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Research paper

Significant wavelengths for prediction of winter wheat growth status and grain yield using multivariate analysis

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ABSTRACT

In order to select significant wavelengths related to winter wheat growth characteristics, field experiments were conducted in three consecutive years. Diffuse reflectance of crop leaves was recorded with other crop variables during growth stages. Multivariate analysis including partial least squares regression (PLSR) and stepwise multiple linear regression (SMLR) procedures were used to determine important wavelengths. The results showed strong relationships between predicted and actual crop variables. The best prediction model built on wavelengths selected by SMLR so that R^2, root mean square error (RMSR) and relative error (RE) for the validation dataset were 0.85, 1.56 and 3.64% for SPAD, 0.89, 413 and 6.21% for grain yield, and 0.84, 0.56 and 4.85% for protein content.

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1. Introduction

Remote sensing has great potential for several applications because it enables wide-area, non-destructive, and real-time acquisition of information on ecophysiological plant conditions (Inoue, 2003). Remotely sensed data, obtained either by satellite or aircraft, can provide a set of detailed and spatially distributed data on plant growth and development (Plant et al., 2000).

Measurements of various crop canopy variables during the growing season provide an opportunity for improving grain yields and quality by site-specific application of fertilizers (Hansen and Schjoerring, 2003). Plant reflectance is affected by leaf surface properties, internal structure, plant stress, and the concentration and distribution of biochemical components; therefore, analysis of remote reflected light may be used to assess plant biomass and the physiological status of a plant (Penuelas and Filella, 1998). Wavelengths in the red and near infrared (NIR) wavebands are frequently used for indirect measurements of plant characteristics (Wood et al., 2003). The majority of agricultural studies use measurements in the visible (400–700 nm) and near infrared (700–2500 nm) regions of the electromagnetic spectrum. The principle is that the majority of red light is absorbed by chlorophyll in the canopy and therefore little is reflected, whereas a high proportion of near infrared light is reflected. As the canopy green area increases, either due to increasing crop density or chlorophyll content, the percentage of red reflectance decreases, while that of near infrared reflectance increases. The position of the red edge can also change, depending on the canopy and soil type, and this spectral shift has been used in some studies (Boochs et al., 1990).

Various methods of mathematical and statistical analyses have been used for setting up linear and non-linear calibration models. Hansen et al. (2002) used multi-way partial least squares regression (N-PLS) to predict grain yield and protein content, and they showed that the relation between reflectance measurements and protein content was slightly better in wheat, where especially N-PLS improved the prediction of grain protein content. They also found that data from repeated measurements of reflectance used in multi-way partial least squares regression before heading improved the prediction of grain yield and protein content in wheat and barley. Card et al. (1988) found that N in dried and ground tree leaves could be determined accurately from reflectance with a laboratory spectrometer. Stepwise multiple linear regression (SMLR) was used to select 580 nm and 480 nm for total nitrogen prediction, and R^2 was 0.90. Lee et al. (2009) found that SPAD (Soil and Plant Analyzer Development, Minolta, Inc.) readings, based on transmittance at 659 and 940 nm, were well correlated with N content in corn ear leaves ($R^2 = 0.962$). They developed prediction models by partial least squares (PLS) regression, principal component regression (PCR), and multiple linear regression (MLR). Their results showed that models built by PLS and PCR were better than models established from MLR and that the standard errors of prediction (SEP) for ear leaf N were

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0.16%, 0.15%, and 0.20% for PLS, PCR, and MLR, respectively. Tumbo et al. (2002) used a back-propagation neural network model for corn nitrogen prediction in field conditions. The model used 201 spectral bands as input, covering a range of 407–940 nm, and results proved that the neural network model could considerably reduce interfering effects of cloud cover and solar angle. The model showed good correlation between predicted and actual chlorophyll meter readings of the training set ($R^2 = 0.91$). A good relationship was also found in the validation dataset ($R^2 = 0.74$). There has been little reported research regarding spectral characteristics and nutrient assessment in citrus.

Yield and protein content are two important key factors for bread wheat production and marketing (Jenner et al., 1991). Protein concentration is known to influence the bread-making quality of wheat (Johnsson et al., 2001). Protein concentration in wheat is determined by the genetic background and also, to a large extent, by environmental factors such as nitrogen, water access and temperature conditions (Johnsson et al., 2001). In barley used for malt, the grain protein content should be lower than 11.5% (Bertholdsson, 1999). This may be difficult as the protein content is influenced by cultivation practices and by environmental factors such as availability of nitrogen and stress situations caused by drought (Birch et al., 1997). Prediction of grain protein for the prospective wheat and barley harvest would therefore be of value to farmers when deciding if the field should be divided into different management zones in order to harvest and deliver the targeted qualities. Grain yield and quality can however be influenced by late season fertilizer and fungicide application (Bertholdsson and Stoy, 1995), but the net profit for the farmer depends on application costs, yield response and crop value. There is therefore a need to predict grain quality during the growing season to improve decision-making concerning management practice. The objectives of this study were I) to establish a step-by-step multivariate analysis method to determine important wavelengths in the spectral reflectance data for assessing N status, protein content and grain yield of winter wheat, II) to develop prediction models in terms of N status, protein content and grain yield using partial least squares regression (PLSR), and III) to select individual significant wavelengths using stepwise multiple linear regression (SMLR) analysis.

