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Spectroradiometric determination of wheat bio-physical variables Comparison of different empirical-statistical approaches

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ABSTRACT: Empirical-statistical methods are widely used to estimate bio-physical canopy variables like LAI or canopy chlorophyll content from remotely sensed spectral data. To gain more insight into different approaches, it was decided to intercompare three important linear empirical-statistical methods for their ability to estimate LAI and canopy chlorophyll content from hyperspectral ground reflectance measurements: (i) partial least squares regression (PLSR), (ii) principle component regression (PCR), and (iii) stepwise multiple linear regression (SMLR). Results obtained on a multi-temporal winter wheat data set revealed that PLSR gave the best results, followed by classical SMLR. On the other hand, the use of PCR can not be recommended. The superiority of PLSR compared to SMLR and PCR was explained by the fact that PLSR unifies their advantages, without owning their disadvantages: (1) since PLSR is a "full spectrum" method, noise sensitivity is relatively small compared to SMLR, and (2) since data compression in PLSR considers covariance to the desired bio-physical variables, PLSR performs much better than PCR.

1 INTRODUCTION

The retrieval of bio-physical variables from multi- or hyperspectral, ground-, airborne and satellite based reflectance measurements, is one main area of research at our lab. Involved methods include empirical-statistical approaches (including artificial neural nets) (Atzberger & Schlerf, 2002; 2003; Jarmer et al., 2003), and the inversion of radiative transfer models (Atzberger, 1995; 1997; 2000; 2002; 2003; Atzberger et al., 2003; Schlerf & Atzberger, 2002; Schlerf et al., 2003; Udelhoven et al., 2000). The retrieved bio-physical variables are useful indicators for land users with strong environmental impact, e.g., agriculture and forestry.

The repetitive mapping of bio-physical variables on a small pixel resolution is for example needed in precision farming and forest inventory and modeling. In the concept of precision farming, mapping of bio-chemical (e.g. leaf chlorophyll content) and structural variables (e.g. LAI) may help to assess nutrition status and plant development. The maps can be transfered into management recommondations and decisions that sustain productivity at reduced environmental costs (Schueller, 1992; Moran et al., 1997; Hatfield & Pinter, 1993). Likewise, the mapping of forest related variables can be integrated into forest inventories (and GIS) since the bio-physical variables allow an assessment of forest health and productivity (Schulze, 2000; Franklin, 2001; Howard, 1991; Lucas & Curran, 1999; Treitz & Howarth, 1999). Since vegetation plays a major role in the global gas and energy exchange, the mapping of variables with high physiological and photochemical relevance is also recommended in the research related to global change (Sellers et al., 1995).

The bio-physical variables can be assessed quantitatively by means of physically based approaches (i.e. the inversion of radiative transfer models) (e.g. Jacquemoud et al., 1995; Bicheron & Leroy, 1999), or by means of empirical-statistical methods (e.g. Curran, 1989; 1994; Rondeaux, 1995). In either case, the approaches have to be suitable for multicollinear data – at least when dealing with hyperspectral data sets. From a scientific viewpoint, the radiative transfer based approach is generally prefered over the empirical-statistical approach, because it allows more physical insight into the system behavior (Goel, 1987). This implicitely adds valuable benefits in overall adaptability (e.g. transfer to all kinds of environmental conditions and vegetation types).

Though empirical-statistical methods do not provide any system insight, they nevertheless have an eligibility. For example, one way to evaluate the quality of a radiative transfer model is to compare its predictive power against elaborated empirical-statistical methods (Kimes et al., 1998). Because of their unreached and unlimited function approximation capability, artificial neural nets (ANN) are prime candidates for such empirical benchmark models. However, when dealing with typically small calibration and validation data sets (<100 samples), the proper use of ANNs requires great care to avoid overfitting. In these cases, the use of linear regression models can be helpful.

To gain more insight into different empirical-statistical methods, it was decided to intercompare three important linear empirical-statistical methods, known to be well suited for dealing with small, highly multicollinear data sets: (i) partial least squares regression, (ii), principal component regression, and (iii) stepwise multiple linear regression. The suitability of the different methods will be analyzed in terms of absolute prediction accuracy, and in terms of (unwanted) noise sensitivity. The significance of the results is naturally limited to the case crop studied (winter wheat) and the two bio-physical variables considered (LAI and canopy chlorophyll content).

2 GROUND TRUTH DATA

Four times during the 1999 growing season (Day of Year 119, 130, 162 and 180), four commercial winter wheat fields in the Trier area were analyzed (except DoY 119 where only three fields were probed) (Fig. 1).

