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Spectroscopic estimation of leaf water content in commercial vineyards using continuum removal and partial least squares regression

Ana Belén González-Fernández*, José Ramón Rodríguez-Pérez, Miguel Marabel, Flor Álvarez-Taboada

Geomatics Engineering Research Group, University of León, Av. Astorga s/n, 24401 Ponferrada, León, Spain

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ABSTRACT

Knowing the water status of grape strains is essential for quality wine. Traditional pressure-chamber methods for estimating water stress are laborious and destructive. We evaluated the effectiveness of spectroscopic methods to estimate water content in commercial vine for three grape varieties (Mencía, Merlot and Tempranillo) from vineyards in El Bierzo (NW Spain). We also determined the spectral range, data fitting method and degree of transformation of spectral data necessary to estimate equivalent water thickness (EWT), from the untransformed spectrum (vegetation indices and full spectra) and from the spectrum transformed using continuum removal (CR) (CR reflectance and CR-derived indices). Partial least squares regression (PLSR) and ordinary least squares regression (OLSR) were used to fit the model. The results depended on the range studied, with the best results obtained for Tempranillo. Continuous stretches of the spectrum produced more suitable EWT models than vegetation indices. The models obtained from the transformed spectrum produced more accurate estimates. The best model was obtained using PLSR in the spectrum transformed by CR in the range 1265 nm to 1668 nm ($R^2 = 6.75$ and RMSE = 0.014%). We demonstrate that a field spectroradiometer determines vine water status rapidly and without damaging sampled leaves.

1. Introduction

Water is a key aspect of agriculture and, to produce good quality wine, the level of humidity in the leaves needs to be controlled (Kennedy et al., 2002). Water stress modifies vine leaf pigment composition (Flexas et al., 2010), reduces turgor and increases water potential; cell enlargement also decreases, leading to growth inhibition. It also slows down photosynthesis (since stomatal closure reduces transpiration and gaseous exchange), as well as the uptake and transport of nutrients, retarding plant growth (Lisar et al., 2012) and, in extreme cases, leading to death. Crops are influenced by environmental variations which may lead to changes in phenology or biology. These changes can be detected through reflectance measurements, especially in leaves (Chuvieco Salinero et al., 2000). Authors like Garbulsky et al. (2011), Hall et al. (2011) and Kokaly et al. (2009) have linked water stress to plant spectral responses.

Mediterranean vineyards are cultivated without irrigation systems, so vines – dependent on climatic conditions to obtain water – may suffer water stress. Leaf composition is related to must composition (Serrano et al., 2010), so hydric needs should be fulfilled during bloom. Water stress between bloom and veraison decreases sugar must content, resulting in poor quality wine due to low alcohol content. A certain amount water stress after veraison increases must quality (Chaves et al., 2010; Cramer, 2010) and has a positive impact on wine quality, as a mild water deficit decreases berry growth and size and affects chemical composition (higher tannin and anthocyanin).

Accurate, rapid and non-destructive methods for water content estimation are needed to optimize management practices

Abbreviations: A, area of the three leaf disk (cm^2); BA, band area; CR, continuum removal; CV, coefficient of variation; DM, dry matter (g); EWT, equivalent water thickness (kg/m^2); FM, fresh matter (g); fWBI, floating position water band index; MBD, maximum band depth; NDII, normalized difference infrared index; NDVI, normalized difference vegetation index; NDWI, normalized difference water index; OLSR, ordinary least squares regression; PCA, principal component analysis; PLSR, partial least squares regression; RGI, red/green index; SIPI, structure intensive pigment index; SIWSI, shortwave infrared water stress index; SRWI, simple ratio water index; VI, vegetation index; WI, water index; ZTM, Zarco–Tejada and Miller index.

* Corresponding author. Tel.: +34 987442000; fax: +34 987442070.
E-mail address: agonf@unileon.es (A.B. González-Fernández).