2. Materials and methods

Tests in winter wheat fields were conducted for three years in the farming area of Hokkaido University (43° 4′ N 141° 20′ E), Japan, with annual average precipitation of 1106.5 mm and minimum temperature (−7 °C) in January and maximum temperature (26.4 °C) in August. The size of the field was 40 m × 120 m and the field was divided into 8 areas. Four levels of fertilizer (ammonium nitrate), 0, 30, 60 and 90 kg ha^{1-}, with two repetitions were applied at the reviving stage (growth stage GS 26), (Zadoks et al., 1974) to create a range of crop growth variations. Field in-season measurements including measurements of SPAD value (soil plant analysis development) and canopy reflectance in 2010 at the flag leaf stage (GS 37) and anthesis stage (GS 60) were done in 20 target points as well as in the 2011 (56 target points) and in the 2012 (40 target points) after the stem elongation (GS 36) and anthesis stage (GS 60) growth investigations were performed. The protein content and grain yield were measured after harvesting and threshing a 1 m × 3 m area in each target point in each of the three years.

The SPAD value was determined the relative amount of chlorophyll concentration in plant leaves by measuring the absorbance of the leaf in two wavelength regions of red (650 nm) and near-infrared (940 nm) by using a SPAD meter (MINOLTA Co. LTD.). According to the catalogue of SPAD 502 (Konikaminolta, 2011) there is strong relationship ($R^2 > 0.9$) between SPAD value and leaf nitrogen concentration, and SPAD value has therefore been widely used for estimation crop chlorophyll and nitrogen contents and for guidance of plant health status and topdressing (Zhang et al., 2003). In this study, SPAD value was used as an index of actual nitrogen content in crop leaves.

2.1. Reflectance measurement

Wheat canopy reflectance measurements in the 350–2500 nm wavebands (1 nm in width) were made using a portable spectroradiometer, FieldSpec®3 (FS3) (Analytical Spectral Devices, Inc., USA), under cloudless conditions and as close to solar noon as possible (Rasooli Sharabian et al., 2012). Calibration was done using a standard white board immediately before measuring reflectance value. Five canopy spectral reflectance measurements were obtained from a 2 m radius centered on the geo-referenced point. The viewing angle of FS3 was set at 25° and the height was 150 cm from the ground, which could cover 0.4 m^2 in each measurement. These measurements were then averaged for the particular location. Reflectance data were preprocessed to remove erroneous measurements and improve stability of the regression. Owing to observed noise problems because of absorption by the atmosphere, the first 50 readings (from 350 nm to 400 nm) at the lower visible wavelengths and last the 1150 readings (from 1350 nm to 2500 nm) at the shortwave infrared (SWIR) were deleted due to their low signal-to-noise ratio; thus, the revised spectra began at 400 nm (Fig. 1).

2.2. Dataset arrangement

Datasets for the three years were separated into modeling and validation datasets. The modeling dataset included a combination of 2010 and 2011 samples (20 samples from each year) to make a calibration model. The 2012 samples (40 samples) were used as the validation dataset. Three methods, correlation coefficient spectrum, partial least squares regression (PLSR) and stepwise multiple linear regression (SMLR), were used for wavelength selection.

2.3. Correlation coefficient spectrum

The simplest method was to compute correlation coefficients between reflectance at each wavelength and the actual crop variables. The correlation coefficient spectrum provided a picture of the relationship between reflectance and crop variables. Wavelength regions showing high correlation are regions that should be selected, and regions showing low or no correlation should be ignored. SPSS version 18 (SPSS Inc., Chicago, USA) was used to calculate correlation coefficients (r).

2.4. Regression analysis

Partial least squares regression (PLSR) implemented in Unscrambler version 10.2 (CAMO, Inc., Oslo, Norway) and stepwise multiple linear regression (SMLR) in SPSS version 18 were used to develop calibrations between crop variables and reflectance spectra. Both PLSR and SMLR have been widely used in chemometrics, remote sensing, and spectral data processing to deal with large datasets containing highly correlated variables. Although PLS has been more widely used in recent years, successful SMLR application to soil spectral analysis has also been reported (Vasques et al., 2009).

2.5. Pre-processing for reflectance data

A large amount of spectral data is usually obtained from spectral instruments and yields useful analytical information (Blanco and

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