In each wheat field, three subplots (0.25 m^2) were considered for biological and spectroradiometric measurements. Thus, in total, 45 corresponding spectral and biological measurements were acquired (for more details see also Jarmer et al., 2003; Atzberger et al., 2003).

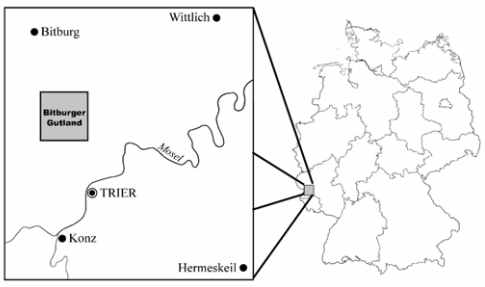

Figure 1. The location of the study region Trier within Germany and test site "Bitburger Gutland" NW of Trier.

2.1 *Reflectance measurements*

The top of canopy reflectance (ρ) was measured with an ASD Field Spec II spectroradiometer from an height of about 1.5 m above ground during favorable weather conditions around solar noon. ASD readings were normalized to bi-directional reflectance by means of a spectralon reference panel of known reflectivity. Integration time was set to 10 seconds. For each sub-plot, five reflectance readings were taken and an average spectrum was calculated. A moving (± 5 nm) Savitzky-Golai filter (Savitzky & Golai, 1964) was applied to the reflectance spectra to eliminate sensor noise. Resampling of field spectra to the central wavebands of the HyMAP sensor ensured application of calibrated models to HyMAP imagery.

Spectral offsets can be removed using spectral derivatives (Demetriades-Shah et al., 1990). Therefore, the reflectance data were transformed into "1st derivatives", which were then normalized to mean of 0 and standard deviation of 1. The first derivative was simply calculated as the reflectance difference between adjacing spectral bands. Only these normalized derivatives were used throughout this study.

2.2 *Biological measurements*

2.2.1 *LAI*

On exactly the same positions within the wheat plots where the canopy reflectance was measured, the above-ground plant material was harvested within the 25 x 25 cm sub-plots and brought to the laboratory. There – using a commercial planimeter – (one-sided) plant surface of the fresh material was determined and used to calculate the leaf area index (LAI; m^2 m^{-2}).

2.2.2 *Canopy chlorophyll content*

Chlorophyll measurements were not taken for each sub-plot, but only for entire fields. At each measurement date, 30 wheat plants per field were randomly selected and SPAD readings from the upper leaves were taken. These SPAD readings were converted into leaf chlorophyll contents by means of an empircal calibration function provided by Markwell et al. (1995). From the 30 individual leaf chlorophyll measurements, the average was calculated and multiplied by the corresponding LAI to obtain the total canopy chlorophyll content for each sub-plot (LAI x CAB; mg m^{-2}). Since the variability of the leaf chlorophyll content was relatively small compared to the LAI variability, canopy chlorophyll content and LAI show a strong positive correlation (not shown).

3 METHODS

Using the multi-temporal empirical data set (Sect. 2), three linear empirical-statistical methods were analyzed in a comparative way:

(i) partial least squares regression (PLSR)
(ii) principal component regression (PCR)
(iii)stepwise multiple linear regression (SMLR)

The methods were selected because they are known to be suitable for small, multicollinear spectral data sets. PLSR and PCR are "full-spectrum" methods since they use all available wavelengths simultaneously. SMLR selects useful wavelengths from the available spectrum; other wavebands are not considered.

The analysis refers to the estimation of leaf area index (LAI) and canopy chlorophyll content (LAI x CAB) (see Sect. 2). The suitability of the different methods will be analyzed in terms of absolute prediction accuracy, and in terms of (unwanted) noise sensitivity. Inputs to the empirical-statistical models were 1st derivatives of ground reflectance measurements resampled to the hyperspectral HyMAP sensor (127 spectral channels between 450 and 2500 nm). To be fully intercomparable, the number of regression factors was fixed to four for all methods.

We will first provide a matrix operation oriented overview, following the excellent work of Martens & Naes (1987) (Sect. 3.1). Next, we describe methodological details referring to the adopted statistical sampling strategy. In Section 3.3 we present the statistical accuracy indicators used to assess the predictive power of the different methods. In Section 3.4 finally, we specify the way we assessed the noise sensitivity of the different methods.

