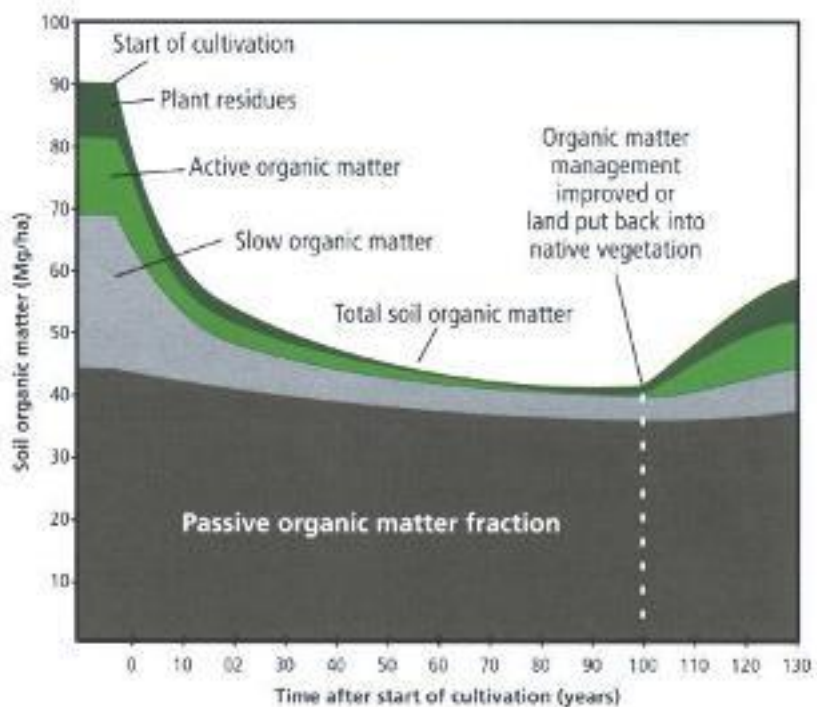# Common Chemometric Indicators for Prediction of Soil Organic Matter Content and Quality from Soil Spectra: A Review and Research Perspectives

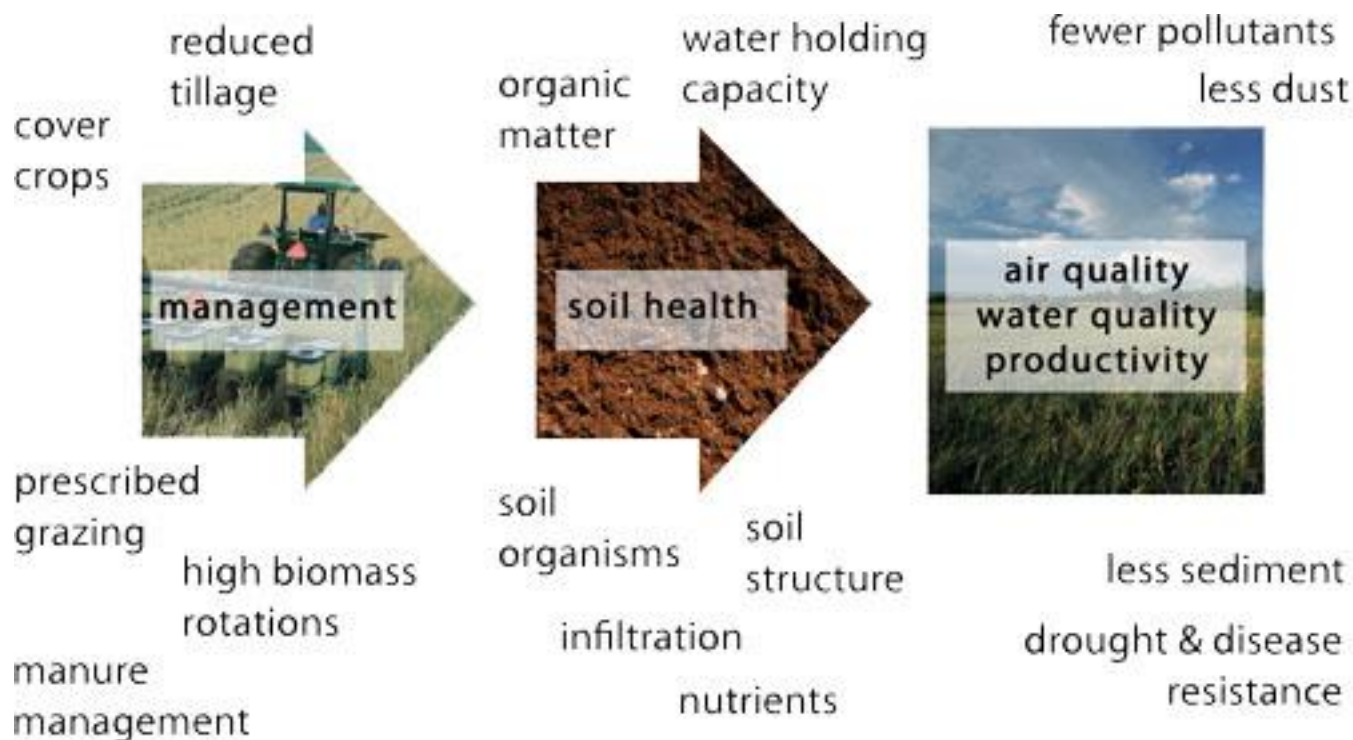Asa Gholizadeh, Luboš Borůvka, M.Mehdi Saberioon

