Computers and Electronics in Agriculture 73 (2010) 165–173

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Comparative analysis of three chemometric techniques for the spectroradiometric assessment of canopy chlorophyll content in winter wheat

Clement Atzberger[a,*], Martine Guérif[b], Frédéric Baret[b], Willy Werner[c]

[a] Joint Research Centre of the European Commission, JRC, Institute for the Protection and Security of the Citizen, IPSC, MARS Unit, Via Enrico Fermi 2749, 21027 Ispra, Italy
[b] Institute Nationale de la Recherche Agronomique (INRA), 84000 Avignon, France
[c] University of Trier, Dept. of Geobotanics, Geozentrum, 54290 Trier, Germany

ARTICLE INFO

Article history:
Received 24 November 2009
Received in revised form 7 May 2010
Accepted 16 May 2010

Keywords:
Data redundancy
Partial least squares regression
Principal component regression
Stepwise multiple linear regression
Canopy chlorophyll content
Noise sensitivity

ABSTRACT

Hyperspectral data sets contain useful information for characterizing vegetation canopies not previously available from multi-spectral data sources. However, to make full use of the information content one has to find ways for coping with the strong multi-collinearity in the data. The redundancy directly results from the fact that only a few variables effectively control the vegetation signature. This low dimensionality strongly contrasts with the often more than 100 spectral channels provided by modern spectroradiometers and through imaging spectroscopy. With this study we evaluated three different chemometric techniques specifically designed to deal with redundant (and small) data sets. In addition, a widely used 2-band vegetation index was chosen (NDVI) as a baseline approach. A multi-site and multi-date field campaign was conducted to acquire the necessary reference observations. On small subplots the total canopy chlorophyll content was measured and the corresponding canopy signature (450–2500 nm) was recorded ($n_{obs} = 42$). Using this data set we investigated the predictive power and noise sensitivity of stepwise multiple linear regression (SMLR) and two 'full spectrum' methods: principal component regression (PCR) and partial least squares regression (PLSR). The NDVI was fitted to the canopy chlorophyll content using an exponential relation. For all techniques, a jackknife approach was used to obtain cross-validated statistics. The PLSR clearly outperformed all other techniques. PLSR gave a cross-validated RMSE of 51 mg m^{-2} ($R^2_{cv} = 0.82$) for canopy chlorophyll contents ranging between 38 and 475 mg m^{-2} ($0.99 \leq LAI \leq 8.74$ m^2 m^{-2}). The lowest accuracy was achieved using PCR ($RMSE_{cv} = 82$ mg m^{-2} and $R^2_{cv} = 0.57$). The NDVI, even using chlorophyll optimized band settings, could not reach the accuracy of PLSR. Regarding the sensitivity to artificially created (white) noise, PCR showed some advantages, whereas SMLR was the most sensitive chemometric technique. For relatively small, highly multi-collinear data sets the use of partial least square regression is recommended. PLSR makes full use of the rich spectral information while being relatively insensitive to sensor noise. PLSR provides a regression model where the entire spectral information is taken – in a weighted form – into account. This method seems therefore much better adapted to deal with potentially confounding factors compared to any 2-band vegetation index which can only avoid the most harmful factor of variation.

1. Introduction

Non-destructive measurements of canopy biophysical variables are required in several applications ranging from precision agriculture (Cox, 2002; Schueller, 1992) to global assessments of the carbon and nutrient cycle (Potter et al., 1999; Bacour et al., 2006). Important biophysical variables are the leaf area index (LAI) and the leaf chlorophyll content (CAB). Both variables influence light interception and photosynthesis. The total canopy chlorophyll content (TC), which is the product of the two variables, shows a close relation to the photosynthetic activity (McDonald, 2003) as well as to the N-status of plants (Houlès et al., 2007; Baret et al., 2007). The assessment of this integrated variable is therefore subject to a number of studies (Combal et al., 2002; Baret and Fourty, 1997; Guérif et al., 2007).

Hyperspectral measurements of vegetation canopies contain useful information for characterizing vegetation status and functioning not previously available with multi-spectral imagery (Curran, 1994; Haboudane et al., 2004; Hatfield and Pinter, 1993; Richter et al., 2009; Lee et al., 2004; Ye et al., 2008; Blackburn, 2007). At the same time, however, these data sets contain large amounts of redundant information (Baret et al., 2000; Schlerf et al., 2005; Grossman et al., 1996). The redundancy directly results from the relatively few parameters (<20) effectively controlling the spectral-directional signatures of vegetation (Widlowski et al., 2007; Im and Jensen, 2008). For example, leaf optical properties

* Corresponding author. Tel.: +39 0332 78 3569.
E-mail address: clement.atzberger@jrc.ec.europa.eu (C. Atzberger).

0168-1699/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.compag.2010.05.006

in the visible to mid infrared (450–2500 nm) are parameterized by most radiative transfer models (RTM) using only 4–6 parameters (Jacquemoud and Baret, 1990; Dawson et al., 1998; Maier et al., 1999). To model the influence of the underlying soil background (Baumgardner et al., 1985), most RTM rely on 1–3 variables to parameterize the soil reflectance (Jacquemoud et al., 1992; Verhoef and Bach, 2007). To describe the canopy structure, three parameters are of prime importance: leaf area index (LAI), the average leaf angle (ALA) and the ratio between leaf size and canopy height (Verhoef, 1984; Kuusk, 1991). In forests with leaves clumped into crowns and open spaces between crowns, three additional parameters permit accurate simulations (Schlerf and Atzberger, 2006). Thus, in total, perhaps 10–15 parameters control most of the observed spectral-directional variability in vegetation canopies (Baret, 1991; Asner, 1998; Jacquemoud et al., 2009). This relatively low number of variables contrasts with the often more than 100 spectral bands available through imaging spectroscopy and from commercially available spectroradiometers.

To deal with hyperspectral data sets two broad approaches were developed (Moran et al., 1997; Baret and Buis, 2008). In the physical based approach, radiative transfer models (RTM) are inverted to retrieve the biophysical parameters of interest (Goel, 1987; Jacquemoud et al., 1995a; Atzberger and Richter, 2009; Houborg and Boegh, 2008; Richter et al., in press). In the second approach, *in situ* reference measurements of the target variable(s) are collected to calibrate statistical models (Darvishzadeh et al., 2008c; Curran, 1994; Thenkabail et al., 2002; Broge and Mortensen, 2002; Schlerf et al., 2010; Yang et al., 2010). Both approaches own specific advantages and disadvantages (Darvishzadeh et al., in press). In the case of RTM the available set of spectral-directional measurements is used simultaneously to derive the parameter(s) of interest. The problem concerning data redundancy is small and (white) noise is partly cancelled out. Problems with the physical based approach derive mainly from two sources (Baret and Buis, 2008): (1) inability to find an appropriate RTM correctly simulating (in the forward mode) the spectral signature of the canopy under study (Jacquemoud et al., 2000; Darvishzadeh et al., 2008b) and (2) the ill-posedness of the inverse problem due to counterbalancing effects between ALA, LAI and soil brightness (Combal et al., 2003; Atzberger, 2004; Darvishzadeh et al., 2008a).

The use of statistical models for the retrieval of vegetation biophysical variables requires that the strong collinearity in the spectral data is taken into account (Martens and Naes, 1987; Williams and Norris, 1987). The most prominent approaches are listed in Table 1 together with some well illustrated studies. Full spectrum methods such as PCA and PLS are widely used in chemometrics (Wold et al., 2001; Geladi and Kowalski, 1986). These techniques transform the spectral feature space such that the resulting (latent) factors account for a maximum of variance in the feature space (PCA), respectively in the covariance with the target variable(s) (PLS). In contrast to the two mentioned full spectrum methods, SMLR selects a minimum set of wavelengths that permit an optimum modelling of the target variable (Chatterjee and Price, 1977; Williams and Norris, 1987). Besides these chemometric techniques the remote sensing community developed over the past 4 decades a large range of spectral indicators (e.g. vegetation indices, red-edge indices), responding strongly to the main vegetation biophysical variables such as LAI or leaf pigmentation (Broge and Mortensen, 2002; Rondeaux, 1995; Jago et al., 1999; Filella and Penuelas, 1994; Darvishzadeh et al., 2009).