3.1 *The empirical-statistical models*

According to Martens & Naes (1987), the calibration of empirical-statistical models consists of two stages (Fig. 2):

(1) the *compression stage*, where the spectral data matrix (X) is compressed into a small number of basic variables ($n_T << n_\lambda$), termed regression factors, T, and

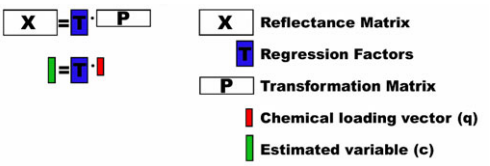

Figure 2. Schematic presentation of the general data model expressed in condensed matrix form (Martens & Naes, 1987). In the *compression stage*, the spectral data are compressed into a small number of regression factors. In the *calibration regression*, regression factors are related to the bio-physical variable.

(2) the *calibration regression*, where regression relationships are established between the regression factors, T, and the bio-physical variable, c.

Data compression gives certain estimated parameters, loading spectra, P, that define how the values of the regression factors, T, are to be calculated. The calibration regression produces estimated parameters, bio-physical loadings, q, that define how the bio-physical variable, c, is determined from the regression factors. Spectral (P) and bio-physical loadings (q) combine mathematically to yield the calibration coefficients for analysis of unknown samples (Martens & Naes, 1987).

The way P and T are estimated is different for the three methods, but q is found always by least square using T. Since in all methods, T is a linear combination of the spectral values, the bio-physical variable, c, can consequently be obtained from an ordinary linear prediction equation. All approaches assume centered spectral and bio-physical data.

3.1.1 *Partial Least Squares Regression (PLSR)*

PLSR is a widely used approach in chemometry (e.g. Beebe et al., 1998) but much less employed in remote sensing. The method is particularly suited for calibration on a small number of samples with experimental noise in both bio-physical and spectral data. In addition, the method can be used even if $n_\lambda > n_{obs}$.

In PLSR, the first loading spectra (i.e., the first row of P) is estimated by matrix operation involving X and c. The solution is then scaled to length 1 and the first column of the regression factor matrix, T, is estimated from the spectral data, X, and this first loading vector, P. Through ordinary (multiple) linear regression, the bio-physical loadings, q, are determined and residuals of the bio-physical variable are computed. With these residuals, the above described calculations are repeated for the second regression factor, and so on.

The resulting PLSR factors, therefore describe important variations in the spectral data themselves but at the same time are relevant for determination of the bio-physical data. This may be expected to lead to more efficient data compression and thus better calibration, compared to other linear empirical-statistical methods.

3.1.2 *Principal Component Regression (PCR)*

Data compression in PCR uses the spectral singular value decomposition of the spectral data to estimate both T and P. Given the centered spectral matrix, X, the first regression factor, T, and the first loading spectra, P, are estimated so that their product accounts for as much as possible of the total variation in the spectral data. The next vectors of T and P are then chosen such that the regression factors are orthogonal to each other while accounting for a maximum of the remaining spectral variance. Thus, the

main spectral variation is described by a few orthogonal regression factors. The factors obtained in this way (here the first four) are then used to calculate the bio-physical loading vector, q, in a subsequent calibration regression stage.

Notice that PCR as described here deletes small eigenvalues. Other versions of PCR that delete eigenvectors because of predictive relevance are also possible but not considered here. Since it is not possible to calculate principle components when the number of wavelengths is higher than the number of observations (i.e. $n_\lambda > n_{obs}$), only each third derivative wavelength was used for analysis.

3.1.3 *Stepwise Multiple Linear Regression (SMLR)*
Although SMLR is not a full-spectrum method like PLSR or PCR it may still be presented under the general framework of Section 3.1. The data compression stage of this method consists in selecting a combination of a few spectral bands as regression factors, T. The regression factor matrix is then used to calcuate the bio-physical loadings, q, by ordinary least square.

In the present study, the derivatives were first regressed sequentially against the bio-physical variables. The derivative with the highest explained variance was then chosen as the first regression factor. With this first regression factor fixed, the next derivative was chosen, and so on. No forward or backward elimination was allowed.

3.2 *Statistical sampling*

In cases where many samples are available (i.e. n_{obs} >100), a meaningful statistical evaluation of statistical models consists in dividing the whole data set into one set of samples used for calibration and the remainder used for independent validation. However, when dealing with small data sets (here: n_{obs} = 45), such a stationary division into calibration and validation samples must lead to biased accuracy indicators, because sample division is to some degree arbitrary. The standard approach is to perform a so called cross-validation, where each sample is estimated by the remaining samples (i.e. the "leave-one-out method"). However, this does not allow to assess the stability of the resulting statistical indicators (e.g., R^2 and RMSE). The statistical accuracy was therefore not only assessed by cross-validation (Sect. 3.2.1), but also by randomized bootstrapping (Sect. 3.2.2).

