# THE ACQUISITION OF SPECTRAL REFLECTANCE MEASUREMENTS UNDER FIELD AND LABORATORY CONDITIONS AS SUPPORT FOR HYPERSPECTRAL APPLICATIONS IN PRECISION FARMING

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### ABSTRACT

Spectral reference measurements in different resolutions are required for many applications in remote sensing. Although, theoretically, in-situ measurements represent the conditions at the time of data acquisition by airborne or satellite sensors in an optimum way, they are strongly influenced by illumination, moisture, geometry, and surface roughness. To minimize these effects laboratory measurements of soil samples are used since they allow to better control the measurement conditions. Therefore, many spectral libraries are based on laboratory measurements and many empirical relations for determining spectrally derived parameters depend on data acquired under laboratory conditions. In this study the reflectance of soil samples under field and laboratory conditions were compared under controlled illumination and geometry conditions. Differences were mainly caused by soil aggregates, which reduce the spectral albedo in the wavelength domain between 600 and 2400 nm. This affects the estimation of the inorganic and organic carbon content from the reflectance data using a partial least square (PLS) regression. Several spectra pre-treatment techniques were tested to reduce the soil aggregate influence and to optimize the modeling results.

### **1 INTRODUCTION**

Bi-directional soil reflectance in the wavelength range between 0.4 and 2.4 µm is a cumulative property, derived from the inherent spectral behaviour of the heterogeneous combination of minerals, water and organic matter. Using statistical methods such as stepwise multiple regression analysis (SMRA) or partial least square (PLS) regression, several authors established relationships between soil reflectance and organic matter (Krishnan et al., 1980, Dalal & Henry, 1986), hygroscopic moisture (Dalal & Henry, 1986), clay content, specific surface and carbonate content (Ben-Dor et al., 1991; Ben-Dor & Banin, 1990, 1994). The possibility of a qualitative and quantitative assessment of soil properties from reflectance data is especially useful for applications in precision farming, where a high spatial resolution in the monitoring of soil and vegetation characteristics is desired. This also includes up-scaling from ground reflectance measurements to routinely acquired multispectral Remote Sensing image data.

Empirical approaches require many ground reference measurements and chemical laboratory data for model calibration. In theory, in-situ measurements represent the conditions at the time of data acquisition by airborne or satellite sensors in an optimum way. However, they are strongly influenced by illumination, moisture, geometry, and surface roughness. To minimise these effects laboratory measurements of soil samples are often preferred, since they allow to better control the measurement conditions. Thus, many spectral libraries are based on laboratory measurements which do not necessarily reflect in-situ environments. In this study a comparison is accomplished between in-situ and laboratory reflectance measurements from soil samples and the consequences on the estimation of soil parameters are investigated.

# 2 METHODS

In a case study an approximately 13 ha large parcel near Trier (West Germany, near the border to Luxembourg) was investigated. 114 in-situ reflectance measurements and soil samples were taken at dry weather conditions in August 1999 after the crop season. The samples were derived from a regular raster of 60 m sampling width to cover the spatial variability of soil characteristics in the parcel. The bi-directional diffuse reflectance measurements were accomplished with an ASD FieldSpec II spectroradiometer with a nominal resolution of 1 nm in the wavelength range of 0.4 - 2.5 µm. An external illumination and measuring device (ASD high intensity reflectance probe, A122000) allowed in-situ reflectance measurements with controlled illumination and geometry conditions. The circular measuring area (radius 10 cm) was planted with an iron masher to reduce the influence of the irregular micro relief on the soil reflectance.

Following the in-situ measurement top soil samples were taken. In the laboratory reflectance measurements were repeated with sieved samples (mesh width 2 mm) and analyzed for organic and inorganic carbon by an infrared cell in a high-frequency induction oven (LECO). The intention was to compare the two chemical soil parameters having different response in the reflectance curve: inorganic carbon is characterized by a well defined absorption feature around 2.35  $\mu$ m (Hunt and Salisbury, 1971), whereas the organic carbon content has an impact on the spectral albedo and the form of the reflectance curve (Baumgardner et al., 1985). Several data pre-treatment techniques were applied on the spectral data sets, including vector normalization, min-max normalization, convex-hull computation and first and second derivative calculation after Savitzky and Goley (1964). The vector norm of a spectra is defined as:

$$\sum_{k} (x_k)^2 = 1 \tag{1}$$

A partial least square (PLS) regression was applied to establish a quantitative relationship between the reflectance measurements and the analytical data. PLS is an extension of the classical principal component regression. In PLS one is concerned with two blocks of data, the matrix X with the independent variables and matrix Y with the dependant variables. The objective is to model X in such a way that the information in Y can be predicted as well as possible. PLS maximizes the covariance between matrices X and Y (for detailed information, see Otto, 1997 and Teppola et al., 1997). The matrix X is decomposed into a score matrix T and a loading matrix P. In a similar way, the matrix Y is decomposed into a score matrix Q:

$$X=TP' + E$$
(2)  
$$Y=UQ' + F$$
(3)

