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# Evaluation of soil quality for agricultural production using visible–near-infrared spectroscopy

Mohammad Sadegh Askari [a,*], Sharon M. O'Rourke [a,b], Nicholas M. Holden [a]

[a] UCD School of Biosystems Engineering, University College Dublin, Dublin 4, Ireland
[b] Faculty of Agriculture and Environment, The University of Sydney, Australia

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ABSTRACT

Soil quality (SQ) assessment has numerous applications for agricultural management. Conventional quantification of SQ is based on laboratory analysis and integrative indices that can be costly and time consuming to obtain. A rapid, quantitative method using soil spectra, following the successful process of soil characterization by visible (VIS)–near infrared (NIR) spectroscopy, can provide a robust approach for soil monitoring.

*Objective:* To predict specific soil indicator properties and soil quality indices for the productive function of the soil using VIS–NIR spectroscopy, and to evaluate the suitability of spectral data for assessing and monitoring the impact of arable and grassland management in a temperate maritime climate.

*Methods:* The study used 40 sites in Ireland under both arable (n = 20) and grassland (n = 20) management systems. Specific indicators and soil quality indices (SQIs) identified by Askari and Holden (2014) and Askari (2014) were used as the reference standard for estimation using VIS–NIR spectra. Partial least-squares regression was used to predict the indicators and SQIs. SQI was predicted from both spectrally derived indicator values and directly from the soil spectra, and accuracy was assessed by comparison with laboratory and field derived measurements.

*Results:* The indicators of SQ could be predicted with excellent (soil organic carbon and carbon to nitrogen ratio in grassland soils; total nitrogen, carbon to nitrogen ratio, extractable magnesium and aggregate size distribution in arable soils), good (bulk density of <2 mm fraction in grassland soils) and moderate (penetration resistance, soil respiration and bulk density in arable soils) accuracy. The SQIs were predicted directly with excellent accuracy under grassland (RPD = 3.04, $R^2 = 0.92$, RMSE = 0.03) and arable (RPD = 2.78, $R^2 = 0.89$, RMSE = 0.04) management. Soil structural quality class, management type and management intensity were differentiable by their characteristic reflectance.

*Conclusion:* The reliability of SQI and key indicators of soil quality, and the ability to differentiate by management practices and soil structural quality confirmed the efficiency of VIS–NIR spectroscopy for monitoring and evaluating SQ as a reliable alternative to conventional laboratory methods.

*Practice:* Spectroscopy has the potential to provide a reliable approach that will allow rapid, low cost, high frequency SQ monitoring for multiple purposes, and can play an important role in sustainable land management.

*Implications:* VIS–NIR spectroscopy was shown to be suitable for quantitative assessment of soil quality, thus paving the way for development of an applied tool that can be used for agricultural management on the context of soil security, soil health, soil protection and soil quality.



## 1. Introduction

Agricultural management practices affect dynamic soil quality by influencing biochemical and physical indicators such as soil organic carbon, biological activity, nutrient supply and aggregate stability (Carter, 2002; Karlen et al., 1997; Magdoff and van Es, 2000). Rapid, low cost and reliable quantification of soil quality under agricultural management is essential to achieve timely monitoring of the effects of management practices on soil conditions, to prevent soil degradation, ensure sustainable soil productivity and soil security (Bone et al., 2010; Khormali and Nabiollahy, 2009; Lal, 2009; McBratney et al., 2014). Different methods have been proposed for monitoring soil quality, from qualitative or semi-quantitative visual approaches (e.g. Ball et al., 2007; Shepherd, 2009) to quantitative methods based on field and laboratory analysis (e.g. Andrews et al., 2004; Karlen et al., 1997; Larson and Pierce, 1994). Of the quantitative approaches, indexing soil quality is perhaps the most common method. This involves the selection of a minimum data set (MDS) from a range of soil properties linked to a

* Corresponding author at: Room 325, UCD School of Biosystems Engineering, University College Dublin, Dublin 4, Ireland.
*E-mail address:* mohammad.askari@ucdconnect.ie (M.S. Askari).