Department of Soil Science and Soil Protection, Faculty of Agrobilogy, Food and Natural Resources, Czech University of Life Sciences Prague

Soil Organic Matter (SOM)

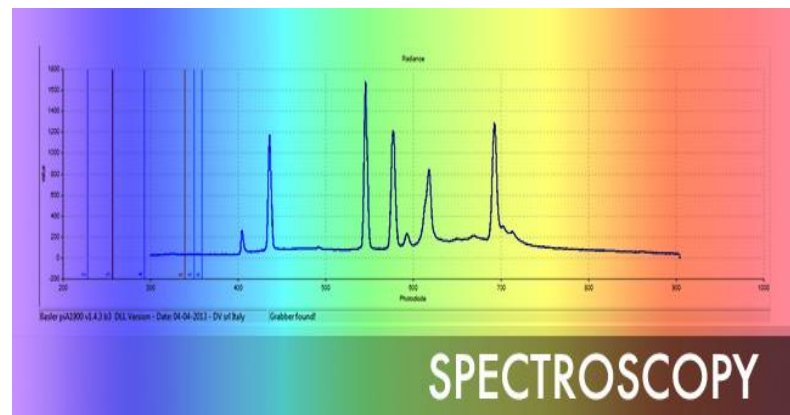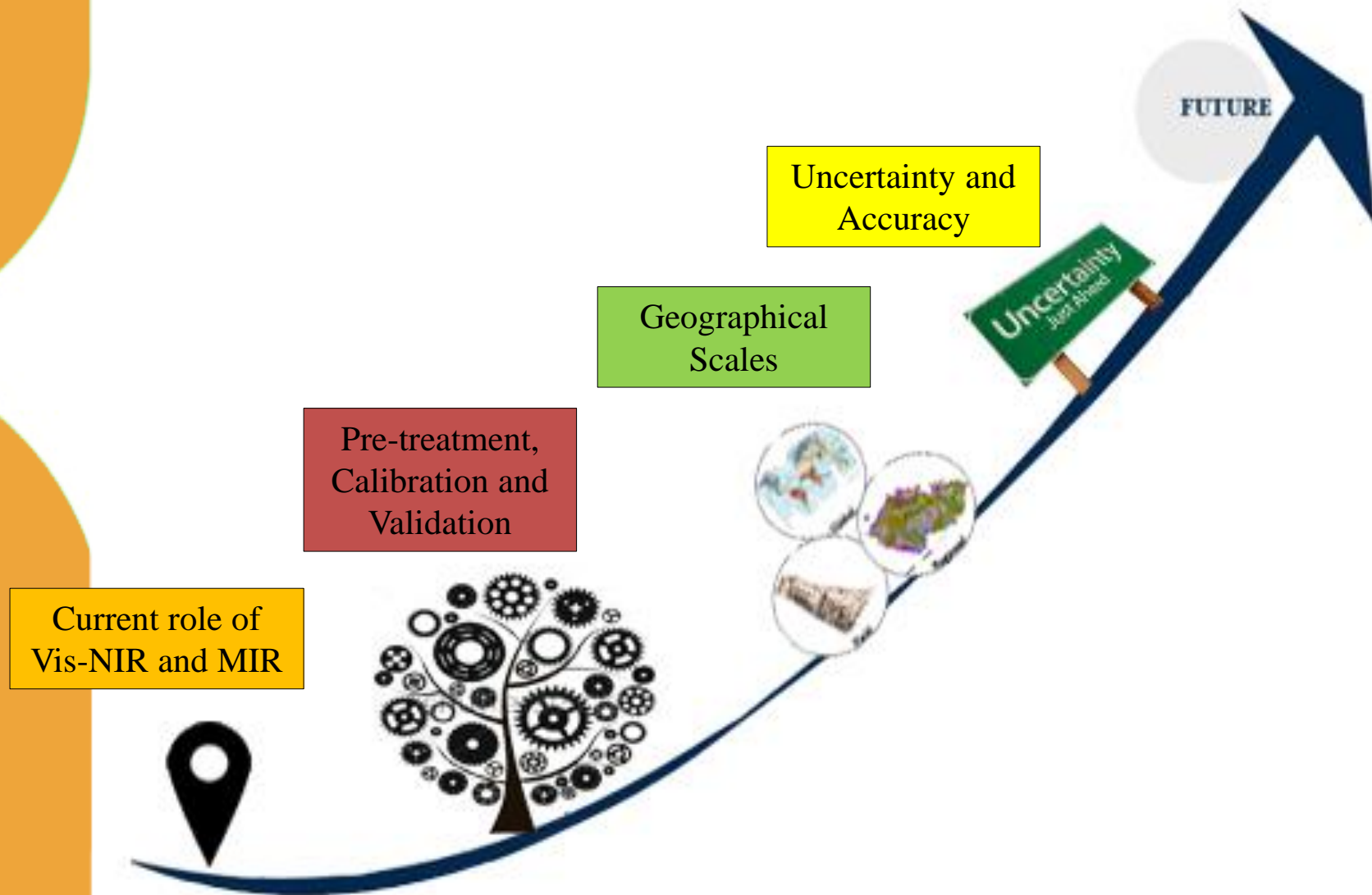**Trend in soil organic matter content (Brady 1999)**

Why focus on SOM?

Managing soil organic matter is the key to air and water quality and also agricultural higher output.

Conventional Methods of Soil Management

Conventional Soil Management Techniques

- High Input & Cost
- Uniform Management
- Low Output
- Time-Consuming
- Environment Pollution
- Labor

Solution → SPECTROSCOPY

Objectives

Uncertainty and Accuracy

Geographical Scales

Pre-treatment, Calibration and Validation

Current role of Vis-NIR and MIR

FUTURE

Uncertainty Just Ahead

Vis, NIR and MIR Spectroscopy for SOM Assessment

Olinger & Griffiths (1993)
- → Vis and NIR are used for the quantitative determination
- → MIR is used for the qualitative determination

Henderson et al. (1992)

Cozzolino & Moron (2006) → Vis had strong correlation with SOM content

Bartholomeus et al. (2008)

Christy (2008)

Cecillon et al. (2009) → NIR had strong correlation with SOM content

Nocita et al. (2013)

Shepherd & Walsh (2002)