Where: X: n\*p matrix of independent variables (n spectra with p data points)

- Y: n\*m matrix of dependent variables (n samples, m variables)
- T, U: n\*d score matrices (with d relevant latent variables)
- P: p\*d matrix of loadings for matrix X
- Q: m\*d matrix of loadings for matrix Y
- E: n\*p matrix of residuals for matrix X
- F: n\*m matrix of residuals for matrix Y

In an inner relation score vector t is regressed against score vector u:

u=tb+g

(4)

Scalar b stands for regression coefficient relating a score vector t into a corresponding score vector u. The first latent variable, which is extracted from the matrix X, explains a maximum of the variance of matrix Y. The second latent variable describes a maximum of the residual variance which has not been described by the first latent variable, and so on. The optimum number d of latent variables to be used in the analysis is determined by predicting an independent set of spectra and comparing the root mean square errors of cross-validation (RMSECV) of the predictions obtained from models with different values of d.

### **3** RESULTS AND DISCUSSION

Figure 1a illustrates the differences between the mean soils' reflectance curves of in-situ and the laboratory measurements. In the wavelength range between 650 and 2400 nm the reflectance of the laboratory samples in the average is significantly higher. Soil reflectance is strongly influenced by illumination, moisture, geometry, and surface roughness (Baumgartner et al., 1985). The first three parameters were kept constant during the experiment, but the reflectance of the in-situ samples is still influenced by soil aggregates. The similarity in the first derivative spectra, plotted in figure 1d, confirm that mainly spectral albedo effects cause the differences between laboratory and field measurements. Derivatives from VIS/NIR-spectra predominately carry the chemical information of the sample, since albedo effects are reduced and overlapping spectral features are resolved. For example, the absorption feature of bound carbon in the carbonate-group in the wavelength region around 2.3  $\mu$ m is more distinct in the derivative spectra than in the reflectance data. The spectral features around 1.4  $\mu$ m, 1.9  $\mu$ m and 2.2  $\mu$ m are derived from combinations and overtone modes of free water's OH-fundamentals (stretching -  $\delta$  and bending -  $\nu$ ) at 1.4 and 1.9  $\mu$ m and the OH-me-OH fundamentals (me = Fe, Mg, Al) in the mineral lattice at 1.45 and 2.2  $\mu$ m (Hunt and Salisbury, 1971). Typical clay minerals that show distinct absorption features at those wavelengths are muscovite, montmorillonite, illite, kaolinite, vermiculite, and chlorite. The lower absorption depths at those wavelengths in the laboratory spectra is a consequence of evaporation losses between sampling time and analysis.



Figure 1: Average spectra of the laboratory and in-situ measurements (a) and effect of min-max normalization (b), vector normalization (c), and calculation of first derivative spectra (d)

Org. carbon	Laboratory		In-situ
RMSECV	Data-pretreatment	RMSECV	Data-pretreatment
0.146	Reflectance spectra	0.179	Reflectance spectra
0.140	Min-max normalization	0.204	Min-max normalization
0.152	Vector normalization (VN)	0.177	Vector normalization (VN)
0.151	First derivative spectra	0.201	First derivative spectra
0.147	First derivative + VN	0.202	First derivative + VN
0.262	Sec. Derivative	0.199	Sec. Derivative
0.198	Convex-hull	0.213	Convex-hull
Inorg. carbon	Laboratory		In-situ
RMSECV	Data-pretreatment	RMSECV	Data-pretreatment
0.258	Reflectance spectra	0.579	Reflectance spectra
0.245	Min-max normalization	0.506	Min-max normalization
0.242	Vector normalization (VN)	0.500	Vector normalization (VN)
0.269	First derivative spectra	0.543	First derivative spectra
0.256	First derivative + VN	0.521	First derivative + VN
0.591	Sec. Derivative	0.596	Sec. Derivative
0 365	Convex-hull	0.736	Convex-hull

Table 1: PLS quantification results (cross-validation) of inorganic and organic carbon from reflectance data, in consideration of several spectral pre-treatment techniques.