The objective of the present study was to evaluate the performance of three chemometric techniques (PLS, PCR and SMLR) for modelling the canopy chlorophyll content from field spectrometer data, resampled to the band setting of the widely used HyMap hyperspectral imager (Cocks et al., 1998). The total canopy chlorophyll content was selected as target variable because of its close relation to photosynthetic activity and plant nitrogen content. As a baseline method, one of the most widely used vegetation indices (NDVI) was used (Tucker, 1979). Randomly generated noise was added to the spectroradiometric data to study the stability of the developed statistical models to unfavourable measurement conditions.

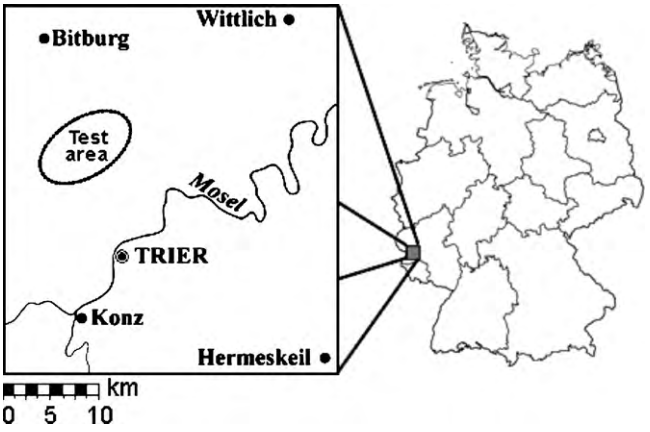

Fig. 1. Study region "Bitburger Gutland" in Germany, northwest of the city of Trier.

2. Material

In 2000, four commercial winter wheat fields (*Triticum aestivum*) were probed. The test area is situated northwest of Trier (Germany) in an agricultural region called "Bitburger Gutland" (Fig. 1). Eutric cambisols from airblown silt over limestone are the typical soils of the area (Udelhoven et al., 2003).

Measurements were taken between mid April and end of June (Day of Year: 115, 129, 160 and 172). On each measurement date, a 5 m × 5 m plot was established in homogeneous parts of the wheat fields. Within these plots, the leaf chlorophyll content was measured using an optical device (Section 2.3). The leaf chlorophyll content was assumed constant within the plot. Within each plot, three subplots (40 cm × 40 cm) were randomly chosen. In these subplots, leaf area index (LAI) and spectral data were recorded. The total canopy chlorophyll content (TC; [mg m^{-2}]) was calculated as the product between LAI and the leaf chlorophyll content. The final data set consisted of 42 TC and reflectance measurements.

2.1. Canopy reflectance measurements

For each subplot, the top of canopy reflectance was measured. Spectral data were recorded between 350 and 2500 nm using an ASD Field Spec Pro© spectroradiometer. Spectral readings were taken in 1 nm intervals with a spectral resolution ranging between 3 nm below 1000 nm and 10–12 nm in the near and shortwave infrared (1000–2500 nm). The hand held measurements were made from a height of about 1.5 m above the ground during favourable weather conditions (clear-sky) around solar noon. A scanning time of 10 s was used to acquire one spectrum. Each spectrum thus represents an average of 100 individual measurements of 100 ms. Applying this averaging increases the signal-to-noise ratio of the resulting measurement. ASD readings with a 24° field of view (bare optic) were converted to bi-directional reflectances by means of a Spectralon© reference panel of known reflectivity. For each subplot, five reflectance readings were taken and averaged. A moving SG filter (Savitzky and Golay, 1964) with a window width of ±5 nm and a polynomial of second degree was applied to eliminate sensor noise. Wavelengths below 420 nm and above 2400 nm were eliminated due to high noise amounts.

Table 1
Valuable examples of chemometric and statistical techniques for estimating vegetation biophysical variables.

Abbreviations	Technique	Examples
PLSR	Partial least square regression	Hansen and Schjoerring (2003), Huang et al. (2004), Nguyen and Lee (2006), Jensen et al. (2007) and Darvishzadeh et al. (2008c)
PCR	Principal component regression	Cohen et al. (2003), Chaurasia and Dadhwal (2004) and Huang et al. (2004)
SMLR	Stepwise multiple linear regression	Jacquemoud et al. (1995b), Yoder and Pettigrew-Crosby (1995), Grossman et al. (1996), Fourty and Baret (1997) and Biewer et al. (2009)
VI	Vegetation indices	Broge and Leblanc (2001), Broge and Mortensen (2002), Thenkabail et al. (2002), Haboudane et al. (2004), Zhao et al. (2005), Zhao et al. (2007) and le Maire et al. (2008)
REIP	Red-edge inflection Point	Filella and Penuelas (1994), Jago et al. (1999), Cho et al. (2007), Cho et al. (2008) and Cho et al. (submitted for publication)
SVM	Support vector machines	Camps-Valls et al. (2006), Clevers et al. (2007), Durbha et al. (2007) and Li et al. (2009)
UNMIX	Unmixing	Asner and Heidebrecht (2002)
NN	Neural nets	Huang et al. (2004), Kalácska et al. (2005), Mas and Flores (2008) and Bacour et al. (2006)

In order to produce statistical models that can be applied to real (airborne or satellite-based) remote sensing data, we resampled the 1 nm ASD spectra to the central wavelengths of the widely used HyMap sensor (Cocks et al., 1998). Only these wavelengths were used for modelling ($n_\lambda = 127$). The analyzed canopy spectra are shown in Fig. 2(a). The strong collinearity in the measured reflectance spectra is depicted in the 2D-correlogram of Fig. 2(b), where large white blocks indicate a high coefficient of determination within and between large wavelengths regions.

2.2. LAI measurements

Destructive LAI measurements were done at exactly the same locations were the spectral measurements were taken. For this purpose, after completion of the reflectance measurements, the above-ground plant material was harvested from the subplots and brought to the laboratory. No distinction between leaves and other green plant material (e.g. stems) was made. This implies that the term LAI should, in the context of this study, be understood as plant area index (PAI) (Breda, 2003). In the laboratory, the one-sided surface of the fresh material was determined using a commercial planimeter. From these measurements, the subplot leaf area index was derived ($m^2\ m^{-2}$).

Measured LAI values ranged between 0.99 and 8.74 with mean of 5.1 and standard deviation of 2.4 (Table 2). The temporal evolution of the measured LAIs is shown in Fig. 3(a). For plotting purposes, the subplot measurements were averaged to better highlight the differences between the four wheat fields.

2.3. Leaf and canopy chlorophyll contents

Thirty wheat plants per plot were randomly selected at each measurement date. From the upper leaves SPAD© readings (Minolta, 2003) were taken and converted into leaf chlorophyll contents (Markwell et al., 1995). The 30 individual leaf chlorophyll measurements were averaged (CAB). Descriptive statistics are reported in Table 2.

To derive the total canopy chlorophyll content of a subplot (TC; $[mg\,m^{-2}]$), the plot-specific leaf chlorophyll contents ($\mu g\,cm^{-2}$) were multiplied by the subplot-specific LAI ($m^2\ m^{-2}$):

$$TC_{ij} = LAI_{ij} \times CAB_i \quad (1)$$

with i subscript for the measurement date ($i = 115$, 129, 160 and 172); j for the subplot identification ($j = 1$, 2 and 3).

