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Removing the effect of moisture from NIR-DRS for prediction of soil carbon content

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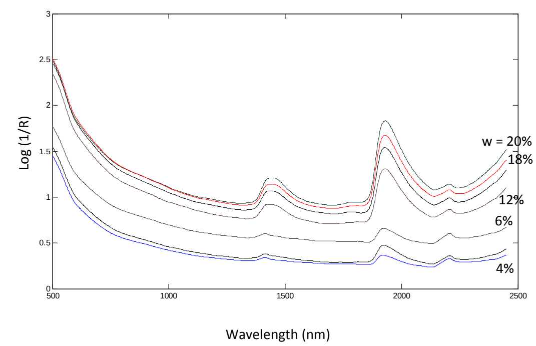
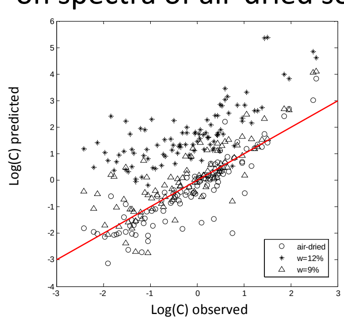
Loamy texture, SOC = 1.1%



Prediction of SOC from PLS calibrated on spectra of air-dried soil



EPO (empirical parameter orthogonalisation)

- S is the m-dimensional (no wavelengths) space of the measured spectra.
- $S = C + G + R$
- C: chemical spectral responses independent of G;
- G : spectra caused by external parameter effect, independent from C;
- R = independent residual

EPO

In matrix form, the spectra can be written as:

$\mathbf{X} = \mathbf{XP} + \mathbf{XQ} + \mathbf{R}$ *[n obs by m wavelengths]*

P is the projection of the useful part of the spectra: $\mathbf{X}^* = \mathbf{XP}$ *[**P** is m by m]*

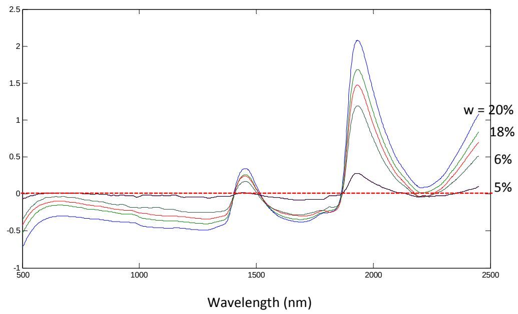
Q is the projection of the not useful part (influenced by moisture) of the spectra: $\mathbf{X}^+ = \mathbf{XQ}$

R is the residual

EPO

- To obtain $\mathbf{X^*} = \mathbf{X}(\mathbf{P})$
- $\mathbf{P} = \mathbf{I} - \mathbf{Q}$ *(m by m* symmetric matrix*)*
- **Q** can be estimated from a matrix of difference spectra **D** *(n by m)*
- $\mathbf{D} = \mathbf{X}_{dry} - \mathbf{X}_{moist}$
- $\mathbf{Q} = \mathbf{G}\,\mathbf{G}^T$ *(**G** is n by m)*
- **G** is estimated by the *c* Principal Components of **D**

Difference spectra (with air-dried)

