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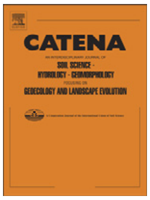

Mid-infrared spectroscopy to support regional-scale digital soil mapping on selected croplands of South-West Germany

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ABSTRACT

Digital soil mapping (DSM) relies on statistical relationships between soil properties and covariates (e.g. terrain attributes, land use class, geology) which may not explain a large proportion of measured soil properties variability. This uncertainty combined with low spatial resolution of existing maps makes it difficult to monitor soils. Diffuse reflectance infrared Fourier transform mid-infrared spectroscopy (midDRIFTS) with partial least square regression (PLSR) may offer an alternative source of high quality data for improved DSM. Previously validated midDRIFTS-PLSR models were used to predict soil total carbon (TC), total inorganic carbon (TIC), total organic carbon (TOC) and texture of 1170 samples from contrasting agroecological regions (~3600 km^2), Kraichgau (K) and Swabian Alb (SA), Southwest Germany. MidDRIFTS-PLSR predictions were integrated with geostatistics for soil property maps (200 m resolution). An average of 93% of the total soil samples were predicted within the confidence intervals of the midDRIFTS-PLSR models for the respective properties. Ordinary kriging (OK) resulted in maps for TC, TIC, TOC and texture with a root mean square standardized error (RMSSE) ~1. Soil organic matter (SOM) (DRIFTS_SOM) and texture (DRIFTS_texture) maps developed in the current study were of higher spatial resolution than previously existing maps. The DRIFTS_SOM and DRIFTS_texture in the both regions showed considerable differences when compared to existing maps. The DRIFTS_SOM in K and SA regions had overlaps of 45 and 69% with the 1:200,000 existing map. While the DRIFTS_texture in K had an overlap of 92% with the 1:1,000,000 existing map, the overlap in SA region was only 11%. We conclude that traditional DSM with covariates can be improved via higher sampling density which is made possible using midDRIFTS-PLSR. Incorporation of mid-infrared spectral data with both remote sensing and other environmental data would be a further application to cope with uncertainty associated to both spectroscopic and spatial modeling.

1. Introduction

Sustainable land use management and planning demands accurate and up-to-date quantitative information on the spatial distribution of essential soil physical and chemical properties at large scales (Banwart, 2011; Lal, 2004). Existing soil maps are often based on soil-landscape models which employ limited numbers of field observations. These maps were created based on statistical relationships between soil properties and covariates (e.g. terrain attributes, land use class, geology) which do not always explain a large proportion of the variation of the measured soil properties of interest (Behrens et al., 2010; Lagacherie et al., 2008). Thus, low resolution and high uncertainty are the main drawbacks of covariate-based soil maps for appropriate soil monitoring and evaluation especially at sub-regional, local, or field scale (Sanchez et al., 2009). These available sources lack detailed information with adequate accuracy to be used for decision making for environmental modeling and protection, especially at smaller scales (Behrens and Scholten, 2006; Gomez et al., 2012). One of the wide-used approaches to assess soil spatial variability and create digital soil maps (DSMs) is geostatistics (Goovaerts, 1999). However, updating the information instead of using the previous "soil survey" method to produce better resolution soil property maps requires a large number of soil samples representative of the region (Brus and de Gruijter, 2011). However, soil quantitative analyses generally rely on labor intensive and time consuming traditional analytical methods (Liu et al., 2006). Hence, a rapid-throughput pedometric approach to produce high-resolution digital soil maps should receive high priority (Behrens and Scholten, 2006). Mid-infrared spectroscopic (MIRS) techniques linked to partial least square regression (PLSR) analysis has been shown to be able to quantify a broad range of physico-chemical soil properties as a compliment to conventional soil analyses (Viscarra Rossel and Behrens, 2010; McDowell et al., 2012; Cécillon et al., 2009).

Although spectroscopic techniques have been widely used in the last 20 years to accurately predict different soil properties, the potential use

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of this technique for digital soil mapping (DSM), especially at the regional scale, has not been extensively explored. Soil in nature is extremely variable and the construction of reliable midDRIFTS-PLSR calibration models needs sufficient samples to represent soil variation at regional or country scale (Brown et al., 2006). These calibration models then can be used to predict target soil properties using only future spatial soil spectra obtained via a statistically design-based sampling strategy (Bellon-Maurel and McBratney, 2011). Therefore, application of midDRIFTS-PLSR to create up to date maps needs i) an efficient sampling strategy in terms of number and distribution where all samples should be analyzed by considering a standard analytical reference analysis and midDRIFTS spectroscopy; ii) calibrated models with high accuracies for each single target properties; and iii) a reliable technique to model spatial variability and distribution.

So far the application of spectroscopy in digital soil mapping is relatively rare and mainly limited to visible and/or near-infrared spectroscopy (V/NIRS). V/NIRS integrated with geostatistics has been applied in few studies for soil property mapping. Wetterlind et al. (2008), Odlare et al. (2005), and Brodský et al. (2013) applied V/NIRS-PLSR models to assess soil spatial variability and create soil organic matter (SOM), soil organic carbon (SOC) and clay content maps. These investigations were carried out at the field or farm level rather than regional scale and no comparison was made with existing maps of properties of interest in the areas. Furthermore, especially at large spatial scales, diffuse reflectance infrared Fourier transform spectroscopy in the mid-infrared range (midDRIFTS) generally has better predictive power for soil carbon fractions and texture than NIRS and V/NIRS (McCarty et al., 2002; McCarty and Reeves, 2006; Soriano-Disla et al., 2014). While vibrations present in the near-infrared spectra are overtones and combinations of fundamental vibrations with less band specificity resulting from overlapping of different vibrations, midDRIFTS spectra contain fundamental molecular vibrations of major soil components (Viscarra Rossel and Lark, 2009). Hence, working on a regional scale with large heterogeneity, NIRS spectra are greatly influenced by different soil types (pedological factors) and may lead to a predictions of low accuracy in PLSR calibration models for soil properties (Bellon-Maurel and McBratney, 2011). Cobo et al. (2010) published a pioneering work on the integration of midDRIFTS-PLSR predicted soil data to compute spatial patterns of several soil properties such as C and N fractions and soil texture across three villages in Zimbabwe. Thus, for accurate prediction of soil properties (McBratney et al., 2003; Viscarra Rossel et al., 2006), spectroscopic techniques could be well suited for assessing agricultural soils and producing soil property maps via integration with geostatistical analysis (Shepherd and Walsh, 2007; Cobo et al., 2010).

