Wheat and maize monitoring based on ground spectral measurements and multivariate data analysis

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Abstract. Improved accuracy in the retrieval of crop biophysical variables is needed to enable a greater contribution of hyperspectral remote sensing data to site-specific crop management. One season of maize and two seasons of wheat field experiments were used to explore the potential of multivariate data analysis for retrieving crop biophysical variables from spectroscopic data. Canopy spectral data at 350–2500 nm were collected during the experiments, in which various seeding densities, fertilization, and irrigation treatments were applied to generate dry biomass, water-content and nitrogen-content variability. Partial least squares (PLS) models that considered the reflectance derivatives (1^{st} and 2^{nd}) and that used only significant wavelengths were evaluated. As the measurements were conducted throughout the whole season, a wide variability was observed, which was critical for obtaining a good calibration model. The use of derivatives and selection of the most significant wavelengths were found to be the best pre-processing methodologies to increase prediction accuracy. Significant predictive power was achieved for the validation dataset, especially for the wheat dry biomass (R^2 ~0.75), for which similar results were obtained, even with data from a different season (R^2 ~0.70). PLS-predicted wheat water content had a correlation of R^2 ~0.60 with the measured values. An advantage was found in the use of PLS models, compared to common vegetation indices. Based on ground spectral measurements, this study confirms the potential of multivariate-data-analysis procedures for the interpretation of hyperspectral remote sensing data.

1 INTRODUCTION

Until recent years, earth observation sensors were not adapted to field-scale monitoring, due to their relatively low spatial resolution, coarse spectral resolution (too broad and too few bands) and low revisit frequency. Therefore, the use of remote sensing technologies was mainly limited to land-use and land-cover studies on regional and continental scales. Recently, satellites with higher spatial and spectral resolutions have been launched and, together with an increasing use of site-specific crop-management technologies [1], they provide a reliable and effective remotely sensed source of information for agriculture. However, commonly used spectral vegetation indices (VIs), such as the Normalized Difference Vegetation Index (NDVI) and other broadband-combinations, have limitations for high biomass, dense cover, high leaf area index (LAI) and/or high chlorophyll values [2-4]. Under these conditions, the aforementioned biophysical variables rapidly reach their maximum values without showing subtle differences among crops (a situation referred to as "saturation constraint"). This problem is crucial when relating, for example, a wide range of biomass measurements with a VI, limiting the prediction of high biomass values [5]. For site-specific-management applications, such as identifying water, nutritional, and/or other stresses after full crop coverage, this "saturation constraint" represents a critical limitation for the use of VIs. The NDVI, for example, saturates when LAI reaches values between 2 and 3 [2]. This LAI value may already be reached after just two months of the wheat-growing season.

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Consequently, alternative methods for the retrieval of biophysical variables under intensive growth conditions are needed. The partial least squares regression (PLS) is a full-spectrum analytical method that has shown good performance in retrieving biophysical variables from forests and field crops using hyperspectral reflectance data [6-10]. One of the basic advantages of the PLS regression over general multiple linear regression is that it can analyze data with strongly co-linear (correlated), noisy and numerous predictor variables [11]. This method is based on reducing the entire spectrum to a series of independent variables, called "latent factors" or "principal components", which are extracted from a matrix of spectral and biophysical variables. Latent factors represent the relevant structural information that is presented in the reflectance measurements and are used to predict the dependent variable [11-13]. This methodology has been widely used in laboratory spectroscopy for chemical and quality characterization of different crops and/or products [12, 14-16]. It has also been used for the identification of spectral differences in ground foliage samples among conifer species, showing better accuracy than other multivariate techniques, such as discriminant analysis [17].

In field crops, PLS models based on reflectance measurements of fresh wheat leaves have shown very promising results in the prediction of leaf water and nitrogen (N) content [18]. By considering the reflectance values as the predictive variables, PLS models identify relevant structural information from the complete spectrum, offering a clear advantage over the use of only certain wavelengths by VIs. In comparison to the latter, PLS models can take into consideration the linear response of near infrared (NIR) reflectance to increases in LAI [19, 20]. Accurate predictions of both biomass and N content were obtained by PLS models from canopy reflectance data of a rice crop, which reached an LAI of 9 [7]. In winter wheat, Hansen and Schjoerring [4] achieved an additional increase in the biomass and N predictive power of hyperspectral data, by using PLS models and found that the models gave better results than VIs.

The main objective of the present study was to explore the suitability of PLS models, by using ground spectral measurements, as a potential tool for spaceborne applications. Specifically, this work was focused on: (1) investigating PLS models for the retrieval of crop biomass, water, and N contents from canopy spectral field measurements; and (2) exploring the best data pre-processing method (e.g., detection of outliers or application of derivatives) and determining the most significant wavelengths to the models.

2 MATERIALS AND METHODS

The study was performed between 2003 and 2005 at the Gilat Research Center, located at 31°21' N, 34°41' E, at an average elevation of 150 m. This semi-arid area is characterized by a mean annual rainfall of 237 mm [21] but also by high inter-annual rainfall variability. This phenomenon is clearly evidenced in the current research, since 190 and 330 mm fell in the 2003/04 and 2004/05 growing seasons, respectively. In order to implement the research objectives, experiments were carried out in one maize and two wheat fields, including a wide range of seeding densities, irrigation and N-fertilization treatments. All experiments included spectral measurements and biophysical characterizations of the crop. Sample collection and subsequent laboratory analyses were performed no more than 2 hours after the spectral measurements had been taken.