The corresponding descriptive statistics are summarized in Table 2 and the temporal evolution of leaf and canopy chlorophyll contents is shown in Fig. 3(b and c).

From Fig. 3(a–c), a relatively strong correlation between the three biophysical variables is evident. Therefore, no attempts were made to study separately the leaf chlorophyll content or LAI.

3. Methods

Using the measured total canopy chlorophyll contents and the corresponding reflectance spectra in the HyMap band setting, three linear statistical methods were analyzed in a comparative way using Matlab's statistical environment (The Mathworks, 2007):

(i) Partial least squares regression (PLSR).
(ii) Principal component regression (PCR).
(iii) Stepwise multiple linear regression (SMLR).

The three methods were selected because they are known to be suitable for small, multi-collinear spectral data sets (Duckworth, 1998; Martens and Naes, 1987). The strong multi-collinearity of the analyzed data set is evident from Fig. 2(b).

PLSR and PCR are "full spectrum" methods as they use all available wavelengths simultaneously. On the contrary, SMLR selects useful wavelengths from the available spectrum and ignores the remaining wavebands during model application. As a baseline method, non-linear regression models between TC and NDVI were studied as well. Despite their known limitations (Gobron, 1997; Baret and Guyot, 1991), vegetation indices like the NDVI are still widely used mainly because of their simplicity.

As predictor variables for the chemometric methods, the 1st derivatives of the field spectra (450–2500 nm) were used ($n_\lambda = 127$). By using spectral derivatives, spectral offsets can be removed (Demetriades-Shah et al., 1990; Yoder and Pettigrew-Crosby, 1995). The derivatives were normalized before modelling to mean of 0 and standard deviation of 1. No attempts were made to reduce the number of input variables through feature selection (Knox et al., 2010; Cramer et al., 2008; Xu et al., 2009).

The suitability of the different methods was assessed in terms of absolute prediction accuracy (RMSE) (y_p: predicted variable; y_o: observed variable):

$$RMSE = \sqrt{\frac{1}{n_\lambda}\sum_{i=1}^{n}(y_p - y_o)^2} \quad (2)$$

and for the amount of explained variance (coefficient of determination, R^2). All statistics were cross-validated using the leave-one-out technique. To be fully intercomparable, the number of regression factors was fixed to four for all methods. A second analysis was run to determine the noise sensitivity of the different approaches.

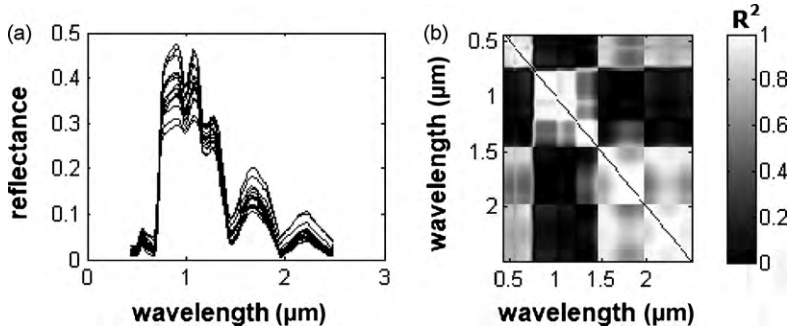

Fig. 2. Spectral data used in the study. (a) Field measured reflectance spectra for the central wavelengths of the HyMap sensor. The spectra were filtered with the Savitzky–Golay filter. To ease the reading, the points were connected by lines. (b) Observed inter-correlation (R^2) between the spectral data in the various HyMap channels. Blocks in bright gray highlight areas of strong correlation.

Table 2
Descriptive statistics (n_{obs} = 42) of the field measured biophysical variables for four winter wheat plots and four measurement dates. LAI is the leaf area index ($m^2\ m^{-2}$), CAB the leaf chlorophyll content ($\mu g\ cm^{-2}$) and TC the total canopy chlorophyll content (LAI × CAB; $mg\ m^{-2}$). The table reports the minimum value (min), maximum (max), mean (mean) and standard deviation (std) of the observations.

	Pooled	Measurement day (DoY)				Plot number			
		115	129	160	172	No. 1	No. 2	No. 3	No. 4
LAI									
Mean	5.05	2.58	6.22	6.24	4.54	6.83	5.25	3.08	5.04
Std	2.36	1.32	1.57	1.91	2.57	2.05	2.20	1.71	1.89
Max	8.74	4.73	8.74	8.71	8.60	8.74	8.71	6.89	7.18
Min	0.99	1.03	3.58	3.25	0.99	2.60	1.40	0.99	2.27
CAB									
Mean	47.9	47.7	49.1	50.8	44.2	50.9	50.0	44.6	45.4
Std	4.7	0.8	2.0	5.1	6.6	3.3	3.0	4.5	6.1
Max	54.8	48.7	51.2	54.8	50.7	54.8	54.5	48.7	50.1
Min	38.5	46.8	47.2	43.9	38.5	46.8	47.8	38.6	38.5
TC									
Mean	247	123	314	324	213	352	265	139	218
Std	134	61	92	118	140	117	117	81	125
Max	475	221	448	475	436	475	474	325	345
Min	38	50	169	143	38	122	67	38	87

Note that for plot no. 4, on DoY 115 no LAI measurements were taken and on DoY 129 no chlorophyll readings.

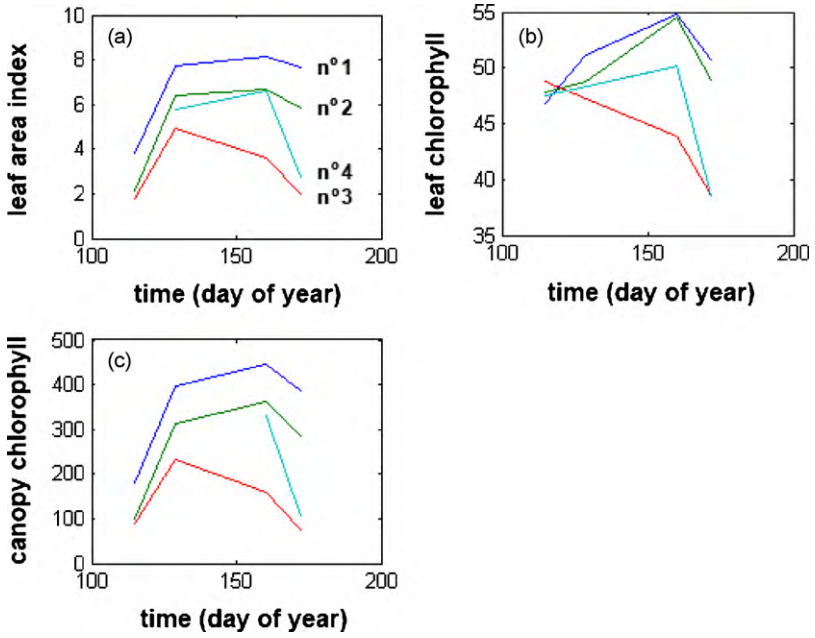

Fig. 3. Biophysical field observations available for the 2000 winter wheat study. For plotting purposes, all measurements were averaged at plot level. (a) Temporal profiles of destructively sampled leaf area indices (LAI) for the four wheat plots, (b) leaf chlorophyll contents ($\mu g\ cm^{-2}$), and (c) canopy chlorophyll contents ($mg\ m^{-2}$). To ease the reading, the points were connected by lines.