Viscarra Rossel et al. (2009) → MIR had strong correlation with SOM content

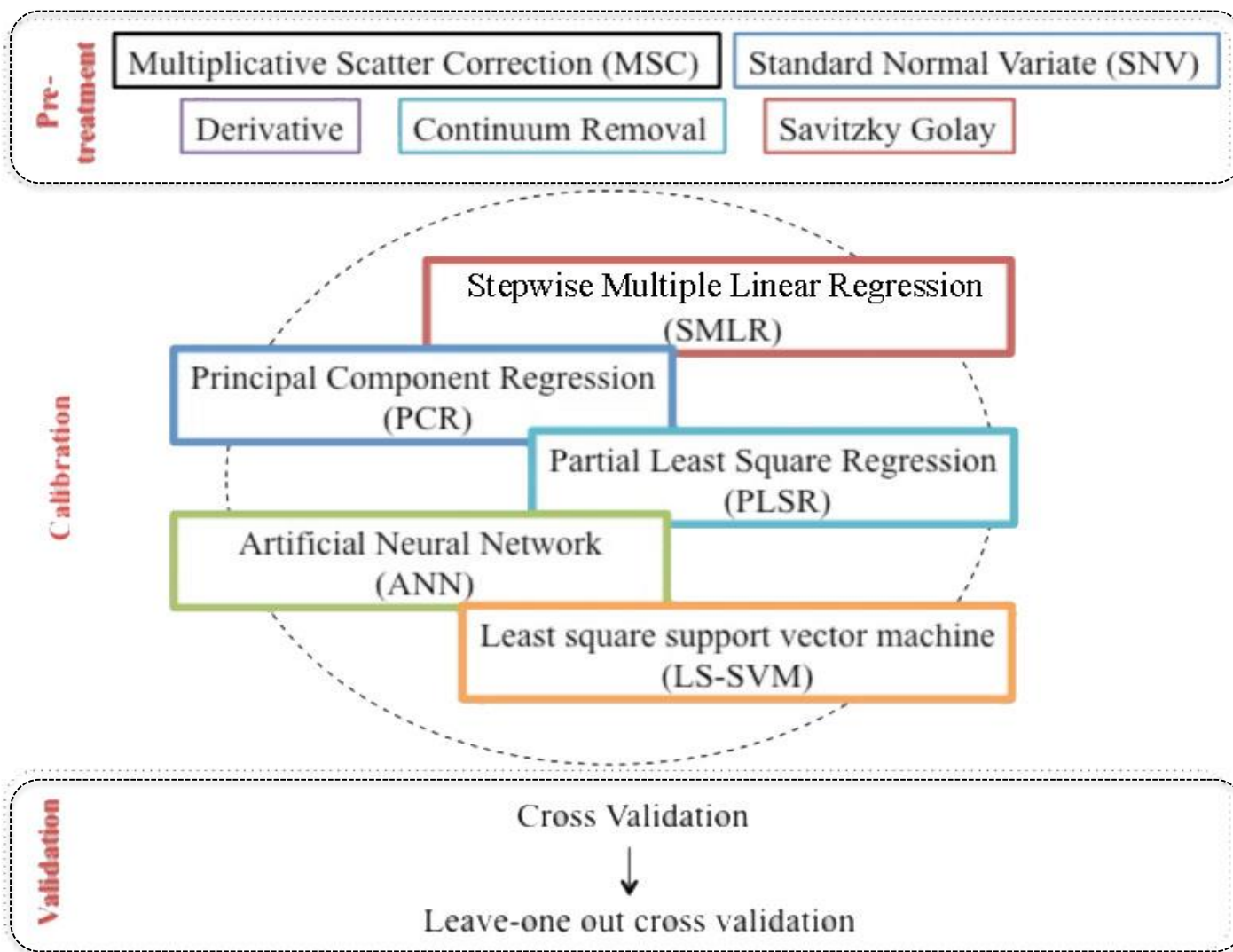Reeves et al. (2006)

