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Simultaneous identification of spring wheat nitrogen and water status using visible and near infrared spectra and Powered Partial Least Squares Regression

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ABSTRACT

The common method of estimating N demand in cereals by spectral measurements may be negatively affected by variation in other crop properties, in particular by crop water status. In this study, we tested whether it is possible to distinguish between N and water status in spring wheat, at the time of split fertilization (plant growth stage – BBCH 32), by means of spectral reflectance data obtained from a sensor with an effective spectral range of 400–950 nm (i.e. without utilizing the distinct short-wave infrared (SWIR) water bands, which requires a more costly sensor). In 2012 and 2013 we ran a spring wheat field experiment in SE Norway. The experiment comprised 36 treatment plots arranged in a split-plot design, with N fertilization on major plots (either 70 or 100 kg N ha^{-1} applied at sowing) and water regime on sub-plots (either limited water supply, natural (rain-fed) water supply, or natural water supply + irrigation). Canopy reflectance was measured on all plots at BBCH 32, using a portable field spectroradiometer (tec5 AG, Germany). Immediately afterwards, aboveground wheat biomass was sampled from 0.25 m^2 quadrats on each plot, and analyzed for total N, fresh and dry matter. The spectral data were first pre-processed by logarithm linearization, 1st derivative filtering using the Savitzky–Golay method and mean normalization. Principal Component Analysis (PCA) performed at the treatment level (i.e. not utilizing ground truth measurements) showed that the first component in all datasets (2012, 2013 and combined) was related to the water regime. The second component in the single year datasets (or the third in the combined dataset) was related to N fertilizer. When combining the spectral information and the ground truth data by means of Powered Partial Least Squares Regression (PPLS), we were able to calibrate models (combined dataset) which fitted well with measured nitrogen at ratio of performance to deviation: RPD = 2.52 (R^2 = 0.86) and water concentration at RPD = 2.35 (R^2 = 0.84) in aboveground spring wheat biomass. The multivariate calibration method revealed several distinct spectral regions containing information related to either wheat plant N or water concentration. This method was superior to an index-based approach, with the best model performance of RPD = 2.26 (R^2 = 0.83) and RPD = 1.49 (R^2 = 0.68) for N and water concentration, respectively.

1. Introduction

Quantitatively speaking, nitrogen is the major yield-determining nutrient required for the crop growth. Crop N use efficiency may vary spatially, mostly due to heterogeneous soil quality (i.e. texture, organic matter content, nutrient status), geomorphology of the terrain, and weather–soil interactions (affecting for example soil moisture availability). Therefore, in order to optimize the profitability of agricultural enterprises, using uniform N fertilizer rates should no longer be a routine practice (Varco et al., 2013). Within-season, site-specific nitrogen application relies on the identification of field areas with various responses to N (Rodriguez et al., 2006).

Plant N status may be estimated using spectral reflectance of electromagnetic (EM) energy in the visible and near-infrared range of the electromagnetic spectrum. The visible region of the EM spectrum (400–700 nm) is influenced by chlorophyll pigments in leaf tissues, which have been found to correlate well with canopy N concentrations (Thomas and Gausman, 1977). The main chlorophyll absorption bands (a and b) are found in the blue (450 nm) and red (670 nm) portion of the spectrum, respectively (Richardson et al., 2002; Raven et al., 2005). However, small

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amounts of chlorophyll are sufficient to saturate the absorption in the 660–680 nm region. Therefore, empirical models for predicting chlorophyll or N concentration are usually based on the reflectance far from pigment absorption maxima, e.g. in the 550 or 700 nm bands (Rodriguez et al., 2006).

The near-infrared (NIR) region of the electromagnetic spectrum covers the range from 700 to 2500 nm. At wavelengths between 700 and 1100 nm the plant's mesophyll cells strongly reflect the incident light (e.g. Tilling et al., 2007). The spectral range between the visible and NIR regions, featuring a characteristic strong positive gradient towards NIR, is named the 'red edge' (Horler et al., 1983). Its position is a strong indicator of chlorophyll content, independent of canopy ground cover. Over many years of research, spectral features in the Vis–NIR region have been incorporated into vegetation indices (VI), in a mathematical combination of reflectance data from two or more spectral bands. These indices have been correlated with plant properties for indirect estimation purposes. Basic VI's integrate a specific spectral absorption band and a neighboring 'reference' band without a spectral feature. The normalized vegetation indices (NDVI, Rouse et al., 1973; NDRE, Barnes et al., 2000) filter the specific information from absorption bands. More complex indices indicate specific waveband positions (e.g. REIP, Clevers, 1994). Progress in VI's includes two dimensional combination of the indices (e.g. CCCI: Barnes et al., 2000) or planar domain indices (e.g. Rodriguez et al., 2006), typically used to improve canopy properties estimation in situations where a changing proportion of bare soil is causing spectral interference. A thorough review of vegetation indices is given by (Thenkabail et al., 2000).