3.2.1 *Cross-validation*
Cross-validated statistics were calculated from estimates which were derived according to the "leave-one-out method" – that is each and every sample is estimated by means of an empirical-statistical model which was calibrated using the remaining (44) samples.

3.2.2 *Randomized bootstrapping*
Cross-validated results do not give any indication about the expected variability of the provided accuracy indicators. For this reason, the prediction accuracy of the different methods was also assessed by dividing the data set into 2 sub-data sets: 2/3 of the samples were used for model calibration and the remaining 1/3 for model validation. Separation into calibration and validation sub-sets was repeated 20 times in a random way. This yields frequency distributions of the accuracy indicators which are useful to assess model accuracy and stability. Results referring to the randomized bootstrapping will be discussed in Section 4.2.

3.3 *Statistical indicators*

To assess the prediction accuracy of the different methods, two classical statistics were calculated: R^2 and RMSE. In the case of cross-validation, these statistics were calculated from the n_{obs}=45 samples, where each sample was estimated by the remaining 44 samples (Sect. 3.2.1) (R^2_{cv}, $RMSE_{cv}$). The statistics using randomized bootstrapping were calculated each time a random division of the data set into calibration (2/3) and validation (1/3) samples was performed. From the resulting frequency distributions, the median value was calculated (R^2_{rb}, $RMSE_{rb}$).

3.4 *Noisy data*

The influence of sensor noise on the stability of the empirical-statistical approaches was assessed using degraded spectral data sets. The models were first calibrated on the original spectral data. Then, a "white" (i.e. wavelength independent) Gaussian noise component (mean of zero) was added to the data set and the formerly calibrated models were used to estimate the bio-physical canopy variables. We applied noise levels with standard deviations of 0.0001, 0.0005, 0.001, 0.005, and 0.01 reflectance units. For comparison, a noise level of 0.001 corresponds for a typical vegetation spectrum to a signal-to-noise ratio (SNR) between 50:1 (red) and 500:1 (nIR).

4 RESULTS

4.1 *Cross-validated predictions*

For both bio-physical variables, the PLSR gave the highest accuracies (Fig. 3 and Tab. 1). The left hand side of Fig. 4 shows the ground measured and estimated canopy chlorophyll contents (LAI x CAB) obtained by this method. The cross-validated R^2 is 0.85 with an RMSE of 51 mg m^{-2}. This corresponds to a relative accuracy ($RMSE_{CAB}/\Delta_{CAB}$) smaller than 10%. Prediction accuracy was similar for LAI (right hand side of Fig. 4).

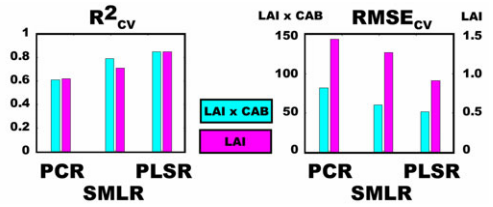

Figure 3. Cross-validated coefficients of determination (R^2) (left) and root mean square errors (RMSE) (right) between ground measured and estimated leaf area index and canopy chlorophyll content for the three empirical-statistical methods analyzed.

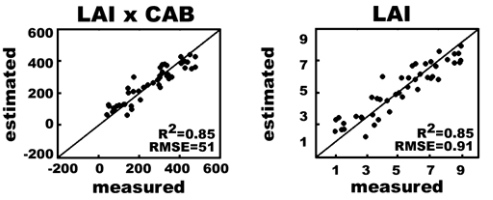

Figure 4. Ground measured versus estimated bio-physical variables using partial least squares regression (PLSR): (left) canopy chlorophyll content; (right) leaf area index. Estimates were obtained by cross-validation.

Comparing the different methods, the worst results were obtained by PCR, whereas SMLR gave acceptable results (Tab. 1).

4.2 *Predictions obtained by randomized bootstrapping*

The above presented cross-validated results indicate only the overall accuracy of the different methods. In contrast, the randomized bootstrapping also allows to assess the stability of the prediction equations (see Sect. 3.2.2). Results obtained using this statistical sampling strategy are summerized in Table 1.

Figure 4 shows the frequency distributions of the coefficient of determination (R^2) between measured and estimated bio-physical variables when division in calibration and validation samples is repeated 20 times in a randomized way. The strong spreading evident for all methods is an indication that an arbitrary (stationary) division of such small data sets in calibration and validation samples will lead to strongly biased results.

The additional information provided by the randomized bootstrapping is for example evident when comparing PLSR and SMLR for their ability to estimate canopy chlorophyll content (Fig. 5). Whereas almost no differences are seen in the cross-validated results (arrows), the frequency distributions obtained by randomized bootstrapping reveal a better performance of PLSR compared to SMLR.