Cecillon et al. (2009) → Vis-NIR had strong correlation with SOM quality

Du & Zhou (2009)

Merry & Janik (2013) → MIR had strong correlation with SOM quality

Spectroscopic Pre-treatment, Calibration and Validation

Pre-treatment
- Multiplicative Scatter Correction (MSC)
- Standard Normal Variate (SNV)
- Derivative
- Continuum Removal
- Savitzky Golay

Calibration
- Stepwise Multiple Linear Regression (SMLR)
- Principal Component Regression (PCR)
- Partial Least Square Regression (PLSR)
- Artificial Neural Network (ANN)
- Least square support vector machine (LS-SVM)

Validation
- Cross Validation
↓
- Leave-one out cross validation

Calibration Techniques

Nicolai et al. (2007) →

SMLR: The estimated regression coefficients vary markedly when the outlying observations are changed or deleted. Furthermore, the variability of the estimated regression coefficients becomes inflated.

Esbensen et al. (2002)

Nicolai et al. (2007) →

PCR: The PCs selected are not essentially the best predictors for the reference data. Moreover, there is no guarantee that the first PCs will include the spectral data related to the specific dependent variable that needs to be modeled.

Zhang et al. (2008) →

PLSR: Not appropriate when the nonlinear models is needed.

Shao et al. (2012) →

ANN: Requires a large number of training data, which always influence the training speed. The over-fitting nature is also a difficulty to conquer in order to create a good result.

LS-SVM as Recommended Calibration Technique

Stevens et al. (2010)

Yasumaru (2011)

→ It has the capability for linear and nonlinear multivariate calibration and solves the multivariate calibration problems in a relatively fast way.

Chen et al. (2012)

→ It is a method with high accuracy, simplicity and robustness.

Shao et al. (2012)

→ The most valuable properties of SVMs are their ability to handle large input spaces efficiently.

Sonali et al. (2013)

→ strike the right balance between accuracy attained on a given finite amount of training patterns and the ability to generalize to unseen data.
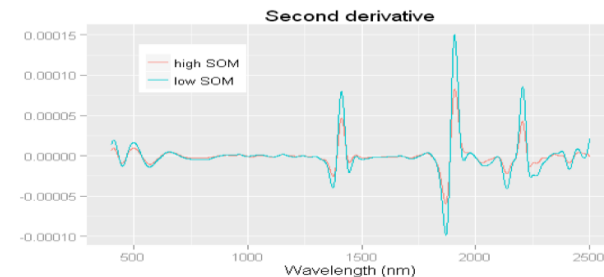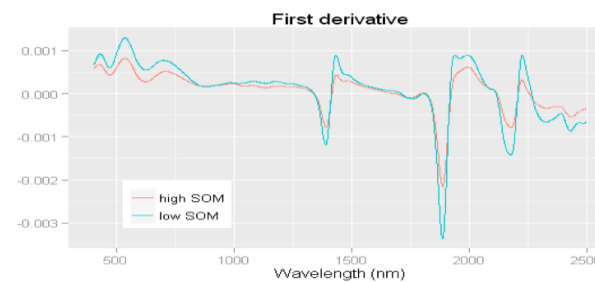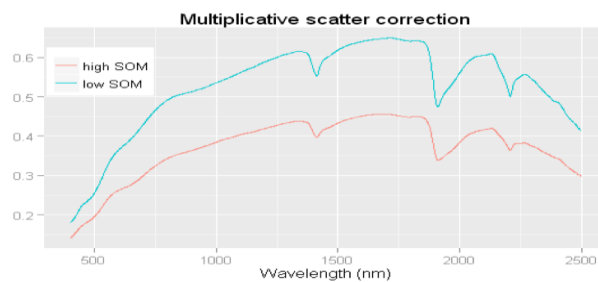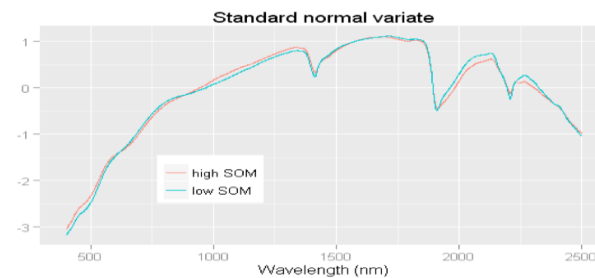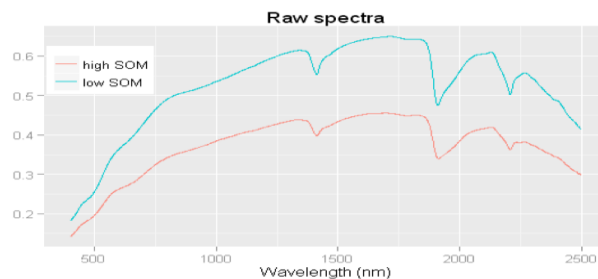
Viscarra Rossel & Behrens (2010)