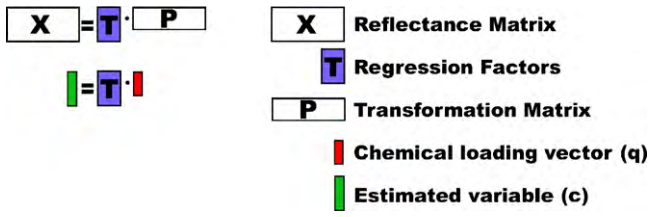

Fig. 4. Schematic presentation of the general data model expressed in condensed matrix form (Martens and Naes, 1987). In the *compression stage*, the spectral data are compressed into a small number of regression factors. In the *calibration regression*, regression factors are related to the biophysical variable.

3.1. Statistical models

According to Martens and Naes (1987), the calibration of any multi-variate statistical model consists of two stages (Fig. 4):

(1) the *compression stage*, where the spectral data matrix (X) is compressed into a small number of basic variables ($n_T \ll n_\lambda$), termed regression factors, T, and
(2) the *calibration regression*, where regression relationships are established between the regression factors, T, and the biophysical 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, biophysical loadings, q, that define how the biophysical variable, c, is determined from the regression factors. Spectral (P) and biophysical loadings (q) combine mathematically to yield the calibration coefficients for analysis of unknown samples (Martens and 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 biophysical variable, c, can consequently be obtained from an ordinary linear prediction equation. All approaches assume centered spectral and biophysical data (i.e. mean of zero).

3.1.1. Partial least squares regression (PLSR)

PLSR is a widely used approach in chemometrics (e.g. Beebe and Kowalski, 1987; Geladi and Kowalski, 1986; Wold et al., 2001). It is also employed in remote sensing for studying vegetation and soil characteristics (Cho et al., 2007; Hansen and Schjoerring, 2003; Farifteh et al., 2007; Nguyen and Lee, 2006). The method is particularly well suited for calibration on a small number of samples with experimental noise in both biophysical 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 biophysical loadings, q, are determined and residuals of the biophysical 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 biophysical 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 (Jackson, 1991). 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 biophysical 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 principal 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 (Chatterjee and Price, 1977) is not a full spectrum method like PLSR or PCR it may still be presented under the general framework shown in Fig. 4. 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 calculate the biophysical loadings, q, by ordinary least square.

In the present study, the derivatives were first regressed sequentially against the biophysical 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. Forward or backward elimination were not investigated.

3.1.4. Normalized difference vegetation index (NDVI)

Two different NDVIs were calculated as baseline approach: (i) the classical NDVI (Tucker, 1979) using red and near-infrared reflectances at 650 and 800 nm and (ii) the leaf chlorophyll sensitive NDVI proposed by le Maire et al. (2008) using wavelengths at 710 and 925 nm.

As the relation between TC and NDVI is non-linear, the exponential model form proposed by Baret and Guyot (1991) was used to relate the two variables:

$$\mathrm{NDVI} = \mathrm{NDVI}_\infty + (\mathrm{NDVI}_{soil} - \mathrm{NDVI}_\infty) \times e^{-k \times \mathrm{TC}} \quad (3)$$

The three parameters of Eq. (3) were fitted iteratively using the *fmins* procedure of Matlab (The Mathworks, 2007). After calibration, the inverse of Eq. (3) was used to estimate the total canopy chlorophyll content from the recorded NDVI value. In the case that the measured NDVI was higher than the infinite NDVI (NDVI_∞), the estimated TC was set to the upper limit of the recorded values (here 600). No attempts were made to test other indices (e.g. Broge and Mortensen, 2002), as the main focus was on full spectrum methods and SMLR.

3.2. Cross-validated statistical indicators

All estimates were obtained according to the "leave-one-out method" (Efron and Gong, 1983). This means, 42 different models were calculated, each time using 41 out of 42 available observations. After calibration, the models were applied to the left-out sample to provide a cross-validated estimate of TC.

To assess the prediction accuracy of the different methods, two classical statistics were calculated between the field measured and

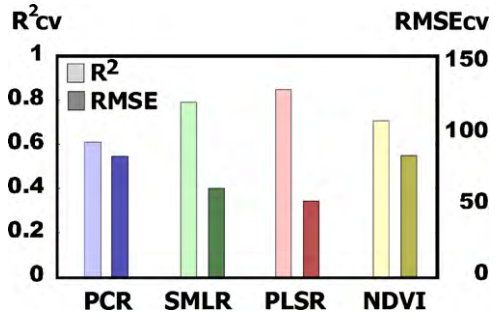

Fig. 5. Cross-validated coefficients of determination (R^2 – left bars) and root mean square errors (RMSE – right bars) between field measured and modelled canopy chlorophyll content using three chemometric techniques. For comparison, the results from the chlorophyll optimized NDVI proposed by le Maire et al. (2008) are also displayed. All statistics are cross-validated.

the modelled canopy chlorophyll content: the coefficient of determination (R^2_{cv}) and the root mean squared error ($RMSE_{cv}$).

3.3. Influence of sensor noise

The influence of sensor noise on the stability of the statistical models was assessed using radiometrically 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 canopy chlorophyll content. We applied noise levels with standard deviations of 0.0001, 0.0005, 0.001, 0.005, and 0.01 reflectance units. For comparison, for a typical vegetation spectrum, a noise level of 0.001 corresponds to a signal-to-noise ratio (SNR) between 50:1 (red) and 500:1 (nIR).

4. Results

Amongst the three investigated chemometric techniques, PLSR performed best (Fig. 5 and Table 3). Compared to PLSR, the two other multi-variate techniques (PCR and SMLR) showed a noticeable decrease in accuracy with SMLR performing somewhat better than PCR.

The excellent performance of PLSR is further accentuated through comparison with the results obtained from vegetation indices. Using the NDVI – and thus only part of the available spectral information (i.e. two bands) – resulted in a strong loss of predictive power. For example, the classical NDVI (Tucker, 1979) yielded only a cross-validated RMSE of 156 mg m^{-2} ($R^2_{cv} = 0.35$) (Table 3). The chlorophyll optimized NDVI proposed by le Maire et al. (2008) reached much higher accuracies ($RMSE_{cv}$ = 79 mg m^{-2}; $R^2_{cv} = 0.73$). However, even this vegetation index – which has been optimized to enhance sensitivity to leaf chlorophyll content – could not reach the accuracy of the partial least square regression technique. Its accuracy was only in the order of the SMLR and PCR (Fig. 5).

The relation between the measured and the modelled canopy chlorophyll content is shown in Fig. 6(a) for PLSR. The cross-validated R^2 was 0.85 with an RMSE of 51 mg m^{-2}. This corresponds to a relative accuracy between 10 and 20%, depending on the way the relative RMSE is calculated (i.e. $RMSE_{TC}/\Delta_{TC}$ or $RMSE_{TC}/\mu_{TC}$). Albeit the maximum LAI was higher than 8 (Table 2), almost no saturation effects were noted when using PLSR. For comparison, Fig. 6(b) shows the scatter plot between measured and modelled TC using the leaf chlorophyll optimized NDVI proposed by le Maire et al. (2008). Albeit the index performed remarkably well it could not reach the accuracy of the full spectrum PLS technique.

Strong differences between the three multi-variate methods were obtained concerning the noise sensitivity (Fig. 7). Particularly for SMLR, the estimation accuracy strongly degraded with increasing noise levels. PCR (and to a lesser extent PLSR) were much less sensitive to "white" noise. As expected, a strong noise sensitivity was also found for the NDVI (not shown), probably because the noise had little chance to cancel out when only two bands were used for modelling.