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defined soil function, normalizing each property value into a unitless score, and integrating the scores into a soil quality index (SQI) (Andrews et al., 2002, 2004; Karlen and Stott, 1994; Mohanty et al., 2007; Qi et al., 2009). To deploy this approach many soil analyses are required, which makes it very time consuming and costly, particularly when monitoring over a prolonged time series (Cécillon et al., 2009a). The visual approach is based on simple and rapid field measurements and/or observations, and as a qualitative or semi-quantitative method has been used as a complementary approach to laboratory analyses focused on soil structural quality (Askari et al., 2013; Ball et al., 2007; Shepherd, 2009).

During the past four decades visible (VIS) and near-infrared (NIR) spectroscopy has been used for determining properties of agricultural systems, especially in food science (Bellon et al., 1994; Huang et al., 2008). Spectroscopic methods have replaced some traditional laboratory analyses such as assessing the composition of cereals (Bellon-Maurel and McBratney, 2011; Williams et al., 1998). The potential in soil science research has also been demonstrated (e.g. Barthès et al., 2008, 2010; Cécillon et al., 2009a). This means that spectroscopy can provide a non-destructive, quantitative approach for the simultaneous prediction of a number of soil quality indicators, and has the potential for multidimensional assessment of soil quality based on the integrated indices of multiple soil variables. The benefits of being rapid and much more cost effective compared to routine analysis are particularly important where large numbers of analyses are required (Bilgili et al., 2011; Hively et al., 2011).

Reviews of literature on the application of VIS–NIR spectroscopic techniques for soil analysis (e.g. Bellon-Maurel and McBratney, 2011; Cécillon et al., 2009a; Malley et al., 2004; Stenberg et al., 2010; Soriano-Disla et al., 2014) have shown that bio-chemical properties tend to be predicted more accurately than physical properties with the exception of soil texture. The prediction of soil properties is possible either by direct interaction with specific absorbance bonds or by indirect correlation with soil properties that are directly linked to soil spectra (Soriano-Disla et al., 2014). Soil organic carbon (SOC), nitrogen, carbon to nitrogen ration (CN) and particle size (percentage of clay, sand and silt) are all considered soil properties that have direct effects on reflectance (Ben-Dor and Banin, 1995; Soriano-Disla et al., 2014; Zornoza et al., 2008). For example, definitive overtone and combination vibrations have been reported for soil nitrogen that relate to specific organic molecules as absorbance signatures (Islam et al., 2003; Morra et al., 1991; Stenberg et al., 2010), while soil particle size affects light reflection and transition (Cécillon et al., 2009a). Correlation between these properties and other soil properties may provide a better understanding of soil spectroscopic methods. To date a small number of investigations on the potential of VIS–NIR spectroscopy for soil quality research have explored single soil or landscape applications, having at most confirmed the ability of the technique. Cohen et al. (2005) successfully predicted SOC, total nitrogen (TN), total carbon (TC), phosphorus (P), pH, cation concentrations, and extracellular enzyme activity using VIS–NIR spectroscopy as indicators of wetland soil quality. They concluded spectroscopy offers both cost and statistical power advantages for integrative assessment of soil quality in wetlands. Kinoshita et al. (2012) investigated multidimensional assessment of soil quality in a Ultisol from a chronosequence in Kenya. They found that laboratory analyses for several biological, chemical and physical indicators could be substituted by spectral analysis with the exception of compaction indicators, and that moderate to good prediction models could be obtained for soil quality scores (Kinoshita et al., 2012). Idowu et al. (2008) evaluated soil quality by 39 chemical, physical and biological soil properties, using a combination of field, laboratory and spectroscopic methods in New York State, USA and stated that to advance the application of VIS–NIR spectroscopy, research should start by establishing the spectral assessment of soil quality across all soil parameters. The use of reflectance spectroscopy for multidimensional assessment of the impact of land-use change on soil quality for three land uses (afforestation, traditional grazing, and agro-pastoral) was presented by Paz-Kagan et al. (2014). This study evaluated the spectral predictability of 14 indicators of soil quality and a summary index and concluded soil spectral data could convey more information than conventional sample analysis. This, as it was suggested, resulted in a better understanding of the impact of land use changes on SQ and degradation mechanisms (Paz-Kagan et al., 2014).