Stevens et al. (2010)

Vohland & Emmerling (2011)

Predictions of different soil properties by LS-SVM using all Vis-NIR wavelengths produced the higher R^2 and smaller RMSE values.
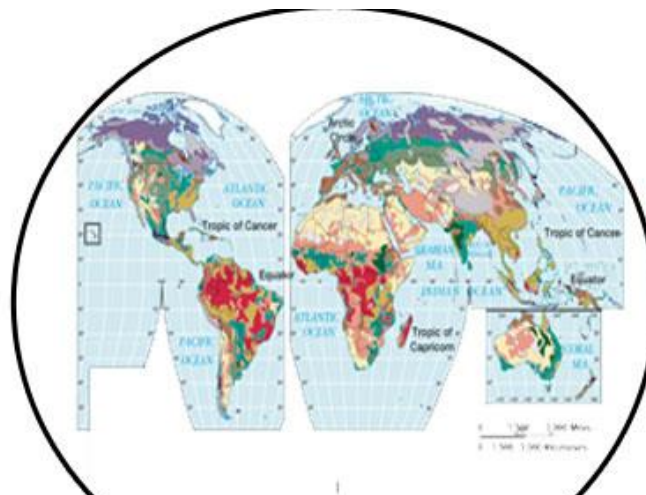
Various Pre-treatment Strategies Results on the Same SOM Data
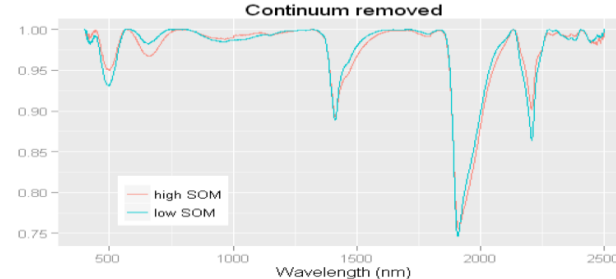
Spectroscopy for SOM Assessment