2.1 Experimental design

Maize (*Zea may*s L.) was planted in 96 cm-wide north-south rows with 10 cm between plants. It was grown under six N-fertilization levels (0, 50, 100, 200, 400 and 600 kg N ha^{-1}) that were applied before seeding. This extreme range of fertilization levels was used in order to create stress due to both nitrogen deficit and excess. The experiment was laid out in a randomized complete-block design with four replicates, in plots measuring 6×24 m each. Two sprinkler irrigation lines were placed 12 m apart along all of the experimental plots, leaving a 6-m border and an effective measurable area of 72 m^2 in each plot. Complete emergence was registered on 12 May 2003, which was designated as the starting point for counting days after emergence (DAE). Irrigation was adjusted to

match a Class A evaporation pan. Two replicates were irrigated only until 52 DAE, receiving a total of 400 mm during the growth season. The other replicates received 60 mm extra until the end of the experiment. During the season, nine sets of measurements were performed, on 13, 21, 27, 31, 43, 48, 56, 63, and 66 DAE.

For both wheat experiments (2003/04 and 2004/05 seasons), spring wheat (*Triticum aestivum* L. cultivar 'Galil') was grown under three treatment factors, each at two levels: rainfed vs. irrigated; seeding at 210 vs. 630 plants per m^2 (2 east-west seeding paths and 1 north-south path); and pre-sowing N fertilization at 0 vs. 50 kg ha^{-1}. The seeding was performed at 18 cm between rows, together with an additional homogeneous basic fertilization of 50 kg N ha^{-1}. The experiments for each water treatment were laid out in 6×16 m plots in a split-strip-block design, with three replicates. During the first season, emergence was registered on 15 Dec. 2003 and heading on 5 Mar. 2004 (DAE 81). Nine measurements were performed during that season, on 6, 16, 21, 34, 45, 59, 72, 84, and 97 DAE. In the second season, emergence was registered on 24 Nov. 2004 and heading on 17 Feb. 2005 (DAE 85). Since the second season was rainy and included many cloudy days that impeded the performance of several instruments, only six sets of measurements were collected, on 12, 27, 47, 54, 63, and 91 DAE. Results from the maize experiment and the two wheat experiments were considered thereafter as three independent datasets. A fourth dataset was established by combining all the wheat data from the 2003/04 and 2004/05 seasons. Combining these two datasets increased the range of biophysical variables and spectral responses, a procedure that was expected to improve the quality of the model.

2.2 Spectral measurements

Canopy radiance was measured with a portable FieldSpec Pro FR spectroradiometer, Analytical Spectral Devices [22], with a spectral range of 350 to 2,500 nm and a 25° field of view (FOV). The spectral resolution was interpolated homogeneously to 2 nm and the water absorption regions (1,350-1,420 nm and 1,800-1,960 nm) were eliminated before analysis. Spectral reflectance was obtained after periodical radiance measurements, using a standard white reference panel (Spectralon Labsphere Inc.). Reflectance data were collected at solar noon ±1 h, under clear sky conditions, in a nadir orientation. The spectrometer was programmed to take 20 readings from each sampling point, automatically saving the average. Each measurement at each sampling date was collected from a different homogeneous point in each plot.

In the maize experiment, throughout the first half of the season, the measurements were performed using a ladder, keeping a sensor-canopy distance of around 1.5 m. Taking into consideration planting pattern, measurement configuration and equipment optics, the FOV included less than a complete theoretical row at canopy surface. According to Daughtry et. al. [23], this generates a problem regarding the variability of the calibration data, given the fact that different percentage of soil coverage would be included in the instantaneous field of view (IFOV). However, due to the plants' size during this period, and the fact that the measurements were performed exactly over the row, the IFOV did include a complete plant while the soil percentage changed considerably. From 31 DAE onwards, the sensor-canopy distance decreased gradually, thus including less than a full row, until the end of the measurements. The spectral measurements of the 63 DAE were performed from a crane at a height of 6 meters above the canopy, therefore including 2.6 complete theoretical rows.

In the wheat experiments, the sensor was held at a constant 1.5 m above the ground, corresponding to an IFOV that included a total of 3.7 rows, at wheat emergence. As the height of the crop increased throughout the season, the IFOV above the canopy was reduced proportionally, but included at least two complete rows during most of the season. Moreover, all treatments reached full coverage between the second and third measurements in both seasons.

2.3 Biophysical variables

Samples for the determination of biophysical variables (biomass, water and N content, and LAI) were collected from exactly the same locations where the canopy reflectances were measured. In the wheat experiments, the samples were collected within a 60×50 cm frame; in the maize experiment, the samples were taken from a 50-cm length in one row, corresponding to a ground area of approximately 96×50 cm. The dry biomass was measured after 48 h at 70°C. Water content was calculated from the fresh and dry weights. N content was determined by the micro-Kjeldhal method [24]. During the wheat experiments, prior to the reflectance measurements, three LAI measurements were collected with a ceptometer AccuPAR LP-80 [25], registering its average.

2.4 Multivariate data analysis

For the multivariate-data-analysis (MVDA) procedure, "The Unscrambler" version 8.0 software [26] was used to define different models and to predict biophysical data. These were considered to be the dependent variables, and the spectrum data the independent ones. For each experiment, this analysis was used to determine the best prediction of the biophysical variables by using PLS regression. These calculated models were obtained by using two-thirds of the dataset, randomly selected, as a calibration subset. For the fourth dataset, i.e., the combined wheat data from 2003/04 and 2004/05, the calibration set was defined by selecting two new thirds of the data from each season independently and combining them, so that the calibration set contained the same proportion of each season's data. The PLS analysis was applied to the reflectance (termed "raw data" from hereon in) and to the 1st and the 2nd derivatives (Savitzky Golay) of the reflectance. This process amplifies the "peakedness," which is considered advantageous for noisy and scattered data [12]. In each dataset, the outliers were designated for each variable as occurring when the relationship between the residuals of a specific sample was higher than 4% of the overall residual for the analyzed variable. They were then omitted. Finally, applying the Martens' uncertainty test [12, 27, 28] before and after outliers had been omitted, the most significant wavelengths were selected. This was applied to the raw reflectance data and to the first and second derivatives.

