EGU22-10092
https://doi.org/10.5194/egusphere-egu22-10092
EGU General Assembly 2022

Compensation of moisture and particle size effects on soil mid-infrared (MIR) reflectance spectra collected in the field with External Parameter Orthogonalization

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Soil spectroscopy in the mid-infrared (MIR) allows the fast and cost-effective derivation of multiple physical and chemical soil properties, e.g., soil organic carbon (SOC) and soil texture, from a single reflectance spectrum. The recent development of extensive soil spectral libraries and field-portable handheld FTIR spectrometers have opened up new opportunities for the widespread application of soil reflectance spectroscopy in the geo- and environmental sciences. Compared to laboratory measurements on pre-treated soil material, field recordings of MIR spectra are impacted by in situ environmental conditions that modify and degrade the measured reflectance signal, most prominently variations in soil moisture and particle size across samples. These conditions prevent leveraging available MIR soil spectral libraries to build predictive models of soil properties directly.

We evaluated the capacity of the External Parameter Orthogonalization (EPO) algorithm to compensate for moisture and particle size-induced effects on MIR reflectance spectra recorded in the field to generate laboratory-equivalent spectra from the in-situ data, which would allow calibrations of predictive soil property models from soil spectral library data to be transferred to field-recorded spectra. An archive of 230 soils collected across five soil regions in Germany covering a broad range of parent materials, soil texture classes and organic carbon contents was used to evaluate the approach. For each soil sample, MIR reflectance spectra had been acquired both in the field, i.e., measured in situ on the soil surface, and in the laboratory on pre-treated (sieved and ground) soil material. Field spectra were corrected for environmental effects by EPO and used to predict SOC and soil texture with predictive models developed on the laboratory spectra.

Analysis of the EPO-transformed spectra showed that the algorithm could compensate for some of the significant environmental effects present in the field data, e.g., non-linear baseline shifts and large-scale water absorption features, effectively reducing variation across the soil samples that is not linked to the physical and chemical soil properties of interest. EPO-transformation of the spectra further allowed a robust transfer of calibrations developed on laboratory spectra of

pre-treated soils to the field spectra. Predictive accuracies for SOC and soil texture were lower than for pure laboratory applications but generally in line with models developed with an extensive regional calibration sample directly on the field MIR spectra.

The correction of field MIR spectra with the EPO algorithm thus represents a promising approach to integrating existing soil spectral libraries into the development of predictive soil property models for in-situ MIR reflectance spectra as it would allow the development of predictive models without requiring a large number of additional regional calibration samples for field application of MIR soil spectroscopy.