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Global Soil Spectral Library: A Spectrally Driven Approach for Assessing Soil Quality Using Infrared Spectra

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Abstract

Identification of degraded landscapes, soil fertility constraints or estimates of soil carbon stocks on a regional or national scale need spatially distributed soil information. Diffuse reflectance infrared spectroscopy is a fast, cheap and reliable method for assessing soil quality of large numbers of samples. A constraint up to today is that local calibrations have to be built for new sets of samples and for individual soil properties. Using global soil spectral libraries that cover the main global variability of agricultural soils could help simplify the procedure and obtain a rapid estimate of basic soil properties for an unknown sample. We tested different spectral pre-treatments including smoothed raw spectra, first derivative spectra and continuum removed spectra for near-infrared (1,250 nm to 2,500 nm) and mid-infrared (2,500 nm to 16,700 nm) spectra. Moreover, we tested different analysing approaches including separation of clusters based on the principal components

using the Expectation-Maximization algorithm, interpretation of spectral classes in terms of soil properties using tree based recursive partitioning and partial least-squares regression. The global soil library (n=971) included agriculturally important groups with a wide range of organic carbon concentrations, texture and pH values from soil archives of the International Soil Reference Information Centre (ISRIC). All computations were done using the “R” free software package to facilitate use of the approaches by developing countries. Partial least-squares regression using first derivative spectra performed best in predicting basic soil chemical and physical properties. Validation statistics (n=291) showed better results for mid-infrared compared to near-infrared spectra. Good predictions in the mid-infrared range (coefficient of determination higher than 0.75 and ratio of reference values standard deviation to root mean square error of prediction higher than 2.0) were achieved for pH value, contents of organic carbon and clay and cation exchange capacity. Predictions for contents of calcium, magnesium and sand were satisfactorily (R^2 0.60 to 0.75; RPD 1.4 to 2.0). The positive results could facilitate the wider use of soil infrared spectroscopy, especially in conjunction with satellite images to improve digital mapping of soil constraints to agricultural production and soil carbon levels.

Keywords: Model performance, near-infrared, mid-infrared, partial least-squares regression