Taking into account all of the aforementioned procedures, 12 models were built for each variable. The statistics, root mean square errors of calibration (RMSEC) and prediction (RMSEP), and coefficient of determination (R^2) were used to compare each models across the various variables [26].

Validation was performed by predicting the remaining one-third of the dataset that formed the validation subset. For the wheat experiments, an extra validation was carried out by using the data from each season to predict the whole dataset of the other season.

2.5 Vegetation indices

Accuracy of the combined dataset (wheat 2003/04 and 2004/05) obtained by the PLS models was compared to several broadband and narrow-band VIs (Table 1).

Both linear and exponential correlation function were considered for the same calibration subset (two-thirds of the complete dataset) used for the PLS calibration. Using the coefficients of each function, the biophysical variables of the validation subset were calculated for each index. The statistics, RMSEP and R^2 were calculated.

Table 1. Vegetation indices

Vegetation indices	Formula	Reference
Normalized Difference Vegetation Index	$NDVI=\frac{R_{800-900}-R_{650-700}}{R_{800-900}+R_{650-700}}$	[29]
Green-NDVI	$GNDVI=\frac{R_{800-900}-R_{540-560}}{R_{800-900}+R_{540-560}}$	[30]
Normalized Difference Green vegetation Index	$NDGI=\frac{R_{540-560}-R_{650-700}}{R_{540-560}+R_{650-700}}$	[31]
Simple Ratio	$SR=\frac{R_{800-900}}{R_{650-700}}$	[32]
Soil Adjusted Vegetation Index	$SAVI=\frac{R_{800-900}-R_{650-700}}{R_{800-900}+R_{650-700}+0.5}(1+0.5)$	[33]
Transformed Chlorophyll Absorption in Reflectance Index	$TCARI=3\left[(R_{700}-R_{670})-0.2(R_{700}-R_{550})\cdot\left(R_{700}/R_{670}\right)\right]$	[34]
Optimized Soil-Adjusted Vegetation Index	$OSAVI=\frac{(1+0.16)(R_{800}-R_{670})}{(R_{800}+R_{670}+0.16)}$	[34]
Red-Edge Position	$REP\dagger=700+40\cdot\frac{R_{re}-R_{700}}{R_{740}-R_{700}}$	[35]
	R970 / 900	[36]
	R900 / 970	[36]
	R900 / 1450	[37]
	R900 / 1530	[38]
	R1080 / 1180	[38]
	R1080 / 1260	[38]
	R1180 / 2170	[38]
	R1260 / 1675	[38]

† R_{re} is the red-edge inflexion point that corresponds to the average between the reflectance at 670 and 780 nm.

3 RESULTS AND DISCUSSION

3.1 Biophysical measurements

The four analyzed variables varied within and between experiments. As expected, gradual increases in dry biomass and LAI were observed (Fig. 1a & 1b). The concurrent standard deviation increase is explained by the larger differentiation between the treatments throughout the season. Considering the coefficient of variations of the wheat experiments at each DAE, it is clear that the first season's variability was much higher than that of the second.

Water status of the crops and its variability were relatively stable during the first half of the season for the three experiments (Fig. 1c). However, from 70 DAE for the wheat and 50 DAE for the maize, the mean water content decreased and the standard deviation

increased, depicting the significant effects of the non-irrigated treatments in wheat, and the cessation of irrigation in maize.

Due to the increase in dry biomass throughout the season, the N content decreased systematically for the three experiments (Fig. 1d), although their standard deviation hardly changed during the growing season.

The difference in biomass development and water conditions between the two wheat seasons is accounted for by the differences in the amount and distribution of the rainfall. During the 2004/05 winter season, the 330 mm of rainfall was concentrated mainly at the beginning of the season, when the temperatures were still high, resulting in optimal growing conditions. By contrast, in the previous wheat season, there were only 190 mm of rainfall, uniformly distributed. This difference explains the fact that in the second wheat season, large quantities of biomass accumulated in a very short period of time. It also accounts for the difference in water content variation throughout the season.

As would be expected, the variability of the water content at each measurement date was much higher during the first wheat season than during the second, indicating that due to the lower rainfall influence, the agronomic treatments were much more evident in the drier season. The strong influence of the natural seasonal growth was confirmed by analyses of variance (data not shown), which revealed significant differences between the various dates for all the biophysical variables. The acquired variability represents the ideal scenario for the current purpose of spectral canopy characterizations.