As mentioned previously, the efficiency of existing maps in monitoring soil physicochemical properties is under question because of their low resolution and lack of consistency. Thus, in areas of low resolution data a high-throughput and cost effective method is needed to produce up-to-date DSMs for sustainable land use management and planning. In the current study we addressed the question of whether midDRIFTS spectroscopy can be used to overcome the lack of high-quality soil spatial data at the regional scale to compliment conventional laboratory analyses and soil surveys for accurate mapping of soil properties at a considerably higher resolution than conventional soil mapping. Previously developed midDRIFTS-PLSR calibrated models (samples, n = 126) at the regional scale in South-West Germany (Kraichgau and Swabian Alb, as described in Mirzaeitalarposhti et al. (2015)) were used to predict total carbon (TC), total organic carbon (TOC), total inorganic carbon (TIC) and soil texture (clay, silt and sand) on a regional scale-based soil sample set using midDRIFTS spectra. The main objectives of this study were: i) to evaluate the robustness of previously calibrated and validated midDRIFTS-PLSR models to accurately predict topsoil (0–30 cm) properties (TC, TIC, TOC, clay, silt, and sand contents) across two contrasting agroecological regions (Kraichgau, Swabian Alb) using only midDRIFTS soil spectra, ii) to apply intensive spectral data sources to improve maps of topsoil soil carbon and texture compared to the currently existing lower resolution maps , and iii) to discuss the possibility of technique to be used from local to global scales.

2. Materials and methods

2.1. Study sites

The study areas were the regions of Kraichgau (K) and Swabian Alb (SA), in the Federal State of Baden-Württemberg, South-West Germany (Fig. 1). Each study region has an area of approximately 1600 km^2. The K region is a fertile and intensively cropped loess-covered hilly region which is situated in a geomorphological basin between 100 and 400 m above sea level (a.s.l.) It is characterized by a mild climate with a mean annual temperature between 9 and 10 °C and mean annual rainfall ranges from 720 to 830 mm (Ingwersen et al., 2011). The main soil types are classified as Luvisols and Regosols (IUSS Working Group WRB, 2015). SA region is a low mountain plateau with elevations between 500 and 850 m a.s.l. This region is characterized by a cooler climate with an annual average temperature of 6 to 7 °C and mean annual precipitation between 800 and 1000 mm. Soils developed mostly in Jurassic limestone, are rich in clay due to strong decalcification and weathering, and are classified mainly as Leptosols, Luvisols and Cambisols (IUSS Working Group WRB, 2015).

2.2. Sample collection and preparation

A probability-based sampling design (e.g. simple randomized and regular grid sampling) (Peterson et al., 1999) was used across both study regions to obtain a spatially dispersed, spatially unbiased sample of soil variables which accounted for both small and large spatial scale variation. To select the sampling points, a land use map of the state of Baden-Württemberg (Ad-hoc-AG Boden, 2005) was overlaid with the boundaries of study areas in ArcView version 10.1 (www.esri.com). For the random selection, a grid of 50 × 50 m was overlaid on the crop land vector layer of each study region separately. Thereafter, 300 sample points were randomly selected in each region. Additionally, 300 points were selected based on a regular 1.5 × 1.5 km grid sampling scheme for each region. This approach combined full study region coverage via the regular grid with additional information at short distances with the random point selection (Peterson et al., 1999). In total, 1170 potential sampling points were selected across two regions: 582 in K and 588 in SA study region (Fig. 1). Finally, the map of the point vector layer for each study region was projected as a KML file in Google Earth (www.earth.google.com) to ensure sampling points were within cropping areas. Points found in unsuitable places for sampling (e.g. road, water way, household, pasture or forest) were re-located (if possible) in adjacent locations within cropped fields. Topsoil (0 to 30 cm) samples were taken during 2012 and geo-referenced using a portable GPS (GPSMAP 62st) with a horizontal accuracy of 1 to 3 m. At each sampling point, five sub-samples within a 15 m radius were bulked to form a composite sample: one central and four others located at a distance of 15 m in the four cardinal directions. The soil samples were taken using a stainless steel soil core sampler with 2.5 cm inside diameter and were placed into plastic bags and kept cool for transport to the laboratory. Soil samples were oven-dried at 32 °C for 48 h, crushed, sieved (<2 mm), and stored at room temperature for further analyses. Approximately, 10 g < 2 mm soils were further ball milled for midDRIFTS analyses described below.

2.3. MidDRIFTS analysis of soil samples and prediction

Samples of ball-milled soils were maintained at 32 °C overnight prior to midDRIFTS analyses according to Demyan et al. (2012) and Rasche et al. (2013). Briefly, each ball-milled soil sample was scanned on a Tensor-27 Fourier transform spectrometer (Bruker Optik GmbH, Ettlingen, Germany) equipped with a potassium bromide (KBr) beam splitter