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The use of near infrared spectroscopy (NIR) for soil quality and soil degradation assessment

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Soil quality is a broad concept involving several aspects. It is well accepted that a soil quality index must comprise physical, chemical and (micro)biological properties. Most of the soil quality indexes recently used, hypothesised and conceptualised, have in common the integration of these properties.

NIR spectroscopy has developed rapidly over the last several decades as low cost, fast and robust analytical method for many agricultural, pharmaceutical and food products. This technique obtains the reflectance spectra of a sample in the range of the near infrared region (750-2500 nm $\approx$ 12000-4000 cm^{-1}). Near infrared radiation is absorbed by the different chemical bonds, such C-H, N-H, C-O and O-H of the organic compounds present in the sample. The infrared spectrum is the result of the overtones and combinations of fundamental vibrational bands for these bonds; as a consequence, an infrared spectrum contains information about the organic composition of the sample. In this sense, NIR coupled with chemometrics techniques has been used to estimate some parameters related to chemical composition of a broad spectrum of samples, including soils.

In the case of soils, many organic fractions such organic C and N, potentially mineralizable C and N, or microbial biomass have been estimated with NIR. Moreover, it has been observed that a NIR spectrum is correlated with some physical and chemical properties of soils (for example the cation exchange capacity).

Somehow, the NIR should be the equivalent of a 'finger-print' of the soil sample, especially in relation to the organic compounds, usually closely related to the soil quality.

A classical approach to soil quality usually includes the assessment of the total and the potentially mineralizable fractions of carbon and nitrogen, pH, enzymatic activities, microbial biomass, bulk density, aggregate stability and available nutrients… Most of these analyses are time-consuming, and in some cases must be carried out using sophisticated and expensive apparatus and chemical reagents. In contrast, NIR is a non-destructive technique which allows in few seconds, and without laborious sample pre-processing, the obtention of the soil spectra. The soil sample pre-treatment is fast and easy, because only needs air-drying and sieving. Thus, several hundreds of soil samples can be measured per day in the laboratory.

Several factors, such as the elimination of the vegetation cover or changes in species composition, forest fires and agricultural practices could modify soil properties, and thus the NIR spectra. The possibility of the use of NIR spectrometry as a rapid and low cost tool (requiring only investment in the spectrometer) in soil quality assessments is hypothesized here.

Each of the spectral points which compose the spectra of a soil sample, contain potentially useful information and could be used as a variable.

Previous to the use of NIR as tool for classifying (and quantifying) the quality of soils, different sets of calibrations using several multivariate statistical techniques must be performed.

For the prediction of individual parameters or properties related with soil quality through NIR (for example the organic carbon or the potentially mineralizable carbon), a model must first be performed. This implies development of a calibration-validation procedure with a broad set of soil samples. Partial least squares (PLS) regression with the data-matrix from the NIR is a common method. For the use of the whole NIR spectra to classify samples according to the severity of the degradation impact, cluster analysis could be performed. Discriminant analysis could be another methodology to apply to degraded and non-degraded soil samples, but the utility of these techniques decreases when samples come from different locations.

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