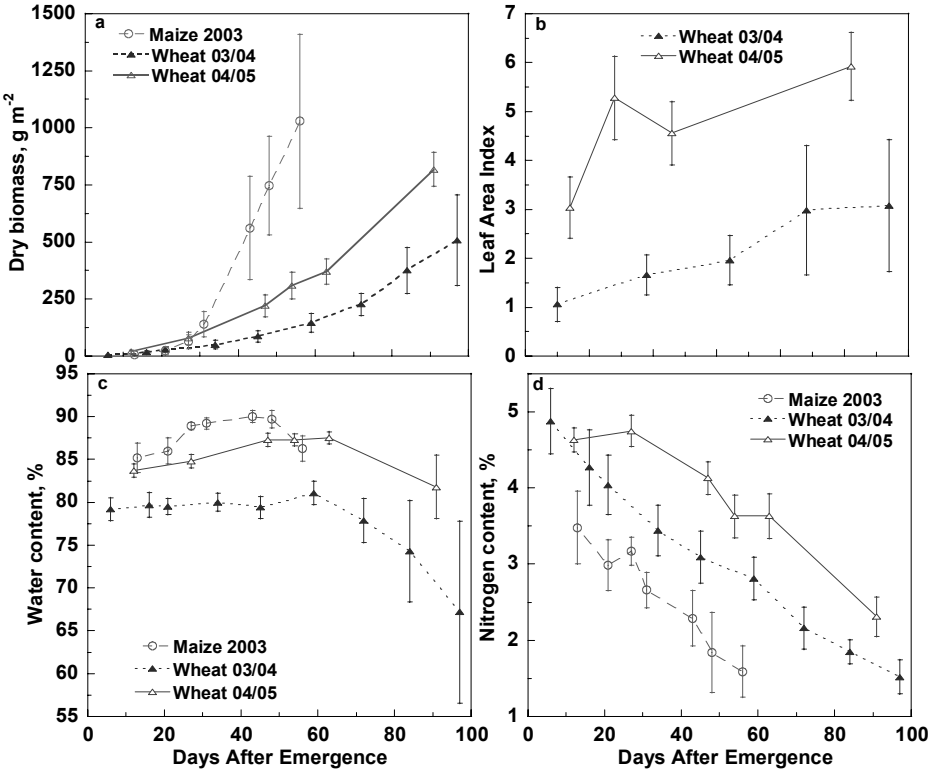

Fig. 1. Mean biophysical values for each experiment: (a) dry biomass; (b) leaf area index; (c) water content; and (d) N content. Error bars correspond to half standard deviation.

The wheat experiments were continued until harvest in both seasons, although there were no spectral measurements towards the end of the seasons. Yields ranged from 60 to 3,200 kg ha^{-1} during the 2003/04 experiment and from 1,600 to 8,100 kg ha^{-1} during the 2004/05 experiment. The very low yields in the first season corresponded to those treatments with high planting density and no supplemental irrigation, in which the plants were under severe water stress during the grain-filling period.

3.2 Spectral characterization

Many spectral measurements were collected during the maize and wheat experiments, covering a wide range of conditions from low to high coverage, and showing typically observed vegetation signatures in those conditions. A decrease in Short Wave Infrared (SWIR) reflectance was observed in the well-watered samples. This is attributed to a higher total water content in the sampled area that increased the amount of energy absorbed in this region of the spectrum [39, 40]. The spectral range was very similar in both maize and wheat experiments, unlike the difference in biomass and its variability between the crops (Fig. 1). This apparent contradiction is explained by the fact that the maize biomass considered the whole plant, although the stem does not actually contribute much to reflectance relative to its important role in biomass. This was especially critical from the middle of the season onwards.

3.3 MVDA calibration

For each of the biophysical variables in each of the four datasets, 12 PLS calibration models were built, in accordance with the respective data-pre-processing methods. Along with the model calculations, a preliminary validation procedure was performed. This full cross-validation process was used to select the best model according to their R^2 and RMSE values (Table 2). For the maize experiment, the data from the crane campaign (63 DAE) were put aside for validation purposes and not included in the calibration. The samples of 66 DAE were also excluded from the calibration, due to the major influence of the dry out on their spectrum. Therefore, neither were these data included in the analysis of the biophysical variables presented in Fig. 1.

Table 2†. Statistics of the best PLS models from calibration and validation datasets.

Model / Dataset	Dry biomass ($g\ m^{-2}$)			Water content (%)			N content (%)			LAI		
	n	R^2	RMSE	n	R^2	RMSE	n	R^2	*e*	n	R^2	RMSE
Maize 2003												
Model	d2 – O			d2 – S			d2 – S					
Calibration	79	0.92	104	88	0.80	1.01	87	0.80	0.32	N/D		
Validation	44	0.69	242	44	0.56	1.55	44	0.64	0.42			
Wheat 2003/04												
Model	d1 – O – S			d1 – O – S			d1 – O – S			d2 – O – S		
Calibration	107	0.96	35	108	0.90	1.50	115	0.91	0.31	84	0.90	0.39
Validation	69	0.92	45	69	0.82	2.50	69	0.85	0.40	69	0.72	0.63
Wheat 04/05	123	0.68	237	123	0.61	3.10	123	0.41	0.80	123	0.49	4.89
Wheat 2004/05												
Model	d2 – O – S			d1 – O – S			d1 – S			d2 – S		
Calibration	70	0.95	59	68	0.84	0.90	82	0.84	0.32	61	0.82	0.55
Validation	41	0.83	108	41	0.65	2.00	41	0.80	0.40	41	0.50	0.86
Wheat 03/04	207	0.05	190	207	0.63	6.30	207	0.64	1.40	207	0.18	1.54
Wheat 03/04 and 04/05												
Model	d2 – O – S			d1 – O – S			d1 – S			d2 – O – S		
Calibration	167	0.88	77	177	0.90	1.67	220	0.82	0.45	130	0.94	0.47
Validation	110	0.78	112	110	0.87	2.49	110	0.82	0.43	110	0.82	0.79

† Symbols and acronyms: d1 = 1st derivative; d2 = 2nd derivative; O = outlier exclusion; S = significant wavelengths exclusively; LAI = leaf area index; n = samples; RMSE = root mean square error (for calibration and validation); N/D = not determined.

