An evaluation of Pre-Processing Techniques for PLS Modelling of Diffuse Reflectance Spectra

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The development of on-the-go soil sensing systems that use near and mid-infrared reflectance to quantitatively measure soil properties is of much interest to the soil science fraternity. However, the complex physical, chemical and biological processes that contribute to soil formation can make the interpretation of their spectra difficult. Furthermore, in a real-time soil sensing situation the effects of light scattering and differences in spectroscopic path length will cause further variation in the sample spectra. These issues make soil spectrometry a challenging prospect.

Recent research has focused on the pre-processing of spectral data to remove non-related spectral variation to improve PLS calibration models [1]. Three broad categories of algorithms exist for this purpose. Normalization methods that correct for the trends and shifts in baseline and curvilinearity or multiplicative interference, smoothing methods for spectral noise reduction and differentiation to correct for peak overlap and/or linear baseline drifts (Fig. 1). These algorithms may be applied autonomously or in unison with each other.

This investigation aims to examine the use of a number of common pre-processing techniques for improving the predictive capability of soil spectra. Pre-processing techniques for soil diffuse reflectance spectra were evaluated using the bootstrap. Results show depending on the soil property investigated, pre-processing can result in more robust PLS calibration models.

References

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