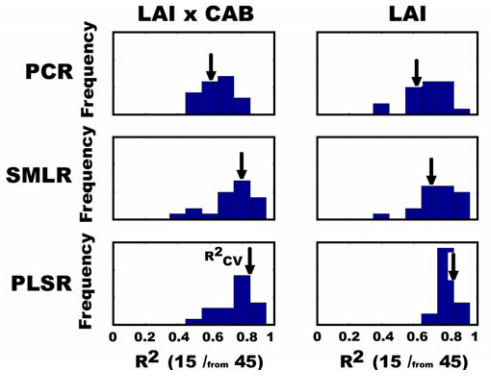

Figure 5. Frequency distributions of the coefficient of determination (R^2) between measured and estimated canopy chlorophyll content (left) and leaf area index (right) obtained by randomized bootstrapping. Thirty out of fourty five samples were used for calibration, the remaining for validation. Arrows indicate the corresponding R^2 values obtained by cross-validation.

Table 1. Statistics (R^2 and RMSE) between estimated and measured leaf area index and canopy chlorophyll content for the three empirical-statistical methods analyzed: (top) cross-validated statistics, (bottom) statistics obtained by randomized bootstrapping (median of the obtained frequency distributions).

		LAI			LAI x CAB		
		PLSR	MSLR	PCR	PLSR	MSLR	PCR
cv	R^2	0.85	0.71	0.62	0.85	0.79	0.57
	RMSE	0.91	1.27	1.44	51	60	82
rb	R^2	0.82	0.76	0.67	0.80	0.76	0.65
	RMSE	1.13	1.25	1.48	68	71	82

4.3 *Noise sensitivity*

Strong differences between the three methods were obtained concerning the noise sensitivity (Fig. 6). Particularily for SMLR, the estimation accuracy strongly degrades with increasing noise levels. PCR (and to a lesser extent PLSR) are much less sensitive to "white" noise.

5 DISCUSSION

Main differences between the three methods can be seen in Figure 7, where the explained variances in the spectral and bio-physical data are shown for the first four regression factors.

Principle component regression (PCR) concentrates the reflectance data only in terms of statistical properties. If important parts of the reflectance variability are due to external effects not included in the regression equation, this unwanted variance (for example due to soil brightness variations) will be concentrated in the first principle components, and thus will be included in the empirical model. Minor, but important factors of variability, will accordingly be placed into the last principle components. Therefore, the prediction accuracy of the PCR in multivariate

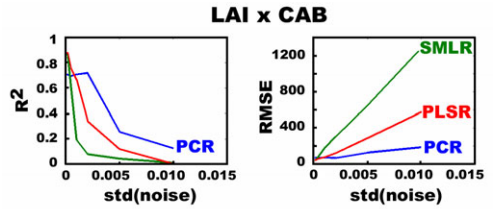

Figure 6. Noise sensitivity of the three empirical-statistical methods in the estimation of the canopy chlorophyll content expressed as a function of the standard deviation of the added "white" noise component: (left) R^2, (right) RMSE.

regressions of spectral data with bio-phyiscal canopy variables was lower compared to the two other investigated methods.The sole advantage of PCR is the relative insensitivity to "white" sensor noise.

This advantage of the PCR is at the same time the major disadvantage of classical stepwise multiple linear regression (SMLR). Since SMLR is not a "full spectrum" method, like PCR and PLSR, sensor noise has little chance to cancel out. On the other hand, SMLR can easily identify the spectral regions which are less affected by unwanted external factors and which enable the establishment of a powerful multivariate regression equation.

The partial least squares regression (PLSR) unifies in a simple and comprehensive manner the advantages of previous approaches without owning their disadvantages: (1) due to the fact that PLSR is a "full spectrum" method, noise sensitivity is relatively small compared to SMLR, and (2) since data compression into regression factors considers covariance to the desired bio-physical variables, PLSR performs much better than PCR.

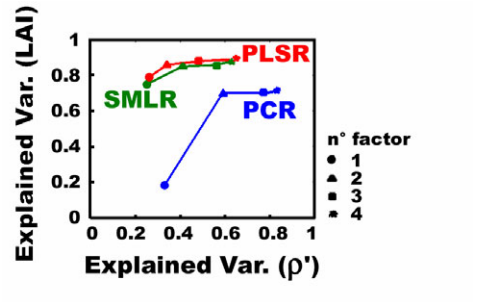

Figure 7. Explained variance in the dependent variable (LAI) and derivative data (ρ') for the three empirical-statistical methods and regression factors one to four. Lines are only to clarify the appearance of data points.

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