For statistically analyzing the different pre-processing methodologies, a multiple ANOVA was applied to all the R^2 values of each model, experiment and biophysical variable. Although removing the outliers was not a significant factor by itself, its combination with the selection of the significant wavelengths improved the accuracy of

the models. As can be inferred from Table 2, samples identified as "outlier" for one variable, were not necessarily thus identified for the others. However, they were consistent between the analyzed variables. Taking the wheat 2003/04 season as an example, 31 samples were omitted as outliers for the dry weight model. Among them, 25 were also outliers for the 30 water content outliers and 19 for the nitrogen content outliers. This result confirms the observation that the methodology used for the outlier selection strongly takes into consideration the variation of the spectrum, but relates to the variation in the dependent variables.

Appropriate wavelength selection significantly improved the correlations in all variables, whereas derivatives and their interaction with selected wavelengths mainly improved the water-content estimation. Therefore, selecting variable-related wavelengths is a basic step towards improving the calibration model due to the enhancement of those ones that relate better with the parameter of interest, and the suppression of the noisier ones. The importance of using derivatives, especially for water content, lies in their suppression of the background spectrum, efficient separation of absorption features, enhancement of function peaks, and removal of confounding linear trends [17, 41, 42].

An analysis for the PLS models of the selected wavelengths of water and N content was performed, based on their weighted regression coefficients (Figs. 2 & 3). The weighted coefficients better illustrate the relative importance of each wavelength, because they take into consideration the influence of the absolute reflectance values on the regression coefficients. For each experiment, Fig. 2 presents the coefficients of those wavelengths that were selected, using the Marten's uncertainty test for the water-content models. Important regions for prediction of water content are those around 1,700, 2,000 and 2,300 nm, associated with water absorption regions [39, 40]. In addition, a certain aggregation of wavelengths in the NIR spectral region (around 900 nm and 1,300 nm) can be seen in the wheat experiments. This differs from the more scattered pattern of selected wavelengths of relatively equal importance in the maize experiment. The fact that the model considered for the maize experiment was based on the 2nd derivatives, which stress very subtle changes in the spectrum, accounts for this difference. The wavelength-aggregation issue might suggest that there was excessive use of hyperspectral data, in light of the achievement of similar performance with the use of broadbands. However, some of the coefficients among those wavelengths around 1,700 nm in the wheat 2003/04 experiment, and around 1,300 and 2,100 nm in the wheat 2004/05 experiment, have different signs (positive and negative). This explains the importance of using separate wavelengths rather than broadbands.

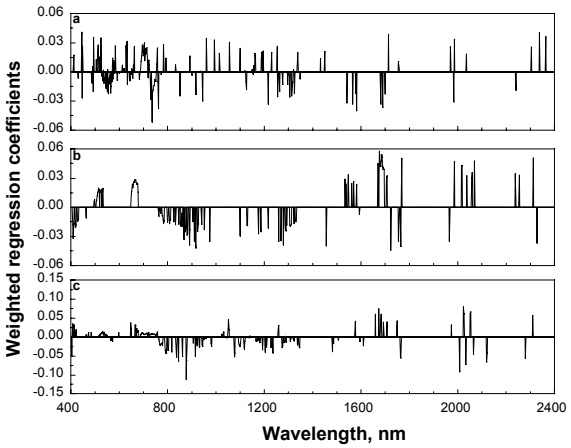

Fig. 2. Weighted regression coefficients of the significant wavelengths used for the selected water-content models. (a) Maize experiment; (b) Wheat 2003/04 experiment; (c) Wheat 2004/05 experiment.

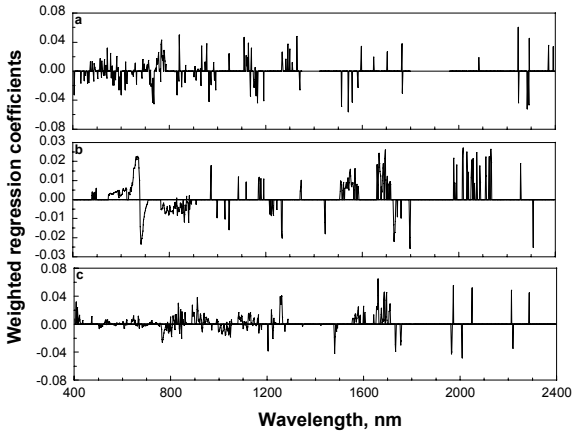

Fig. 3. Weighted regression coefficients of the significant wavelengths used for the selected N-content models. (a) Maize experiment; (b) Wheat 2003/04 experiment; (c) Wheat 2004/05 experiment.

The weighted regression coefficients of those wavelengths that were selected in each experiment for N-content prediction are presented in Fig. 3. For the maize experiment, almost all the visible wavelengths were included in the best model, which was based on the second derivatives. This is because the second derivatives showed almost no variability in the visible range. In the 2003/04 wheat experiment, groups of significant wavelengths can be noticed around 650 nm (red edge area), 1,500 nm, 1,700 nm, and 2,000 to 2,200 nm.

3.4 Validation of the PLS models

Statistics of every variable and every experiment are summarized in Table 2. It can be seen that the predictions of the biophysical variables for the wheat experiments are better than those for the maize experiment. These differences are attributed to the reduced contributions of the stem and lower leaves to the maize spectrum during the middle to late stages of development [19]. The reduced and variable canopy-sensor height in the maize measurements might also be marked as a source of error in the prediction of its biophysical variables from the spectral measurements. However, the fact that a complete plant was included in the IFOV during the first measurements and the fact that the viewing geometry was consistently above the row during the whole experiment, support the quality of this dataset. This was confirmed by data collected from the crane campaign (63 DAE).