5. Discussion

The study proved a high potential of hyperspectral measurements for mapping the canopy chlorophyll content as a proxy for photosynthetic activity and N-status (Baret and Fourty, 1997). Using PLSR the cross-validated RMSE was only ~50 mg m^{-2}. This low RMSE is remarkable for several reasons: (i) all estimates were fully cross-validated, (ii) the sampled wheat canopies covered the full range of LAI values from 1 to 8, and (iii) the field experiment included several wheat fields at different phenological stages. Our results compare well with studies employing radiative transfer models for estimating TC in sugar beet (e.g. Combal et al., 2002). In the study of Combal et al. (2002) somewhat higher accuracies were achieved (15–37 mg m^{-2}). However, their data set covered also a much smaller range of canopy chlorophyll contents (i.e. $0 \leq TC \leq 100$ mg m^{-2} instead of $38 \leq TC \leq 475$ mg m^{-2} in this study). This demonstrates the potential of chemometric techniques for mapping this important biophysical variable.

The study confirmed method-inherent differences between the three investigated chemometrical methods (Martens and Naes, 1987; Huang et al., 2004). Principal component regression concentrates the reflectance data only in terms of their statistical properties (Chaurasia and Dadhwal, 2004). Hence, it is not assured that the most relevant information is included in the first few principal components (PC) that are later used as regression factors during the calibration stage. On the contrary, it may happen that important factors of variability (for a given variable of interest) will be placed into higher PC not used in the predictive equation (Cohen et al., 2003). This explains why the prediction accuracy of the PCR

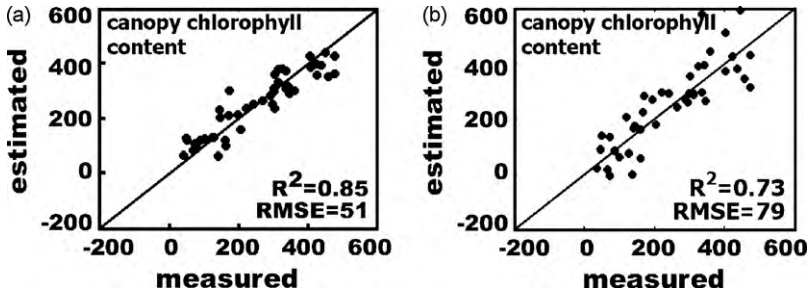

Fig. 6. Field measured versus modelled canopy chlorophyll content. (a) Results obtained from partial least squares regression (PLSR) and (b) results from leaf chlorophyll specific NDVI proposed by le Maire et al. (2008). All estimates and statistics are cross-validated.

Table 3
Cross-validated statistics (R^2 and RMSE) between the estimated and the measured canopy chlorophyll content (TC). Three chemometric techniques (PCR, SMLR and PLSR) are compared with two 2-band vegetation indices using band settings proposed by Tucker (1979) and le Maire et al. (2008), respectively.

	Chemometric techniques			NDVI-based	
	PLSR	SMLR	PCR	Tucker	le Maire
R^2_{cv}	0.85	0.79	0.57	0.35	0.73
$RMSE_{cv}$	51	60	82	156	79

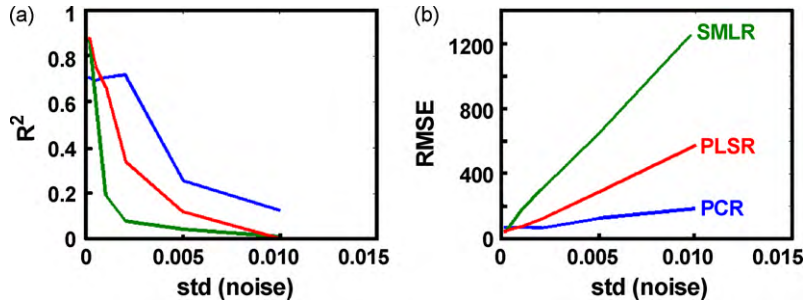

Fig. 7. Sensitivity of three chemometric techniques for estimating the canopy chlorophyll content (TC) as a function of the radiometric noise level: (a) noise sensitivity of the estimated TC in terms of R^2 and (b) noise sensitivity of the estimated TC in terms of RMSE. The noise is expressed as the standard deviation of the added "white" noise component.

for the canopy chlorophyll content was lower compared to the two other investigated methods. The sole advantage of PCR in this study was the relative insensitivity to "white" sensor noise which was well cancelled out.

This advantage of the PCR was at the same time the major disadvantage of the classical stepwise multiple linear regression (SMLR). Since SMLR is not a "full spectrum" method, like PCR and PLSR, sensor noise had little chance to cancel out (Jacquemoud et al., 1995b; Grossman et al., 1996). The same holds also for 2-band vegetation indices such as the investigated NDVI. The advantage of SMLR is that it permits the user to focus on spectral regions with known (direct or indirect) links to the variable of interest (Fourty and Baret, 1997). The obtained regression coefficients can be easily checked for plausibility and significance. Also, SMLR models can be easily implemented in standard (image) processing software.

The partial least squares regression (PLSR) unified in a simple and comprehensive manner the advantages of SMLR and PCR without owning their disadvantages: (1) due to the fact that PLSR is a "full spectrum" method, noise sensitivity was relatively small compared to SMLR and (2) since data compression into regression factors considers covariance to the desired biophysical variable(s), the first few PLSR derived regression factors had a closer relation to the variable of interest compared to PCR. This explains the more accurate results obtained through PLSR compared to SMLR and PCR. As this study only dealt with winter wheat crops the results are naturally restricted to this species. However, from theoretical considerations similar findings are expected for other plant species (Huang et al., 2004). A disadvantage of PLSR is that it is not yet implemented in all commercial (image) processing software packages.

It is known that several biophysical and biochemical variables determine the spectral signature of vegetation canopies (Asner, 1998; Baret, 1991). Thus, a simple 2-band combination cannot cancel out all possibly intervening confounding variables (Baret and Guyot, 1991). This was confirmed using the classical NDVI with bands located in the red and near-infrared (Tucker, 1979). Amongst all techniques, the NDVI yielded the highest cross-validated RMSE, more than 3-times higher than what was obtained from PLSR. Problems with the NDVI relate mainly to the location of the band in the red spectral range, near to the chlorophyll absorption maximum. The use of the red band increases sensitivity to low canopy LAI and low leaf chlorophyll contents (Baret and Guyot, 1991). With the present study, however, we investigated relatively dense canopies (mean LAI of 5.1) with 'normal' leaf chlorophyll contents (around 50 $\mu g\,cm^{-2}$). Thus, the classical NDVI saturated quickly explaining the poor performance of this widely used indicator. The same argumentation explains the higher accuracies obtained by the NDVI optimized for mapping the leaf chlorophyll content (Zhao et al., 2007). Indeed, with this index one band is still located on the near-infrared shoulder (at 925 nm). However, the second band is located at 710 nm and thus in the red-edge where the chlorophyll absorption is strongly reduced compared to the red wavelength. This increases the sensitivity of the index to the canopy chlorophyll content and explains the relatively good results obtained in this study.

Concerning the optimized NDVI it has however to be considered that the relatively good results were only possible using an exponential fit, whereas all other techniques relied on linear transformations. This is a disadvantage of the method as the use of an exponential relation can lead to situations where an observed vegetation index is higher than the fitted (infinite) value ($NDVI_\infty$ in Eq. (3)). In this case the inverse of the relation is *Inf* requesting a user-defined input. This also happened in this study, where one left-out sample was higher than the fitted ND_∞.

6. Conclusions

To make full use of hyperspectral data suitable techniques have to be used. The techniques must deal efficiently with the strong multi-collinearity present in the spectral data and should not be too sensitive to sensor noise. Our study assessed the spectroradiometric prediction of the canopy chlorophyll content as a proxy for the canopy photosynthetic activity. Three commonly used chemometric techniques were assessed in a jackknife procedure and applied to reference observations collected in a multi-site and multi-date field campaign. The results demonstrated that the two objectives can be well met using partial least square regression (PLSR). Compared to principal component regression (PCR) and stepwise multiple linear regression (SMLR), PLSR showed the lowest cross-validated RMSE while being relatively insensitive to artificial (white) noise. PLSR also clearly outperformed a chlorophyll optimized vegetation index that was used as a baseline approach. The advantage of the latter is that it is easily implemented in standard (image) processing software. On the contrary, many

software packages do not yet include routines for calibrating and applying PLSR models.

