From spectra to traits

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1 Ramblings

Because leaf spectra integrate over many morpho-anatomical and chemical properties of leaves, they have been widely used to infer ecologically relevant leaf traits such levels of nitrogen, carbon and concentration photosynthetic pigments.

Those inferences are generally drawn based on PLSR models. Although PLSR has been successfully applied in chemometrics and spectroscopy, there are potential drawbacks. PLSR is designed as a predictive model instead of an explanatory model, and may fail to recover the true underlying model.

Bayesian model averaging has been suggested an alternative approach ...

Goals: Compare the performance of PLSR and BMA in chemistry / morphology inference:

1. Fit: do they explain different amounts of the variation?
2. Explaining trait / spec relationship: Do they identify the same regions of the spectra to be related to a given trait?
3. Predictive accuracy: How well do these methods predict chemistry?
4. Robustness: Which method is more robust to misspecification (or say noise / bias in spectra such as illumination effects)