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Comparison between artificial neural network and partial least squares for on-line visible and near infrared spectroscopy measurement of soil organic carbon, pH and clay content

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ABSTRACT

Soil organic carbon (OC), pH and clay content (CC) can be measured with on-line visible and near infrared spectroscopy (vis-NIRS), whose calibration method may considerably affect the measurement accuracy. The aim of this study was to compare artificial neural network (ANN) and partial least squares regression (PLSR) for the calibration of a visible and near infrared (vis-NIR) spectrophotometer for the on-line measurement of OC, pH and CC in two fields in a Danish farm. An on-line sensor platform equipped with a mobile, fiber type, vis-NIR spectrophotometer (AgroSpec from tec5 Technology for Spectroscopy, Germany), with a measurement range of 305–2200 nm was used to acquire soil spectra in diffuse reflectance mode. Both ANN and PLSR calibration models of OC, pH and CC were validated with independent validation sets. Comparison and full-point maps were developed using ArcGIS software (ESRI, USA). Results of the on-line independent validation showed that ANN outperformed PLSR in both fields. For example, residual prediction deviation (RPD) values for on-line independent validation in Field 1 were improved from 1.93 to 2.28, for OC, from 2.08 to 2.31 for pH and from 1.98 to 2.15 for CC, after ANN analyses as compared to PLSR, whereas root mean square error (RMSEP) values decreased from 1.48 to 1.25%, for OC, from 0.13 to 0.12 for pH and from 1.05 to 0.96% for CC. The comparison maps showed better spatial similarities between laboratory and ANN predicted maps (higher kappa values), as compared to PLSR predicted maps. In most cases, more detailed full-point maps were developed with ANN, although the size of spots with high concentration of PLSR maps matches the measured maps better. Therefore, it was recommended to adopt the ANN for on-line prediction of OC, pH and CC.

1. Introduction

Air pollution, soil erosion and intensive farming practice and the subsequent deposition of acidifying substances such as nitrogen and sulfur compounds have enhanced the acidification of soil. This acidification can result in an imbalanced nutrient supply and increased aluminium toxicity, leading to reduced nutrient uptake by crops (Ingerslev, 1997). Hence, maintaining the optimum pH level in the topsoil in all parts of the field is important to achieve optimum yields and consistent soil quality. If soil acidity is not regulated, it can cause poor crop growth and large yield losses. In addition, over-use of lime is wasteful and costly and can create problems to the availability of some micronutrients (Department for Environment, Food and Rural Affairs, 2010). Though pH is the main indicator to soil acidity, the accurate characterisation of within-field variation of soil OC and soil CC is also critical for variable rate lime application, as to increase pH by one unit, clay and organic soils need more lime than sandy soils (Department for Environment, Food and Rural Affairs, 2010). Hence, a robust, cost-effective, quick and accurate approach to measure soil OC, pH and CC simultaneously is the key success for implanting variable rate lime application.

Recent advances in proximal soil sensing techniques indicate that on-line sensors are capable of providing trustful and high resolution data on some fundamental soil properties including soil OC, pH and CC. Among available techniques, the visible and near infrared (vis-NIR) spectroscopy proved to be the most capable technology for on-line characterisation and

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quantification of within field variation in soil properties (Bricklemyer and Brown, 2010,b; Kuang and Mouazen, 2013a,b; Kweon and Maxton, 2013; Mouazen et al., 2007; Shi et al., 2006; Shibusawa et al., 2001).

Similar to OC, along with soil total carbon, soil total nitrogen, soil moisture content, CC has been clarified into the category of soil properties with direct spectral response in the near infrared range (Kuang et al., 2012; Stenberg et al., 2010). Compared to OC less effort has been put on vis-NIR measurement of CC. Although pH has no direct spectral response in the near infrared range, it attracted numerous researchers' interest, as it indicates soil acidity and nutrient uptake. Many studies have reported on-line measurements of OC or soil organic matter (OM) with vis-NIRS at different geographic scales (e.g. Bricklemyer and Brown, 2010; Kuang and Mouazen 2013b; Kweon and Maxton, 2013; Mouazen et al., 2007; Muñoz and Kravchenko, 2011). Less success was reported for on-line measurement of soil pH (Kodaira and Shibusawa, 2013; Marin-González et al., 2013; Mouazen et al., 2007; Tekin et al., 2013), whereas very limited studies on CC were reported (Bricklemyer and Brown, 2010; Mouazen et al., 2013). All these studies have used partial least squares regression (PLSR) for the modeling of on-line collected spectra.