The current study focused on the three most widely used chemometric techniques plus one well known vegetation index. The next step consists in assessing the impact of feature selection and to test some newer techniques such as SVM (support vector machines) and non-linear approaches based on artificially neural nets (NN). To confirm the findings for a broader range of species and environments, a simulation experiment based on synthetic spectra generated by physically-based radiative transfer models will be conducted.

Acknowledgements

The funding provided by the German Research Foundation and the University of Trier is acknowledged. Thanks to the colleagues from University of Trier who helped in acquiring the field data.

References

Asner, G.P., 1998. Biophysical and biochemical sources of variability in canopy reflectance. Remote Sensing of Environment 64, 234–253.

Asner, G.P., Heidebrecht, K.B., 2002. Spectral unmixing of vegetation, soil and dry carbon cover in arid regions: comparing multispectral and hyperspectral observations. International Journal of Remote Sensing 23, 3939–3958.

Atzberger, C., 2004. Object-based retrieval of biophysical canopy variables using artificial neural nets and radiative transfer models. Remote Sensing of Environment 93, 53–67.

Atzberger, C., Richter, K., 2009. Geostatistical regularization of inverse models for the retrieval of vegetation biophysical variables. Proceedings of SPIE 7478, 74810, doi:10.1117/12.830009.

Bacour, C., Baret, F., Beal, D., Weiss, M., Pavageau, K., 2006. Neural network estimation of LAI, fAPAR, fCover and LAI × Cab, from top of canopy MERIS reflectance data: principles and validation. Remote Sensing of Environment 105, 313–325.

Baret, F., 1991. Vegetation canopy reflectance: factors of variation and application for agriculture. In: Hunt, D. (Ed.), Physical Measurements and Signatures in Remote Sensing. Courchevel, France, pp. 145–167.

Baret, F., Buis, S., 2008. Estimating canopy characteristics from remote sensing observations. Review of methods and associated problems. In: Liang, S. (Ed.), Advances in Land Remote Sensing: System, Modeling, Inversion and Application. Springer, Netherlands, pp. 172–301.

Baret, F., Fourty, T., 1997. Radiometric estimates of nitrogen status of leaves and canopies. In: Lemaire, G. (Ed.), Diagnosis of Nitrogen Status in Crops. Heidelberg, Springer-Verlag, Germany, pp. 201–227.

Baret, F., Guyot, G., 1991. Potentials and limits of vegetation indices for LAI and APAR assessment. Remote Sensing of Environment 35, 161–173.

Baret, F., Houles, V., Guerif, M., 2007. Quantification of plant stress using remote sensing observations and crop models: the case of nitrogen management. Journal of Experimental Botany 58, 869–880.

Baret, F., Weiss, M., Troufleau, D., Prévot, L., Combal, B., 2000. Maximum information exploitation for canopy characterisation by remote sensing. Aspects of Applied Biology 60 – Remote Sensing in Agriculture, 71–82.

Baumgardner, M.F., Silva, L.F., Biehl, L.L., Stoner, E., 1985. Reflectance properties of soils. Advances in Agronomy 38, 1–44.

Beebe, K.R., Kowalski, B.R., 1987. An introduction to multivariate calibration and analysis. Analytical Chemistry 59 (17), 1007–1017.

Biewer, S., Fricke, T., Wachendorf, M., 2009. Development of canopy reflectance models to predict forage quality of legume–grass mixtures. Crop Science 49, 1917–1926.

Blackburn, G.A., 2007. Hyperspectral remote sensing of plant pigments. Journal of Experimental Botany 58, 855–867.

Breda, N.J.J., 2003. Ground-based measurements of leaf area index: a review of methods, instruments and current controversies. Journal of Experimental Botany 54, 2403–2417.

Broge, N.H., Leblanc, E., 2001. Comparing prediction power and stability of broadband and hyperspectral vegetation indices for estimation of green leaf area index and canopy chlorophyll density. Remote Sensing of Environment 76, 156–172.

Broge, N.H., Mortensen, J.V., 2002. Deriving green crop area index and canopy chlorophyll density of winter wheat from spectral reflectance data. Remote Sensing of Environment 81, 45–57.

Camps-Valls, G., Bruzzone, L., Rojo-Álvarez, J.L., Melgani, F., 2006. Robust support vector regression for biophysical variable estimation from remotely sensed images. IEEE Geoscience and Remote Sensing Letters 3, 339–343.

Chatterjee, S., Price, B., 1977. Regression Analysis by Example. Wiley, New York.

Chaurasia, S., Dadhwal, V.K., 2004. Comparison of principal component inversion with VI-empirical approach for LAI estimation using simulated reflectance data. International Journal of Remote Sensing 25, 2881–2887.

Cho, M., Skidmore, A., Atzberger, C., 2008. Towards red-edge positions less sensitive to canopy biophysical parameters for leaf chlorophyll estimations using properties optique spectrales des feuilles (PROSPECT) and scattering by arbitrarily inclined leaves (SAILH) simulated data. International Journal of Remote Sensing 29, 2241–2255.

Cho, M.A., Skidmore, A., Corsi, F., van Wieren, S.E., Sobhan, I., 2007. Estimation of green grass/herb biomass from airborne hyperspectral imagery using spectral indices and partial least squares regression. International Journal of Applied Earth Observation and Geoinformation 9, 375–391.

Cho, M.A., Mathieu, R., Ramoelo, A., Main, R., Asner, G., Atzberger, C., submitted for publication. Quantifying shifts in the spectral red edge using spectral angle measure (SAM) for canopy chlorophyll concentration. Remote Sensing of Environment.

Clevers, J.G.P.W., Van Der Heijden, G.W.A.M., Verzakov, S., Schaepman, M.E., 2007. Estimating grassland biomass using SVM band shaving of hyperspectral data. Photogrammetric Engineering and Remote Sensing 73, 1141–1148.

Cocks, T., Jenssen, R., Stewart, I., Willson, I., Shields, T., 1998. The HyMap(TM) airborne hyperspectral sensor: the system, calibration and performance. In: Schaepman, M., Schlapfer, D., Itten, K. (Eds.), Proceedings 1st EARSeL Workshop on Imaging Spectroscopy. Zürich, Switzerland, pp. 37–42.

Cohen, W.B., Maiersperger, T.K., Gower, S.T., Turner, D.P., 2003. An improved strategy for regression of biophysical variables and Landsat ETM+ data. Remote Sensing of Environment 84 (4), 561–571.

Combal, B., Baret, F., Weiss, M., 2002. Improving canopy variables estimation from remote sensing data by exploiting ancillary information. Case study on sugar beet canopies. Agronomie 22, 2–15.

Combal, B., Baret, F., Weiss, M., Trubuil, A., Macé, D., Pragnère, A., Myneni, R., Knyazikhin, Y., Wang, L., 2003. Retrieval of canopy biophysical variables from bidirectional reflectance using prior information to solve the ill-posed inverse problem. Remote Sensing of Environment 84, 1–15.

Cox, S., 2002. Information technology: the global key to precision agriculture and sustainability. Computers and Electronics in Agriculture 36, 93–111.

Cramer, J.A., Kramer, K.E., Johnson, K.J., Morris, R.E., Rose-Pehrsson, S.L., 2008. Automated wavelength selection for spectroscopic fuel models by symmetrically contracting repeated unmoving window partial least squares. Chemometrics and Intelligent Laboratory Systems 92, 13–21.

Curran, P.J., 1994. Imaging spectrometry. Progress in Physical Geography 18, 247–266.