Various multivariate analyses, termed “Chemometrics” (Geladi, 2003), are used for modeling the relationship between spectra and soil properties. Among these, partial least squares regression (PLSR) is perhaps the most commonly used technique (McCarty et al., 2002; Viscarra Rossel et al., 2006). The spectral analysis procedure involves preparation of soil samples, spectral acquisition, pre-processing of spectral data and selection of an appropriate statistical model, and each step can affect the accuracy of the model for each individual indicator (Butkutė and Šlepetienė, 2006; Mouazen et al., 2010; Park et al., 1997). Different pre-processing techniques have been applied to improve prediction ability (i.e. Mouazen et al., 2010; Vasques et al., 2008) such as mean normalization, baseline offset, maximum normalization (Mouazen et al., 2005), first derivatives (Coûteaux et al., 2005; Shepherd and Walsh, 2002) and second derivatives (Fystro, 2002). Such methods usually remove noise, baseline effects and reduce the impact of particle size (Kinoshita et al., 2012; Martens and Naes, 1989). Choosing the best performing pre-processing technique depends on the data set and requires testing to ascertain an effective pre-processing method (Kuśnierek, 2011). Increasing the number of soil samples can result in a greater $R^2$ and ratio of prediction deviation (RPD), reduction in RMSE and greater spectral predictability that might result in better detection of soil variability (Shepherd and Walsh, 2002; Viscarra-Rossel et al., 2008; Guerrero et al., 2010), but this also increases the cost and time of analyses considerably. Wetterlind et al. (2008) indicated a successful prediction model of soil carbon could be obtained from only 25 soil samples, and Kuang and Mouazen (2012) suggested a minimum of 50 samples for good accuracy and minimum cost in a farm scale spectral prediction of organic carbon, moisture content and total nitrogen. It is reasonable to assume that 100 soil samples can provide enough information for developing soil spectral models at an acceptable cost for agricultural systems in Ireland within a relatively narrow range of soil types.

Previous research on soil quality under temperate maritime agricultural management has shown that visual evaluation of soil structure (VESS) data was closely related to a number of biochemical and physical soil properties and could be used for overall evaluation of soil quality under arable and grassland management (Askari et al., 2013; 2015). Furthermore, it was found that soil quality could be assessed using CN, SOC and bulk density (BD) as a minimum data set (MDS) under grassland management (Askari and Holden, 2014) and using BD, CN, TN, aggregate size distribution (ASD), extractable magnesium (Mg), penetration resistance (PR), and soil respiration (SR) as a MDS under arable management (Askari, 2014). The SQIs for productivity under arable and grassland management were also identified. Askari et al. (2015) also showed that VIS–NIR spectra could predict soil indicators associated with soil structural quality with good reliability. The final step for this work was the prediction of SQI directly from soil spectral data. The objective of this research was to evaluate the predictability of soil indicator properties and soil quality indices for the productive function of the soil using VIS–NIR spectroscopy and to assess the suitability of soil spectra for monitoring soil quality under agricultural management in a temperate maritime climate. A sub-objective was to differentiate soils by structural quality classes and management practices using soil spectral data to confirm the reliability of the methodology.

## 2. Materials and methods

### 2.1. Experimental design and measured soil properties

The study was conducted from September to December 2011 on forty sites under both grassland ($n = 20$) and arable ($n = 20$)