mainly focuses on soil structural factors including size, shape, strength and porosity of soil aggregates (Ball et al., 2007). Many soil functions such as biological diversity and activity, soil productivity and soil physical stability that support plant growth, nutrient and carbon cycling are affected by soil structural quality (Kavdır and Smucker, 2005). Guimarães et al. (2013) showed that VESS was able to differentiate structural quality and could be used for the evaluation of soil physical quality. Ball et al. (2013) reported that the visual assessment techniques could explain more than soil structure and included various soil properties associated with crop and environmental conditions, and Askari et al. (2013) indicated that VESS could be used as a practical and rapid method for detecting the impact of arable management systems on Irish soils. Mueller et al. (2013) concluded that soil visual evaluation method could be used for general soil quality rating. Despite the capability of visual approaches for assessing of soil quality, these methods are qualitative or semi-quantitative and can be used as a complementary approach to laboratory analyses, which are time consuming and expensive (Askari et al., 2013; Ball et al., 2007; Shepherd, 2009). In addition, subjectivity is still a controversial issue regarding the visual assessment of soil, and using the methods appropriately requires gaining practical experience (Guimarães et al., 2011).

Over the past three decades, Visible (VIS) and near-infrared (NIR) spectroscopy have been shown to be an effective alternative to conventional laboratory analysis, and can provide time and cost effective approaches for the prediction of several soil properties (Cécillon et al., 2009; Chodak, 2011; Viscarra Rossel et al., 2006). Spectroscopy has the potential to simultaneously characterize a number of soil attributes associated with soil quality, thus requiring less time and expensive sampling procedure (Viscarra Rossel et al., 2006). The advantage of using spectroscopy becomes evident when quantifying soil quality, which requires large amounts (in terms of sample numbers and number of properties measured) of soil data across management systems. Spectral data are often suitable for the estimation of biochemical soil quality indicators such as soil organic carbon, total nitrogen and microbial biomass that can be indirectly linked to soil structure (Chang et al., 2001; O'Rourke and Holden, 2012; Yang et al., 2012). Contradictory results have been reported for the prediction of soil physical properties, which are directly associated with soil structural quality (Cécillon et al., 2009). Cañasveras et al. (2010) concluded that reflectance was useful for prediction of soil aggregate stability, and the spectral prediction of aggregate stability indices was better than indices predicted by pedotransfer functions using basic soil attributes (organic matter, texture, pH, iron oxides and calcium carbonate). Gomez et al. (2013) found that laboratory Vis–NIR spectroscopy could be used as an alternative approach for assessing soil aggregate stability. They indicated the soil aggregate stability had a strong correlation with soil organic carbon. Partial least squares regression (PLSR) is the most commonly used multivariate analysis technique among calibration methods employed for soil spectral analysis (Chang and Laird, 2002; McCarty et al., 2002; Viscarra Rossel et al., 2006). PLSR can provide an accurate method for modeling the relationship between soil spectra and indicators of soil structural quality (Janik et al., 2009). Soil structure is usually highly associated with soil properties, which are predicted well from spectral data (such as SOC, e.g. O'Rourke and Holden (2011, 2012)), and this correlation can be used for determination of soil structural quality from spectral data sets.

For this study, VESS, VIS–NIR spectroscopic and chemometric analysis were employed for classification and assessment of soil structural quality. The objectives were to relate soil structural quality to indicators typically used to describe soil quality in general, and to evaluate the efficiency of soil VIS–NIR spectra for prediction of those indicators closely related to soil structural quality.

2. Materials and methods

2.1. Site characterization and experimental design

The study was conducted on 40 sites under different agricultural management systems in Ireland. Twenty sites were selected on arable and twenty on pasture between latitude 52°8′ N and 54°20′ N and longitude 6°22′ W and 8°19′ W. The mean daily temperature was between 4.0 °C to 15.7 °C, and average annual precipitation ranged from 750 to 1000 mm (http://www.met.ie). Calcification, leaching and gleying were the dominant soil forming processes in the study area and the soils mainly consisted of Grey Brown Podzolics, Brown Podzolics, Brown Earths, Gleys, Rendzinas and Lithosols (Gardiner and Radford, 1980). Field sampling was conducted in a 30 m^2 plot laid out with random orientation where soil and land cover were uniform based on visual examination on arrival in the field. At each plot, five sub-plots 2 m^2 were selected based on walking a 'W' between the end points of the main plot for sampling and field measurements, and unusually dry or wet areas, headlands, gateways and highly compacted areas were avoided. Soil samples ($n = 200$) were taken from the top 10 cm of soil, sealed and stored in cool, dark conditions prior to laboratory analysis.

2.2. Field and laboratory analyses

Soil chemical, physical and biological properties, which were considered as potential indicators of soil quality based on published literature (e.g. Ditzler and Tugel, 2002; Doran and Parkin, 1994; Karlen and Stott, 1994; Karlen et al., 1997; Larson and Pierce, 1994; Lima et al., 2013; Masto et al., 2008; Qi et al., 2009), were measured in order to explore the relationship between soil structural quality and overall soil quality. Measured indicators were: near-surface penetration resistance determined using a portable soil compaction meter (FIELDSCOUT SC900) to 10 cm depth (Lowery and Morrison, 2002); sorptivity measured according to the method presented by Philip (1957); bulk density (BD) determined by the core method (Grossman and Reinsch, 2002); the bulk density of the 2 mm fraction (BD_{2mm}); total porosity determined by gravimetric methods (Flint and Flint, 2002); soil water content determined by oven drying at 105 °C overnight (Topp and Ferre, 2002); particle size distribution measured using 2 mm air dried soil samples by the pipette method (Gee and Or, 2002); aggregate size distribution by dry sieving (Nimmo and Perkins, 2002) presented as the mean weight diameter (MWD); microbial respiration measured as an indicator of biological activities using fresh soil and calculating the amount of CO_2 evolution at 20 °C (Horwath and Paul, 1994); total nitrogen (TN) and total carbon (TC) measured according to the combustion