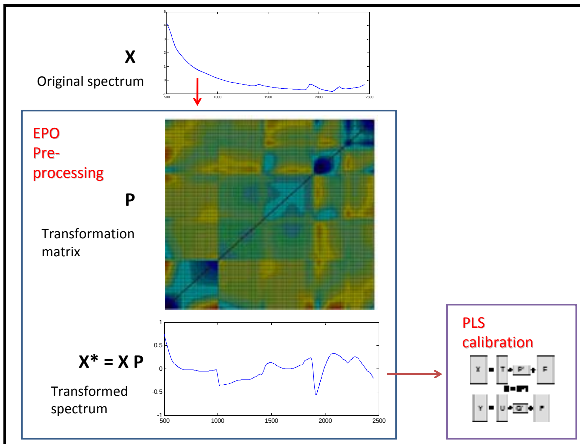


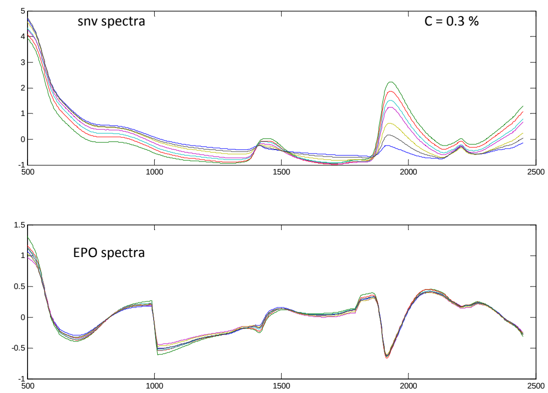
Calibration strategy

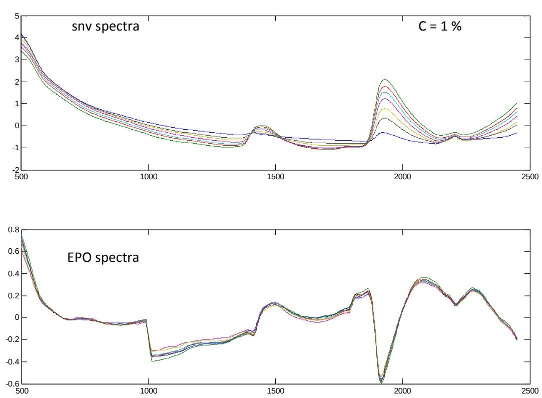
EPO Development Dataset
Contain spectra of soil under
various field conditions (varying moisture)
and
Spectra at standard moisture condition
(air-dried)
n = 60-100
SPECTRA -> EPO Spectra

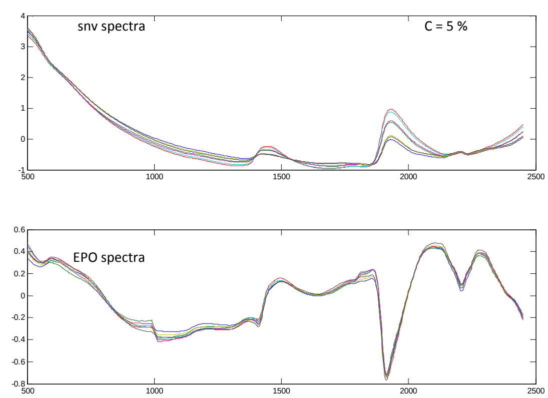
Model calibration Dataset
Contain measured SOC and spectra
of soil under standard moisture condition
(e.g at air-dried)
SPECTRA -> EPO -> DEVELOP e.g. PLS
n > 200

Validation dataset
Contain measured SOC and spectra
of soil under
various moisture conditions
SPECTRA -> EPO -> APPLY PLS
n ~ 20-100

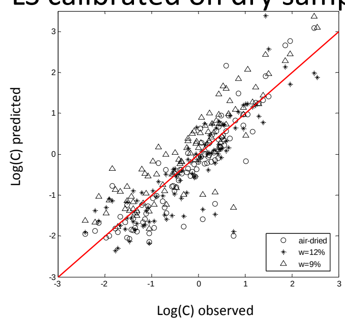






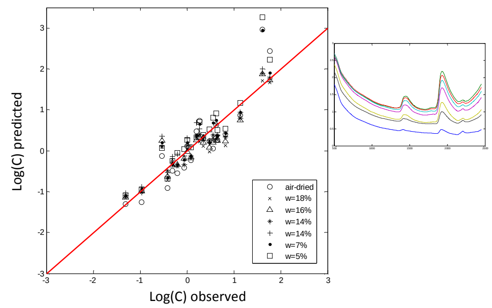


Perform PLS on transformed spectra PLS calibrated on dry samples



EPO development data, 100 samples

Prediction on independent samples
(20 samples, each with 7 different moisture content)



Conclusions

- This first experiment shows a practicable and robust method to predict soil organic carbon independent of (field) moisture content.
- Pre-processing the data with the EPO method allows removal of the moisture effect, to a large degree, which improves the quality of the prediction model.
- We propose 3 independent datasets for the field NIR calibration procedure:
  - The calibration dataset
  - The EPO development dataset
  - The validation dataset
- We need to further investigate the effect of the EPO spectral transformation on the prediction of other soil properties.

- Budiman Minasny, Alex. B. McBratney, Veronique Bellon-Maurel, Jean-Michel Roger, Alexia Gobrecht, Laure Ferrand, Samuel Joalland. **Removing the effect of soil moisture from NIR diffuse reflectance spectra for the prediction of soil carbon**. *Geoderma* (Submitted)

Acknowledgment

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