Figure 2: Spatial pattern of measured and PLS estimated organic carbon contents (%), based on vector normalised reflectance curves.



Figure 3: Spatial pattern of measured and PLS estimated inorganic carbon contents (%), based on vector normalised reflectance curves.

A min-max- or vector normalisation of the reflectance curves (figure 1b, 1c) already reduces the influence of the soil aggregates of the in-situ measurements considerably, whereas the spectral albedo differences within the average spectra are retained. Beside soil aggregate effects, spectral albedo differences between the samples are caused by several reasons. The general relationship between organic matter and soil brightness and colour have long been recognized. The shape of the reflectance curve in the VIS and NIR at higher contents of organic carbon (2-3%) may turn from a convex into a concave shape (Baumgardner et al., 1985). Additional factors which affect the spectral albedo are soil moisture, content of iron, or mafic minerals and soil texture. Organic matter is also characterised by broad spectral features from the functional groups. The absorption bands of organic compounds in the near and shortwave infrared largely originate as harmonics and overtones of the fundamental stretching frequencies of C-H, O-H and N-H bonds in the middle infrared-region together with various combination bands (Martens, 1989). Both, the form of reflectance curve and structural information, which are preserved in min-max or vector-normalised spectra, are used for modelling the organic carbon content.

As an additional distinctive feature the PLS estimations for inorganic and organic carbon (table 1) from the spectral data sets were taken into account, with respect to the different spectral pre-treatment techniques. Obviously, the min-max- or a vector-normalisation of the spectra improves the PLS estimations from reflectance data, whereas the prediction accuracy of inorganic carbon is considerably higher. In general, better predictions were obtained with the laboratory spectra. This demonstrates that the soil aggregate effects could not be completely removed from the in-situ samples.

The derivative and convex-hull spectra resulted in distinct worse PLS estimations for inorganic and organic carbon. These data pre-treatment techniques reduce, respectively, eliminate albedo differences within a spectra. This result was expected for organic carbon, where spectral albedo is an important predictor variable, but not for inorganic carbon. It shows that spectral albedo to some extent also carries information about calcareous mineral compounds such as calcite and dolomite.

A further reason for the poor prediction quality of the second derivative spectra is the declining signal-to-noise ratio in these spectra.

A root mean square error for cross-validation (RMSECV) of 0.14, attained for the optimal organic carbon PLS model using min-max normalised laboratory spectra, corresponds to 60% common variance of measured and predicted contents. This is not enough to preserve the spatial pattern of the measured organic carbon contents in the test area. This is visualised in figure 2, where a spline interpolation of the measured and the estimated organic carbon concentrations is shown. A reason for the medium prediction quality is probably the low dynamic organic carbon concentration range of only one percent in the investigated parcel (minimum concentration = 1.4%, maximum concentration = 2.4%). Thus, other optically active soil minerals such as iron oxides with a higher variability may dominate the spectral albedo. Similar to organic carbon, an increase of iron oxides leads to a decrease of overall reflection in the visible and near infrared (Obukhov, and D.S. Orlov, 1994; Jarmer and Schütt, 1998). The prediction quality declines dramatically for the organic carbon estimations based on the in-situ measurements (R<sup>2</sup>=0.17), despite the use of vector normalised reflectance spectra.

In contrast to the organic carbon contents, PLS estimations of inorganic carbon where accurate for both, vector normalised in situ spectra ( $R^2$  0.88) and laboratory spectra ( $R^2$  of 0.95). Figure 3 illustrates that the spatial pattern of the measured concentrations are persevered with the estimated quantities of both approaches.

# 4 CONCLUSIONS

- Under controlled conditions of illumination and geometry spectral differences between in-situ and laboratory measurements mainly originate from albedo effects from macroscopic soil aggregates.
- A vector-normalization of the reflectance spectra reduces spectral differences between the two approaches. It also improves the prediction quality for PLR estimations of inorganic and organic carbon contents.
- PLS estimations of inorganic carbon, characterized by well defined absorption features, is more accurate than the estimation of the organic carbon content.
- A relationship of in-situ reflectance data and soil properties for precision farming applications can be developed within a soil landscape only if the soil texture is not too variable.

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