Spectroscopic determination of leaf traits using infrared spectra

Introduction

Leaf traits are relevant to differentiate plant species but also to assessment plant health. Conventional methods of measuring leaf traits, especially at the molecular level (e.g., water, lignin, and cellulose content) are expensive and time-consuming. Spectroscopic methods allowing the estimation of leaf traits through are becoming a tool for accurate estimation of molecules from organic material.

Leaf traits and leaf spectra measured in 19 herbaceous and woody species

This study measured emissivity for 6612 narrow bands from the short to the long wave infrared (1.4-16.0µm) from 19 plant species including herbaceous, woody, temperate and tropical plants. At the same time, we measured 14 leaf traits that characterize the status of a leaf, including chemical (e.g. leaf water content, nitrogen, cellulose) and microscopic features (e.g. leaf and cuticle thickness).

Why Thermal Infrared Spectroscopy?

In the visible range it is possible to measure plant stress based on the reflected energy of the leaves, related to water, pigments and some biochemicals. The emissivity generated by the leaves is related to the biochemistry and the microstructure. Changes in the internal composition of the leaf generated by stress might therefore alter the emissivity spectra.

Reducing models for each leaf trait from 6612 spectral bands to few bands

Optimized partial least squares regression models (PLSR) were fitted to derive models with as few variables as possible while still describing the leaf traits well. The models are selected before the R-squared drops more than 15%. Most stable models have a high R-squared until supported by few final bands.

Selected bands for lignin, cellulose and water, compared with the pure spectra.

The selected bands from PLSR models for the organic molecules match the most conspicuous features of lignin and cellulose.

Final models for each leaf trait

Most selected bands for leaf traits are located at wave numbers where the emissivity varies when leaf trait values changes.

Conclusion

1. This study finds the fingerprints of leaf traits in TIR spectra, by simplifying PLSR models to the minimum number of variables.
2. The selected bands for molecules of cellulose, lignin and water match visible features of these pure compounds and also known molecular bonds of these molecules.
3. The spectra of all leaves share the same strong absorption features in the SWIR, which are strongly associated to organic molecules of lignin and cellulose, but have different features in the MWR and LWR.
4. Most bands selected to estimate leaf traits are located in regions with visible differences between low and high levels of leaf traits.