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Research Paper

# Evaluation of the performance of portable visible-infrared instruments for the prediction of soil properties

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Good soil management requires large amounts of soil data which are expensive to provide using traditional laboratory methods. Soil infrared spectroscopy including portable/miniaturized visible-infrared spectrometers offers a cost-effective solution. There is a need to test and compare the performance of portable/miniaturized mid-infrared (MIR) and visible-near-infrared (vis-NIR) spectrometers for the prediction of soil properties across a range of soils. For this assessment, 458 soil samples from Australia were scanned by four vis-NIR and MIR portable/miniature spectrometers and partial least squares regressions (PLSR) applied for the prediction of 17 properties in soils dried at 40 °C and sieved to <2 mm. The performance of these instruments was tested and compared to a reference benchtop MIR/NIR instrument. Mid-infrared handheld instruments provided the best performance, the vis-NIR instrument the next most successful, and the miniature NIR instrument with a restricted spectral range (950–1650 nm) being less successful. When models using the same spectral range obtained by different instruments were compared, similar performance was achieved, thus the spectral quality provided by different instrumentation was not decisive in determining prediction accuracy. Many new portable infrared instruments have restricted spectral ranges, thus a number of different spectral ranges in both the MIR and vis-NIR were assessed to determine the optimal range for prediction of soil properties. It was concluded that the range 1650–5000 nm would be ideal.



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## 1. Introduction

The need to increase food production globally over the next 30 years requires that we have better information on soil condition, in both developed and developing economies. Sustainable intensification of agricultural production requires that we develop better management strategies for soils. In order to support the development and application of optimum management strategies, there is a need to increase the spatial density of soil analytical data (Nocita et al., 2015; Palm, Sanchez, Ahamed, & Awiti, 2007; Viscarra Rossel et al., 2016). This demand for large amounts of soil data is enhanced by the fact that soils are highly heterogeneous and diverse temporally, spatially and to depth (Palm et al., 2007; Reimann, Birke, Demetriades, Filzmoser, & O'Connor, 2014; Viscarra Rossel et al., 2016), requiring the adoption of soil management decisions for each specific situation.

Traditional laboratory methods of soil analysis are unable to satisfy such demands because they are expensive and time-consuming. *Infrared spectroscopy, using* the mid-infrared (MIR: 4000–400 $cm^{-1}$, 2500–25,000 nm), the near-infrared (NIR: 700–2500 nm, 14,286–4000 $cm^{-1}$) and/or the visible (vis: 400–700 nm, 14,286–25,000 $cm^{-1}$) regions, in combination with multivariate regression methods, offers a practical alternative (Nocita et al., 2015; Shepherd & Walsh, 2007; Soriano-Disla, Janik, Viscarra Rossel, MacDonald, & McLaughlin, 2014). Infrared soil analysis techniques, described extensively in previous publications (e.g. Janik, Merry, & Skjemstad, 1998; Stenberg, Viscarra Rossel, Mouazen, & Wetterlind, 2010), are non-destructive and relatively cost-effective, rapid, and precise. This allows the prediction of many soil properties through the use of multivariate regression. Thus, the technique is well suited to provide an assessment of key soil attributes such as texture, mineralogy, cation exchange capacity (CEC) and organic C (OC) and N contents (Palm et al., 2007).

Recent improvements in instrumentation have seen the field of soil spectroscopy to develop rapidly, opening up the opportunity to take the technique from the laboratory to the field using portable, handheld and now miniature spectrometers (Alcalà et al., 2013; Knadel, Stenberg, Deng, Thomsen, & Greve, 2013; Kuang et al., 2012; Reeves, 2010; Yang & Mouazen, 2012). However, the performance of portable/miniature instruments can be compromised by technical limitations. As discussed by Mouazen, Saeys, Xing, De Baerdemaeker, and Ramon (2005) and Soriano-Disla et al. (2014), instrument performance is dependent on technical specifications such as type of energy source and detector, resolution, sampling accessories, instrument and energy intensity. Thus, for the same set of soils and reference soil properties, different instruments could have different performance, which could be detrimental for the further development of predictive regression models (Mouazen et al., 2005; Reeves, 2010).

Instrument performance is also related to the spectral range used (Kuang et al., 2012; Mouazen et al., 2005; Reeves, 2010) where more accurate predictive models have generally been obtained by using the MIR range as compared with NIR (e.g. as summarised by Reeves, 2010; Soriano-Disla et al., 2014; Viscarra Rossel, Walvoort, McBratney, Janik, & Skjemstad, 2006). This has been related to the fact that more information is provided by MIR spectra. Conversely, the NIR peaks are much less intense, being the result of overtones and combination bands of fundamental vibrations in the MIR region (Nguyen, Janik, & Raupach, 1991; Stenberg et al., 2010).

However, there are some soil properties for which the vis-NIR region seems to perform better than MIR (e.g. soil biological properties or cation exchange related properties; Soriano-Disla et al., 2014). In addition, the MIR region is more susceptible to variable water content in field samples (Kuang et al., 2012; Reeves, 2010) and, in some cases, the absorbance from some soil compounds (e.g. quartz) is so intense that it overlaps other relevant soil information (Nguyen et al., 1991). This can be detrimental for the accuracy of the predictions (Rabenarivo et al., 2013).

In terms of the performance of portable/miniature instruments, there are very few studies which evaluate the performance of portable MIR instruments (Dhawale et al., 2015; Forrester et al., 2015; Ji et al., 2016). This is mainly attributed to the fact that MIR instruments have been generally restricted to the laboratory until relatively recently (Dhawale et al., 2015; Forrester et al., 2015; Reeves, McCarty, & Hively, 2010). Comprehensive studies comparing the potential of different portable infrared spectrometers covering vis-NIR and MIR ranges for the prediction of soil properties in a range of soils are lacking.

Hence, the main objective of this study was to provide an assessment of the performance of portable and miniature MIR and vis-NIR spectrometers to predict soil properties. The assessment included an analysis of the impact of the quality of the spectra on the performance of predictions and the optimal region across MIR and vis/NIR ranges for such predictions.

## 2. Material and methods

### 2.1. *Soil sampling*

The samples used in this study were obtained from the Australian CSIRO National Soil Archive (CNSA, http://www.clw.csiro.au/aclep/archive/) and can be found in http://www.asris.csiro.au/(APSRU reference sites). The final selection comprised 80 soil profiles (n = 458 samples) from South Australia (66%) and New South Wales (34%) (Supplementary Fig. 1). Soil samples were dried at 40 °C and sieved <2 mm. Samples were sourced from variable depths, most of the samples (n = 315) represented the first 100 cm, the rest (n = 143) representing depths from 100 to 180 cm. Samples represented 9 soil orders which are commonly used for cropping in Australia, mostly Calcarosols, Chromosols, Dermosols, Sodosols and Vertosols. Minor contributions of Dermosols, Kandosols, Kurosols, Ferrosols and Tenosols were observed.

### 2.2. *Soil laboratory analysis*

The following properties (Table 1) were determined by the methodology described in Rayment and Higginson (1992) and Rayment and Lyons (2011): Exchangeable bases calcium ($Ca^{2+}$), magnesium ($Mg^{2+}$), potassium ($K^{+}$) and ($Na^{+}$), alcoholic 1M ammonium chloride at pH 8.5, pre-treatment for soluble salts,