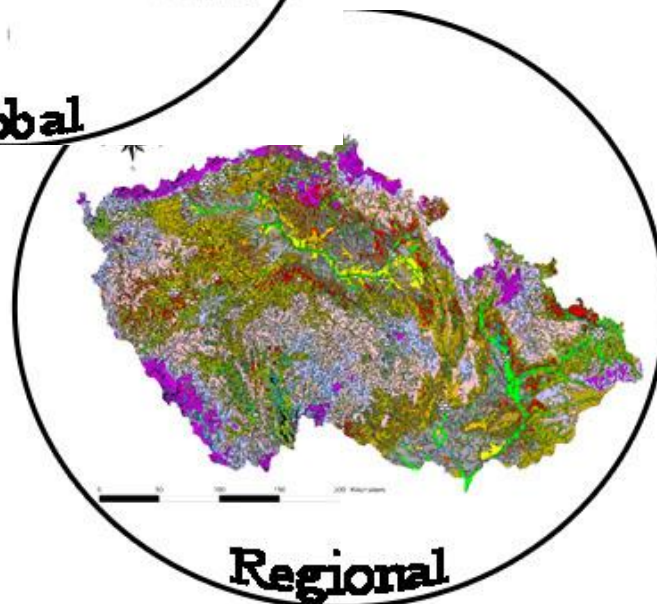| No.	Vis/NIR/MIR	Sample	Data Processing	Validation Set	SEP (%)	Range in μm	Reference
1	Vis-NIR	Lab/Fresh	PLSR	70%	0.39	0.4-2.5	Van Vuuren et al., 2006
2	NIR	Lab/Ground (Moisturized)	MLR	33%	0.19	1.65-2.5	Sudduth & Hummel, 1993
3	Vis-NIR	Lab (Oven Dried)/Ground	1stD- PLSR	LooCV	4.6	0.4-2.5	Rinnan & Rinnan, 2007
4	NIR	Field/On-the-go	SNV- 1stD- PCR	LooCV	0.4	0.7-1.7	Christy, 2008
5	Vis-NIR	Field/Hole and Trench	MSC-1stD- PLS	22%	2.1	0.4-2.45	Ben-Dor et al., 2008
6	MIR	Lab (Oven Dried)/Ground	PLSR	LooCV	0.72	2.5-25	Masserschmidt et al., 1999

Calibration Scales: Field, Regional or Global
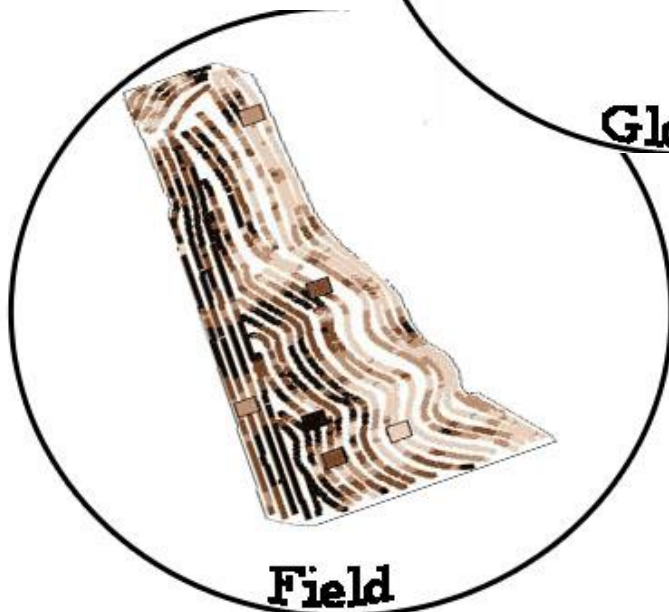
Accuracy and Uncertainty in Soil Spectroscopy

Conclusions

➢ For the determination of SOM quantity and quality, MIR spectroscopy is often more accurate and produces more robust calibrations than Vis-NIR spectroscopy.

➢ Finding suitable data pre-treatment and calibration strategies for the application of Vis-NIR or MIR spectroscopy is dramatically eye-catching.

➢ Smoothing (mostly Savitzky-Golay) and LS-SVM algorithms lead to over-optimistic performance in the assessment of SOM.

➢ A global soil spectral libraries will improve the predictive ability of spectroscopy for soil quantity and quality attributes whatever the soil type.

➢ Inaccuracy and uncertainties occur in different steps within the prediction procedure such as soil sampling, spectra collecting, building the prediction model (number of training samples and model parameters) and final spatial prediction.

Future Works

➤ Standardization of Vis-NIR and MIR spectroscopy calibration is needed and it would allow the identification of soil properties including SOM quantity and quality that are possibly spectroscopy predictable and would lead to an enhanced acceptance of Vis–NIR and MIR spectroscopy in soil analyses.

➤ Internal standards, a standard protocol and controlled conditions can assist in sharing and comparing soil spectra worldwide with higher accuracy.

➤ An urgent research need is the development of global soil spectral libraries.

Thank you