Darvishzadeh, R., Atzberger, C., van Wieren, S., Skidmore, A., 2008a. Estimation of vegetation LAI from hyperspectral reflectance data: effects of soil type and plant architecture. International Journal of Applied Earth Observation and Geoinformation 10, 358–373.

Darvishzadeh, R., Skidmore, A.K., Schlerf, M., Atzberger, C., 2008b. Inversion of a radiative transfer model for estimating vegetation LAI and chlorophyll in a heterogeneous grassland. Remote Sensing of Environment 112, 2592–2604.

Darvishzadeh, R., Skidmore, A.K., Schlerf, M., Atzberger, C., Corsi, F., Cho, M.A., 2008c. LAI and chlorophyll estimated for a heterogeneous grassland using hyperspectral measurements. ISPRS Journal of Photogrammetry and Remote Sensing 63, 409–426.

Darvishzadeh, R., Atzberger, C., Skidmore, A.K., Abkar, A.A., 2009. Leaf area index derivation from hyperspectral vegetation indices and the red edge position. International Journal of Remote Sensing 30 (23), 6199–6218.

Darvishzadeh, R., Atzberger, C., Schlerf, M., Skidmore, A.K., in press Mapping vegetation leaf area index with airborne hyperspectral imagery in a Mediterranean grassland: from statistical models to inversion of radiative transfer models. Remote Sensing of Environment.

Dawson, T.P., Curran, P.J., Plummer, S.E., 1998. LIBERTY – modeling the effects of leaf biochemical concentration on reflectance spectra. Remote Sensing of Environment 65, 50–60.

Demetriades-Shah, T.H., Steven, M.D., Clark, J.A., 1990. High resolution derivative spectra in remote sensing. Remote Sensing of Environment 33, 55–64.

Duckworth, J., 1998. Spectroscopic quantitative analysis. In: Workman, J., Springsteen, A.W. (Eds.), Applied Spectroscopy. A Compact Reference for Practitioners. Academic Press, San Diego, pp. 93–164.

Durbha, S.S., King, R.L., Younan, N.H., 2007. Support vector machines regression for retrieval of leaf area index from multiangle imaging spectroradiometer. Remote Sensing of Environment 107, 348–361.

Efron, B., Gong, G., 1983. A leisurely look at the bootstrap, the jackknife, and cross-validation. The American Statistician 37, 36–48.

Farifteh, J., Van der Meer, F., Atzberger, C., Carranza, E.J.M., 2007. Quantitative analysis of salt-affected soil reflectance spectra: a comparison of two adaptive methods (PLSR and ANN). Remote Sensing of Environment 110, 59–78.

Filella, I., Penuelas, J., 1994. The red edge position and shape as indicators of plant chlorophyll content, biomass and hydric status. International Journal of Remote Sensing 15, 1459–1470.

Fourty, T., Baret, F., 1997. Vegetation water and dry matter contents estimated from top-of-the-atmosphere reflectance data: a simulation. Remote Sensing of Environment 61, 34–45.

Geladi, P., Kowalski, B.R., 1986. Partial least-squares regression: a tutorial. Analytica Chimica Acta 185, 1–17.

Gobron, N., 1997. Theoretical limits to the estimation of the leaf area index on the basis of visible and near-infrared remote sensing data. IEEE Transactions on Geoscience and Remote Sensing 35, 1438–1445.

Goel, N.S., 1987. Models of vegetation canopy reflectance and their use in estimation of biophysical parameters from reflectance data. Remote Sensing Reviews 4, 1–112.

Grossman, Y.L., Ustin, S.L., Jacquemoud, S., Sanderson, E.W., Schmuck, G., Verdebout, J., 1996. Critique of stepwise multiple linear regression for the extraction