Figure 4 presents the biomass predictions based on the same-season validation datasets. Figure 4a shows 3 samples of the maize crane measurements, which fit almost perfectly, confirming that the short sensor-canopy height represents only a minor source of error. The rest of the samples of this campaign were underestimated. This underestimation is explained by the fact that such high biomass samples were not included within the calibration dataset. Moreover, it could also be influenced by the inclusion of the stem in the total biomass measurement, which supports the conclusion that in order to represent the biomass that affects the spectrum, the stem and leaves need to be analyzed separately.

In the case of the wheat experiments, the absence of a significant stem means that underestimation from 60 DAE onwards springs only from the presence of lower leaves. In the case of the 2003/04 wheat experiment (Fig. 4b), this can be confirmed by noting that even the prediction of the largest biomass sample was precise. In the 2004/05 wheat experiment (Fig. 4c), the cloud of data points that can be seen among the samples of about 800 g m^{-2} produced a much less accurate fitting. This can be explained by the saturation of red reflectance (chlorophyll absorbed energy), limiting the biomass

prediction under such strong development conditions. This factor also contributed to the underestimation at dry biomass densities over 600 g m^{-2} in the combined wheat experiments (Fig. 4d).

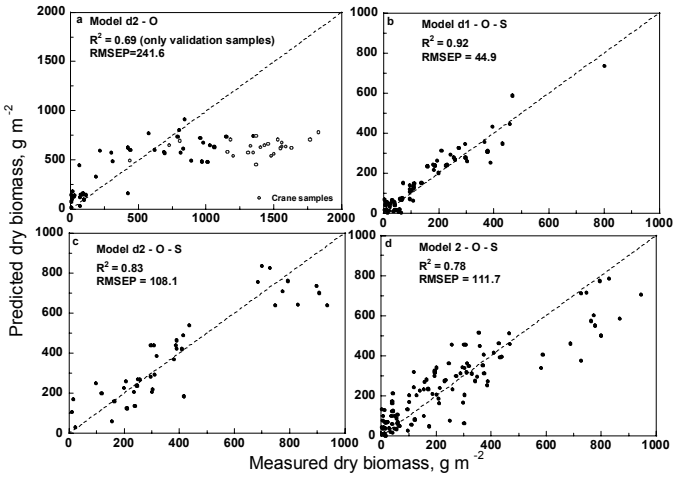

Fig. 4. Dry biomass prediction of the validation dataset. (a) Maize 2003, empty symbols represent samples taken from the crane; (b) Wheat 2003/04; (c) Wheat 2004/05; (d) Combined wheat 2003/04 and 2004/05. Symbols: d1 = 1^{st} derivative; d2 = 2^{nd} derivative; O = outlier exclusion; S = significant wavelengths.

The prediction of the 2003/04 wheat dry biomass on the basis of the 2004/05 model (inter-season validation) results in a very low correlation and high error (Table 2). This could be a result of the extremely different growing conditions. All samples that were used for calibration (2004/05) correspond to plants that had a good water status. In the validation set (2003/04), some of the late sampling data represent drier conditions that did not exist in the calibration dataset. However, despite these differences, the variability in the 2003/04 wheat experiment enabled its data to yield better prediction of the biomass produced in the 2004/05 wheat experiment. Despite significant correlation, a high error given by a considerable shift (overestimation) was observed in the predicted data during almost the entire season. The 2004/05 wheat data include higher NIR reflectance values than those from the previous season (data not shown), which accounts for this overestimation. This problem represents a definite limitation in the use of the model, because it occurs during the critical period of crop development, when it is still possible to make some decisions concerning fertilization or crop use [43].

The water-content predictions in the maize experiment (Fig. 5a) exhibit the highest errors among the lowest water-content values. These samples correspond to the later stages of development, when the stem effect also plays a significant role. The high error in the prediction of the samples from the crane campaign is explained by the fact that from 50 DAE the water content started to decrease (Fig.1c), and only a few samples were included in the calibration at such a low level of water content. From Figs. 5b and 5c, it can be seen that the wider range of stress, in measured values that prevailed in the 2003/04 wheat experiment, resulted in better correlation with the predicted values than those of the maize and the 2004/05 wheat experiment (R^2 = 0.82 vs. 0.56, and 0.65, respectively). This result shows that these models can predict differences among widely varying water contents better than those among less variable ones. The strong influence of biomass density on the spectral changes resulted in a small increase in the RMSEP of those dryer samples from the 2003/04 experiment, which in fact contributed to improving the overall correlation. Therefore, fine-tuning can be performed, by including in the calibration dataset extra samples that are similar in biomass content but differ in water content.