Spectral N status measurements have been performed by optical reflectance spot-sensors, tested both handheld (e.g. Gebbers et al., 2013) and tractor-mounted (Schmidhalter et al., 2003; Varco et al., 2013). Various passive (using solar irradiance) and active (including artificial light source) reflectance sensors are currently available. Gebbers et al. (2013) list the VI's used by specific commercially available sensors. These sensors provide only basic indices for N status and biomass such as NDVI, NDRE and REIP. A challenge using such indices is that they may also be influenced by several other factors, such as canopy biomass, plant height, disease and weed infestation and water status (Schepers et al., 1996). Moreover, the effects of these factors may co-occur. For example, Moran et al. (1989) found that due to reduced canopy density, the water stressed canopies had lower spectral reflectance in the red and NIR ranges instead of an expected increase. This has potential implications for the calculation of optimum N fertilizer rates, in systems where remotely sensed information on site-specific N status is coupled with agronomic decision models. The determination of a precise fertilization rate may be particularly confounded by the crop water status (Osborne et al., 2002). Nitrogen requirements increase with water availability and misdiagnosing crop N deficiency and water stress may result in over-fertilization and reduced yields, respectively (Reese et al., 2010).

Many studies have addressed spectral determination of canopy water status. In general, leaf reflectance of drought-stressed plants increases over the entire spectrum (Linke et al., 2008), but some bands in the short-wave infrared (SWIR) region (1100–2500 nm) contain more water-related information (e.g. Ceccato et al., 2001). Sensors covering the SWIR range are typically built of relatively expensive materials; low-cost silicon sensors typically cover the Vis–NIR range outside SWIR (400–1100 nm). From a cost perspective, it is thus of interest to explore possible water absorption bands in the Vis–NIR range.

Water absorption bands from the SWIR region have their overtones (i.e. weaker absorption bands caused by molecular transition to higher energy state) in Vis–NIR region, with the intensity diminishing towards shorter wavelengths. A distinct water absorption band centered at 960 nm has, however, gained much interest. This band was later used in the WI index (Penuelas et al., 1993), which became a commonly used water status indicator (e.g. Rodriguez et al., 2006). Another index tested for plant water content signalling is the fluorescence based PRI index (Penuelas et al., 1995), which utilizes a band at 530 nm. This index has, however, also been shown to be sensitive to changes in chlorophyll (Thenot et al., 2002). In an indoor study on canopy drought stress, Linke et al. (2008) showed distinct differences in stressed canopy spectra in the well-known SWIR water bands (1400 and 1900 nm) and in three bands in the visible range (520–530, 570–590, 690–710 nm).

A number of studies have thus shown that both N and water status may be identified separately using Vis–NIR spectral reflectance. For practical use (i.e. site-specific fertilization), however, we need to be able to separate between N demand and water stress occurring simultaneously. Some studies have addressed this challenge. Rodriguez et al. (2006) used an index based approach to spectrally estimate N status in wheat at 33 BBCH irrespective of the plant water status. Their study included four N fertilizer rates as well as an irrigated and a rain-fed water regime. Their models explained up to 69% of the observed variability in the nitrogen nutrition. Another index-based approach was presented by Liu et al. (2004), who estimated plant water content in three winter wheat cultivars with varying crop status (four N treatments and four irrigation regimes). They explained 34–75% of the measured variation in plant water content. Other studies have included ancillary data, such as thermography (Tilling et al., 2007) or image-based sensors (Gebbers et al., 2013), and thereby managed to increase the efficiency of indices-based separation of water and N-status to over 80%. Using these techniques involves more instrumentation, data processing and integration.

An alternative to index-based approach, where only a few spectral bands are used, is multivariate analysis utilizing the entire spectrum. Not many studies have used multivariate analysis in order to separate the N and water information in the spectral signal. Pimstein et al. (2007) combined Partial Least Squares (PLS) regression and reflectance measurements to estimate nitrogen and water status of fresh wheat leaves. Common for these studies, was that their spectral measurements also comprised the SWIR-region. To our knowledge, no studies have been published, which separate plant water and nitrogen status on the basis of multivariate analyses of spectral measurements in the low-cost Vis–NIR range.

PLS is a common choice when analyzing multivariate data. A more recent method is the Powered Partial Least Squares (PPLS, Indahl, 2005). This method has a strong ability to weigh the most significant variables with respect to the response variables, and may be used for automatic pre-selection of spectral bands to optimize multivariate calibration. The PPLS-method was shown to be the most robust method for estimating spring wheat yields based on canopy reflection in the Vis–NIR range (Overgaard et al., 2010).

The objective of the present study was to test the possibility of separating nitrogen and water status in spring wheat at the time of split fertilization (BBCH 32) by means of PPLS-regressions and spectral canopy measurements obtained from a quartz sensor with an effective spectral range of 400–950 nm, i.e. without utilizing the distinct SWIR water bands which require a more costly sensor.

2. Materials and methods

As a part of a larger project (the "MULTISENS-project", www.bioforsk.no/multisens), a two-year (2012–2013) field trial in spring wheat (*Triticum aestivum* L., cv. "Bjarne") was performed at Apelsvoll research farm in SE Norway, a part of Bioforsk Arable Crops Division.