of leaf biochemistry information from leaf reflectance data. Remote Sensing of Environment 56, 182–193.
Guérif, M., Houlès, V., Baret, F., 2007. Remote sensing and detection of nitrogen status in crops. Application to precise nitrogen fertilization. In: Proceedings 4th International Symposium on Intelligent Information Technology in Agriculture, Beijing, China.
Haboudane, D., Miller, J.R., Pattey, E., Zarco-Tejada, P.J., Strachan, I.B., 2004. Hyperspectral vegetation indices and novel algorithms for predicting green LAI of crop canopies: modeling and validation in the context of precision agriculture. Remote Sensing of Environment 90, 337–352.
Hansen, P.M., Schjoerring, J.K., 2003. Reflectance measurement of canopy biomass and nitrogen status in wheat crops using normalized difference vegetation indices and partial least squares regression. Remote Sensing of Environment 86, 542–553.
Hatfield, J.L., Pinter Jr., P.J., 1993. Remote sensing of crop protection. Crop Protection 12, 403–413.
Houborg, R., Boegh, E., 2008. Mapping leaf chlorophyll and leaf area index using inverse and forward canopy reflectance modeling and SPOT reflectance data. Remote Sensing of Environment 112, 186–202.
Houleš, V., Gueïrif, M., Mary, B., 2007. Elaboration of a nitrogen nutrition indicator for winter wheat based on leaf area index and chlorophyll content for making nitrogen recommendations. European Journal of Agronomy 27, 1–11.
Huang, Z., Turner, B.J., Dury, S.J., Wallis, I.R., Foley, W.J., 2004. Estimating foliage nitrogen concentration from HYMAP data using continuum removal analysis. Remote Sensing of Environment 93, 18–29.
Im, J., Jensen, J.R., 2008. Hyperspectral remote sensing of vegetation. Geography Compass 2/6, 1943–1961.
Jackson, J.E., 1991. A User's Guide to Principal Components. Wiley, New York.
Jacquemoud, S., Bacour, C., Poilvé, H., Frangi, J.-P., 2000. Comparison of four radiative transfer models to simulate plant canopies reflectance: direct and inverse mode. Remote Sensing of Environment 74, 471–481.
Jacquemoud, S., Baret, F., Hanocq, J.F., 1992. Modeling spectral and bidirectional soil reflectance. Remote Sensing of Environment 41, 123–132.
Jacquemoud, S., Baret, F., 1990. PROSPECT: a model of leaf optical properties spectra. Remote Sensing of Environment 34, 75–91.
Jacquemoud, S., Baret, F., Andrieu, B., Danson, M., Jaggard, K., 1995a. Extraction of vegetation biophysical parameters by inversion of the PROSPECT + SAIL models on sugar beet canopy reflectance data. Application to TM and AVIRIS sensors. Remote Sensing of Environment 52, 163–172.
Jacquemoud, S., Verdebout, J., Schmuck, G., Andreoli, G., Hosgood, B., 1995b. Investigation of leaf biochemistry by statistics. Remote Sensing of Environment 54, 180–188.
Jacquemoud, S., Verhoef, W., Baret, F., Bacour, C., Zarco-Tejada, P.J., Asner, G.P., François, C., Ustin, S.L., 2009. PROSPECT + SAIL models: a review of use for vegetation characterization. Remote Sensing of Environment 113 (Suppl. 1), S56–S66.
Jago, R.A., Cutler, M.E.J., Curran, P.J., 1999. Estimating canopy chlorophyll concentration from field and airborne spectra. Remote Sensing of Environment 68, 217–224.
Jensen, T., Apan, A., Young, F., Zeller, L., 2007. Detecting the attributes of a wheat crop using digital imagery acquired from a low-altitude platform. Computers and Electronics in Agriculture 59, 66–77.
Kalácska, M., Sánchez-Azofeifa, G.A., Caelli, T., Rivard, B., Boerlage, B., 2005. Estimating leaf area index from satellite imagery using Bayesian networks. IEEE Transactions on Geoscience and Remote Sensing 43, 1866–1873.
Knox, N.M., Skidmore, A.K., Schlerf, M., De Boer, W.F., Van Wieren, S.E., Van der Waal, C., Prins, H.H.T., Slotow, R., 2010. Nitrogen prediction in grasses: effect of bandwidth and plant material state on absorption feature selection. International Journal of Remote Sensing 31 (3), 691–704.
Kuusk, A., 1991. The hot spot effect in the leaf canopy. In: Digest – International Geoscience and Remote Sensing Symposium (IGARSS), vol. 3, pp. 1555–1557.
le Maire, G., François, C., Soudani, K., Berveiller, D., Pontailler, J.-Y., Bréda, N., Genet, H., Dufrêne, E., 2008. Calibration and validation of hyperspectral indices for the estimation of broadleaved forest leaf chlorophyll content, leaf mass per area, leaf area index and leaf canopy biomass. Remote Sensing of Environment 112, 3846–3864.
Li, H., Liang, Y., Xu, Q., 2009. Support vector machines and its application in chemistry. Chemometrics and Intelligent Laboratory Systems 95 (2), 188–198.
Lee, K.-S., Cohen, W.B., Kennedy, R.E., Maiersperger, T.K., Gower, S.T., 2004. Hyperspectral versus multispectral data for estimating leaf area index in four different biomes. Remote Sensing of Environment 91, 508–520.
Maier, S.W., Luedeker, W., Guenther, K.P., 1999. SLOP: a revised version of the stochastic model for leaf optical properties. Remote Sensing of Environment 68, 273–280.
Markwell, J., Osterman, J.C., Mitchell, J.L., 1995. Calibration of Minolta SPAD-502 leaf chlorophyll meter. Photosynthetic Research 46, 467–472.
Martens, H., Naes, T., 1987. Multivariate calibration by data compression. In: Williams, Norris (Eds.), Near-Infrared Technology in Agriculture and food industries. Americal Association of Cereal Chemists, MS, pp. 57–87.
Mas, J.F., Flores, J.J., 2008. The application of artificial neural networks to the analysis of remotely sensed data. International Journal of Remote Sensing 29, 617–663.
McDonald, M., 2003. Photobiology of Higher Plants. John Wiley, Chichester, West Sussex, England.
Minolta, 2003. Chlorophyll Meter SPAD-502: Instruction Manual. Minolta Camera BeNeLux BV, Maarssen, The Netherlands.
Moran, S.M., Inoue, Y., Barnes, E.M., 1997. Opportunities and limitations for image-based remote sensing in precision crop management. Remote Sensing of Environment 61, 319–346.
Nguyen, H.T., Lee, B.-W., 2006. Assessment of rice leaf growth and nitrogen status by hyperspectral canopy reflectance and partial least square regression. European Journal of Agronomy 24, 349–356.
Potter, C.S., Klooster, S., Brooks, V., 1999. Interannual variability in terrestrial net primary production: exploration of trends and controls on regional to global. Ecosystems 2, 36–48.
Richter, K., Atzberger, C., Vuolo, F., Weihs, P., D'Urso, G., 2009. Experimental assessment of the Sentinel-2 band setting for RTM-based LAI retrieval of sugar beet and maize. Canadian Journal of Remote Sensing 35, 230–247.
Richter, K., Atzberger, C., Vuolo, F., D'Urso, G., in press. LAI retrieval accuracy for wheat, sugar beet and maize from future ESA Sentinel-2 data. IEEE Journal of Selected Topics in Applied Earth Observation and Remote Sensing.
Rondeaux, G., 1995. Vegetation monitoring by remote sensing: a review of biophysical indices. Photo-Interpretation 3, 197–216.
Savitzky, A., Golay, M.J.E., 1964. Smoothing and differentation of data by simplified least square procedure. Analytical Chemistry 36, 1627–1638.
Schlerf, M., Atzberger, C., 2006. Inversion of a forest reflectance model to estimate structural canopy variables from hyperspectral remote sensing. Remote Sensing of Environment 100, 281–294.
Schlerf, M., Atzberger, C., Hill, J., 2005. Remote sensing of forest biophysical variables using HyMap imaging spectrometer data. Remote Sensing of Environment 95, 177–194.
Schlerf, M., Atzberger, C., Hill, J., Buddenbaum, H., Werner, W., Schueler, G., 2010. Retrieval of chlorophyll and nitrogen in Norway spruce (*Picea abies* L. Karst.) using imaging spectroscopy. International Journal of Applied Earth Observation and Geoinformation 12, 17–26.
Schueller, J.K., 1992. A review and integrating analysis of spatially-variable control of crop production. Fertilizer Research 33, 1–34.
The Mathworks, 2007. Matlab 7 (Computer Program). The Mathworks, Natick, MA.
Thenkabail, P.S., Smith, R.B., De-Pauw, E., 2002. Hyperspectral vegetation indices and their relationships with agricultural crop characteristics. Remote Sensing of Environment 71, 158–182.
Tucker, C.J., 1979. Red and photographic infrared linear combinations for monitoring vegetation. Remote Sensing of Environment 8, 127–150.
Udelhoven, T., Emmerling, C., Jarmer, T., 2003. Quantitative analysis of soil chemical properties with diffuse reflectance spectrometry and partial-least-square regression. Plant and Soil 251, 319–329.
Verhoef, W., 1984. Light scattering by leaf layers with application to canopy reflectance modeling: the SAIL model. Remote Sensing of Environment 16, 125–141.
Verhoef, W., Bach, H., 2007. Coupled soil-leaf-canopy and atmosphere radiative transfer modeling to simulate hyperspectral multi-angular surface reflectance and TOA radiance data. Remote Sensing of Environment 109, 166–182.
Widlowski, J.-L., Taberner, M., Pinty, B., Bruniquel-Pinel, V., Disney, M., Fernandes, R., Gastellu-Etchegorry, J.-P., Xie, D., 2007. Third Radiation Transfer Model Intercomparison (RAMI) exercise: documenting progress in canopy reflectance models. Journal of Geophysical Research D: Atmospheres, 112 (art. no. D09111).
Williams, P.C., Norris, K.H., 1987. Near-Infrared Technology in the Agricultural and Food Industries. American Association of Cereal Chemists, St. Paul, Minnesota, USA.
Wold, S., Sjöström, M., Eriksson, L., 2001. PLS-regression: a basic tool of chemometrics. Chemometrics and Intelligent Laboratory Systems 58, 109–130.
Xu, H., Liu, Z., Cai, W., Shao, X., 2009. A wavelength selection method based on randomization test for near-infrared spectral analysis. Chemometrics and Intelligent Laboratory Systems 97, 189–193.
Yang, F., Li, J., Gan, X., Qian, Y., Wu, X., Yang, Q., 2010. Assessing nutritional status of Festuca arundinacea by monitoring photosynthetic pigments from hyperspectral data. Computers and Electronics in Agriculture 70, 52–59.
Ye, X., Sakai, K., Okamoto, H., Garciano, L.O., 2008. A ground-based hyperspectral imaging system for characterizing vegetation spectral features. Computers and Electronics in Agriculture 63, 13–21.
Yoder, B.J., Pettigrew-Crosby, R.E., 1995. Predicting nitrogen and chlorophyll content and concentration from reflectance spectra (400–2500 nm) at leaf and canopy scales. Remote Sensing of Environment 53, 199–211.
Zhao, D., Huang, L., Li, J., Qi, J., 2007. A comparative analysis of broadband and narrowband derived vegetation indices in predicting LAI and CCD of a cotton canopy. ISPRS Journal of Photogrammetry and Remote Sensing 62, 25–33.
Zhao, D.H., Li, J.L., Qi, J.G., 2005. Identification of red and NIR spectral regions and vegetative indices for discrimination of cotton nitrogen stress and growth stage. Computers and Electronics in Agriculture 48, 155–169.