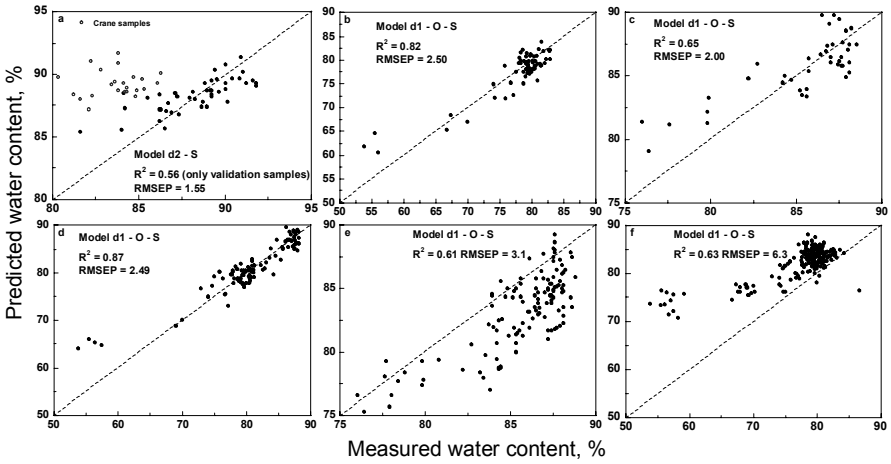

Fig. 5. Water content prediction. (a) Maize 2003, empty symbols represent samples taken from the crane; (b) Wheat 2003/04; (c) Wheat 2004/05; (d) Wheat 2003/04 and 2004/05; (e) Wheat 2004/05 dataset based on 2003/04 model; (f) Wheat 2003/04 dataset based on 2004/05 model. Symbols: d1 = 1st derivative; d2 = 2nd derivative; O = outlier exclusion; S = significant wavelengths.

Figure 5e shows a bias problem created by the underestimation of the predicted water content for the 2004/05 wheat data using the 2003/04 wheat model. On the other hand, there was an overestimation among the low values of water content in the 2003/04 wheat data, as predicted by the 2004/05 wheat model (Fig. 5f). This can be explained by the fact that, as already noted, the water content was lower in the first season than in the second - 52 to 85% vs. 75 to 90%, respectively. Since these models cannot extrapolate efficiently beyond the information included in the calibration, their prediction capability is limited. Therefore, all the samples of the second season were concentrated in the small range of the first season. This demonstrates that the greater the variability of the calibration data, so that they cover a wider range of possible scenarios, the more accurately the model can predict. This is the main reason why the combined dataset yielded higher R^2 and lower RMSEP values (Table 2). A comparison between the predictions of the 2003/04 wheat data and the 2004/05 model yields a much better performance in predicting water content than in predicting biomass.

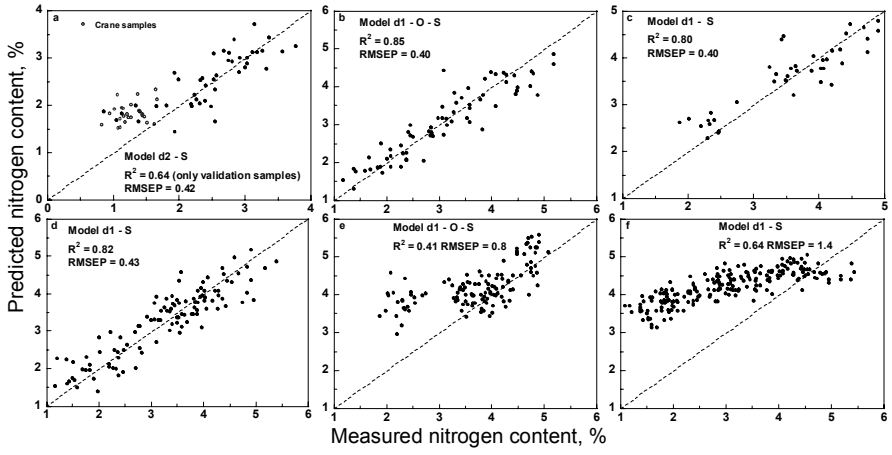

Fig. 6. Nitrogen content prediction. (a) Maize 2003, empty symbols represent samples taken from the crane. (b) Wheat 2003/04. (c) Wheat 2004/05. (d) Wheat 2003/04 and 2004/05. (e) Wheat 2004/05 dataset based on 2003/04 model. (f) Wheat 2003/04 dataset based on 2004/05 model. Chosen model: d1, 1st derivative; d2, 2nd derivative; O, outlier exclusion; S, significant wavelengths.

The predicted and measured results for the N content were somewhat better than those for the water content (Fig. 6). In the maize experiment (Fig. 6a), the main source of error in the validation lies in the low N-content samples, where an overestimation can be noted. The accurate prediction of the crane samples confirms that, despite the fact that canopy-sensor height was not optimal, yet, due to the adequate criteria used in the measurement configuration, the results were representative. Moreover, if the crane samples are taken into consideration, the overall accuracy analysis of the prediction of N-content, R^2 increases from 0.64 to 0.72.

For the wheat validation (Fig. 6 b, c, d), the prediction reached very high levels of accuracy. In the case of the inter-season validations (Fig. 6 e, f), overestimation of the low values can be seen in both cases. However, it was clearer and more extended in predictions of the 2003/04 dataset from the model of the 2004/05 dataset (Fig. 6f). This could be attributed to the rapid growth that occurred at the beginning of the 2004/05 wheat season, which generated conditions of high N content at a stage at which biomass development was already much more advanced than in the previous season.

3.5 PLS vs. vegetation indices

To determine the net improvement given by the PLS models in the prediction of the measured biophysical variables over standard methodologies, the prediction results were compared to those obtained with known VIs. As mentioned, this analysis was performed for the 330 samples of the combined wheat dataset of the 2003/04 and 2004/05 season. After calculating the VIs for the complete dataset, the calibration subset (taking out the same outliers that were not considered in the PLS models) was used for fitting each of the VIs to the biophysical variables with both a linear and an exponential model. Table 3 presents the correlation of the best model (linear or exponential) for each VI between the measured and predicted variables of the validation subset. Although were included indices that had been correlated to all of the analyzed variables, only the accuracy obtained for the biomass and LAI reached similar levels to the results achieved by the PLS methodology.

Table 3. Biophysical estimation accuracy by analysis of vegetation indices. Statistics based on validation dataset of the wheat 2003/04 and 2004/05 combined experiment.