Although the linear PLSR analyses is the most common technique for spectral calibration and prediction (Viscarra Rossel et al., 2006), nonlinear techniques e.g. artificial neural networks (ANN) have got much less attention and were rarely explored for the spectral analysis in soil sciences. Mouazen et al. (2010) have shown considerable improvement for the vis-NIR prediction accuracy of key soil properties by combing PLSR and Back-propagation neural network. Similarly, Li et al. (2012) introduced hybrid modeling of PLSR and ANN for quantifying lunar surface minerals. Other nonlinear calibration techniques implemented in soil sciences were regression trees (Brown et al., 2006; Vasques et al., 2008; Viscarra Rossel and Behrens, 2010), multivariate adaptive regression splines (Shepherd and Walsh, 2002; Viscarra Rossel and Behrens, 2010), support vector machine regression (Stevens et al., 2010; Viscarra Rossel and Behrens, 2010), and penalized-spline signal regression (Stevens et al., 2010). The ANN was one of the most adopted methods. Few examples on the use of the ANN technique for soil analysis with NIR spectroscopy could be found in literature. Fidêncio et al. (2002) have implemented the radial basis function networks (RBFN) in the NIR region (1000–2500 nm) and Daniel et al. (2003) have used ANN in the vis-NIR region (400–1100 nm). Later, Mouazen et al. (2010) and Viscarra Rossel and Behrens (2010) combined PLSR with ANN and discrete wavelet transform (DWT) with ANN, respectively. All these reports were for laboratory collected soil spectra. Among the wide range of non-linear calibration techniques presented, ANN seems be one of the most suitable techniques to model on-line collected vis-NIR spectra (Stenberg et al., 2010). This is attributed to its potential to provide stable calibrations, and to the availability of commercial software to run the analyses. To date, no literature can be found on the use of the ANN to model on-line collected vis-NIR soil spectra. The aim of this study is to compare the performance of PLSR and ANN modeling techniques for on-line prediction of OC, pH and CC in two fields in a Danish farm.

Fig. 1. On-line visible and near infrared (vis-NIR) soil sensor (Mouazen, 2006).

2. Materials and methods

2.1. Experimental site

Two experimental fields (56°22′21.15″N, 9°33′47.03″E) located in Vindumovergaard Farm, Viborg, Denmark were used in this work. Detailed information about these fields is provided in Table 1. Both fields were drilled with spring barley in spring 2013, with the intention to establish a lime application experiment to regulate the soil acidity. The soil texture in these two fields can be classified as sandy loam according to the United State Department of Agriculture (USDA) texture classification system. Field 1 was of 18 ha area while Field 2 was of 30 ha area.

2.2. On-line measurement

The on-line measurement system designed and developed by Mouazen (2006) was used (Fig. 1) to measure the two experimental fields in Denmark. It consists of a subsoiler, which penetrates the soil to the required depth, making a trench, whose bottom is smoothed by the downward forces acting on the subsoiler. The optical probe is housed in a steel lens holder. This is attached to the backside of the subsoiler chisel and acquires diffuse reflectance spectra from the smooth bottom of the trench. The subsoiler was retrofitted with the optical unit and attached to a frame. This was mounted onto the three point linkage of the tractor (Mouazen et al., 2005). An AgroSpec mobile, fiber type, vis-NIR spectrophotometer (Tec5 Technology for Spectroscopy, Germany) with a measurement range of 305–2200 nm was used to measure soil spectra in diffuse reflectance mode. Detailed information about the system can be found in Kuang and Mouazen (2013a).

Blocks of 230 m by 800 m and 500 m by 600 m were laid out in Field 1 and Field 2, respectively. Each measured line was 600–800 m long with 20 m intervals between adjacent transects (Fig. 2). The travel speed of the tractor was around 2 km/h and the measurement depth was set at 15 cm. Examining Fig. 2 reveals that there are gaps along the measurement transects, where no spectra are available. Indeed, the quality of soil spectra at these points was

Table 1
Information of the two experimental fields in Vindumovergaard Farm, Denmark.

Field	Area (ha)	Crop	Sample number	Texture type	Sand (%)	Silt (%)	Clay (%)
Field 1	18	Spring barely	132	Sandy loam	70.6	24.6	4.8
Field 2	30	Spring oat	80	Sandy loam	68.6	21.9	9.5