Indices	Dry biomass g m^{-2}			Water content %			N content %			LAI		
	M	R^2	RMSE	M	R^2	RMSE	M	R^2	RMSE	M	R^2	RMSE
NDVI	E	0.46	151	E	0.20	5.47	E	0.15	0.93	E	0.74	0.96
GNDVI	E	0.52	143	E	0.18	5.52	E	0.15	0.93	E	0.81	0.82
NDGI	L	0.36	169	E	0.37	4.83	ns	ns	1.01	L	0.64	1.15
SR	L	0.43	162	L	0.34	4.93	ns	ns	1.01	L	0.77	0.93
SAVI	E	0.46	158	E	0.24	5.33	ns	ns	0.96	E	0.73	1.04
TCARI	ns	ns	ns	E	0.11	5.76	E	0.12	0.95	ns	ns	ns
OSAVI	E	0.47	152	E	0.22	5.40	E	0.12	0.95	E	0.76	0.93
REP	L	0.69	118	E	0.16	5.60	ns	ns	0.98	L	0.86	0.70
R970/900	E	0.62	139	E	0.29	5.16	ns	ns	0.98	E	0.84	0.79
R900/970	E	0.63	142	E	0.29	5.15	ns	ns	0.99	L	0.83	0.78
R900/1450	L	0.36	171	E	0.35	4.92	ns	ns	1.01	L	0.67	1.13
R900/1530	L	0.39	167	E	0.33	4.97	ns	ns	1.01	L	0.70	1.07
R1080/1180	E	0.57	156	E	0.23	5.35	ns	ns	0.97	L	0.82	0.81
R1080/1260	L	0.55	144	E	0.26	5.26	ns	ns	0.98	E	0.81	0.90
R1180/2170	L	0.39	166	E	0.31	5.08	ns	ns	1.00	L	0.66	1.13
R1260/1675	L	0.42	162	E	0.27	5.21	ns	ns	0.98	L	0.68	1.10

Symbols and acronyms: ns = not significant; M = Model; E = Exponential; L = Linear; RMSE = root mean square error

Regarding the model type, it can be seen from Table 3 that, for the prediction of dry biomass and LAI, several indices better fitted an exponential model, while several better

fitted a linear model. For the dry biomass, the best PLS model of the combined dataset had higher R^2 and smaller RMSEP values than any of the analyzed VIs (R^2 = 0.78 & RMSEP = 112 vs. 0.69 & 118 for the red edge position index). It should be noted that several indices (REP, GNDVI, R970/900, R1080/1180, R1080/1260, etc.) predicted LAI values similar or even better than those from the PLS model (R^2 = 0.82 & RMSEP = 0.79). Although several of these last indices were developed for water content, they yielded much better results for the prediction of biomass variables than for the water content itself. In the case of water content, the PLS model was much more accurate than any of the analyzed VIs. Although it was originally developed for monitoring crop N conditions [31], the exponential model using NDGI was relatively the best index for the water-content prediction (R^2 = 0.37 & RMSEP = 4.8 vs. 0.87 & 2.5 for the PLS model). Finally and surprisingly, almost all of the indices were nonsignificant ($p > 0.001$) for the N-content prediction, in comparison to accurate estimation by PLS (R^2 = 0.82 & RMSEP = 0.43). The lack of accuracy in the prediction of water and nitrogen content, presented by the VIs, shows their lack of ability to build multi-year models due to their high sensitivity to different levels of biomass presence. In comparison, although the two analyzed season were very different, the combined PLS models provided significantly better prediction than those achieved by the VIs. Therefore, the PLS was the only method that enabled accurate estimation of all biophysical variables.

4 CONCLUSIONS

PLS regression methods are a suitable tool for retrieving crop-condition indicators from spectral data at the canopy level. High accuracy, using PLS models, was achieved for the prediction of several biophysical variables of one maize and two wheat crops. However, this accuracy is highly dependent on the quality and variability of the calibration dataset. The observed variability among the three experiments and throughout each of their seasons highlights the importance of data variability and of its spread across the widest possible range, in order to achieve the best calibration model. With regard to data pre-processing, considerable improvements were achieved by using spectrum derivatives instead of raw reflectance data. Another important aspect of pre-processing is the elimination of samples that deviate widely from the main core of the dataset (outliers). However, the most important pre-processing procedure is definitely that of appropriate wavelength selection - reducing the number of wavelengths involved in the model - yields much better results. Nevertheless, there were some differences in behavior among the various biophysical variables; in the maize experiment, the best method involved the use of significant wavelengths after application of the second derivative. In the wheat experiments, the best method involved the successive determination of the first derivative, elimination of outliers, and selection of significant wavelengths.

With the exception of the R970/900 and R900/970 indices for LAI prediction, the selected wheat PLS models showed better accuracy than any of the analyzed VIs for all of the biophysical variables. This is consistent with what has been previously documented for the prediction of water and N content of wheat leaves by the use of PLS models with NIR spectrometry at the leaf level [18].

In addition to the discussed “saturation constraint” of the VIs, this lack of accuracy when using multi-year functions for the prediction of biophysical variables, such as water or nitrogen content, enhances the comparable potential of PLS models. This is especially important in those areas where regional support programs are being offered to the growers to improve the efficiency of their operations. In these cases, in order to build reliable and representative databases for the decision making process, data from several years is needed. Based on these results, PLS models represent a better methodology for the retrieving of crop biophysical variables that can be confidently applied in different field crop decision support systems. This conclusion is especially relevant today, when airborne hyperspectral images are more available and cheaper, thus becoming a real option for commercial applications.

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