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(especially irrigation) in viticulture. Spectroscopic analysis is widely applied in agriculture for disease inspection, nutritional status evaluation, fruit quality assessment and category discrimination (Chaves et al., 2010). The usual approach to estimating water content is by measuring leaf water potential (which includes leaf osmotic potential, apoplastic water content and/or plant cell elasticity) using a pressure chamber (Turner, 1988). However, this method is slow and is influenced by temperature, light, size and position of the leaf (Serrano et al., 2010). Water content can alternatively be estimated by remote sensing at different scales using vegetation indices (VI), physical models and continuum removal (CR) analysis. Gaulton et al. (2013), Santos and Kaye (2009) and Suárez et al. (2010) demonstrated the usefulness of reflectance to evaluate water stress.

Several studies have found a relationship between water leaf content and VI calculated from spectral values. Dzikiti et al. (2010) and Serrano et al. (2010) demonstrated than VI can be used to control drought, monitor irrigation and help harvest management, given the relationship between VI and variables describing must quality or vine vigour (Meggio et al., 2010; Serrano et al., 2012; Suárez et al., 2010). In those studies, the relationship between spectral information (i.e. VI or spectral bands) and leaf water was determined using ordinary least squares regression (OLSR), obtaining models that use the 430–650 nm wavelength range.

A drawback to measuring leaf reflectance is that measurements are influenced by the light inclination angle for the leaf (Zarco-Tejada et al., 2005). One way to overcome this problem is to use an integrating sphere, as it corrects reflectance and transmittance measurements and measurements leaf parts (Zarco-Tejada et al., 2005); however, the drawback is that the integrating sphere is very fragile. One solution is to use a plant probe accessory (ASD Inc., 2012), which always arrives with the same angle and intensity; its structure is also sufficiently strong to be able to use it in the field.

Hyperspectral data sets contain useful information for characterizing vegetation. However, leaf water content depends on many different factors (e.g. crop, cultivar, plant density, canopy form, management techniques, atmospheric effects and climatic conditions) and variations are hard to relate to narrow-band indices, which only take into account a small part of the spectral data. VI require only two bands and do not use all information content contained in spectral data (Cho et al., 2007), there by weakening the relationship with the studied variable. Statistical methods like multiple linear regression are useful to predict vegetation parameters with more than two variables but, when hyperspectral data is used, multicollinearity is sufficiently high to invalidate the results (Curran et al., 2001). Another problem is that the number of studied variables is smaller than the number of wavebands used in the analysis (Atzberger et al., 2010). Other common methods are principal component analysis (PCA) and partial least squares regression (PLSR), which transform the spectral feature space to obtain latent factors for a model with maximum variance in the feature space (Atzberger et al., 2010). When a dependent variable is specified for regression, PLSR is more effective than PCA for dimension reduction, due to the supervised nature of its algorithm. PLSR – rather than decomposing the spectra into a set of eigenvectors and scores and then regressing these against the response variables – uses response variable information during the decomposition process (Cho et al., 2007; Zhang et al., 2012), so the relationship is enhanced and error is less than with PCA. PSLR suitability for estimating water leaf content was corroborated by Cho et al. (2007), who estimated biomass from airborne hyperspectral imagery using spectral indices and PLSR. It was concluded that PLSR based on airborne hyperspectral data was a better alternative to univariate regression. Zhang et al. (2012) also found that PLSR in combination with preprocessing methods could construct accurate models and provide accurate predictions of water content and other biochemical parameters. Mirzaie et al. (2014) obtained a higher correlation with water content prediction using PLSR. For hyperspectral remote sensing of some 80 species across the world, Zhao et al. (2013) used PLSR to determine equivalent water thickness (EWT).

Prediction models can also be improved by pre-processing spectral data in order to improve the signal-to-noise ratio and the accuracy of prediction models (Vasques et al., 2008). The CR transformation, which is the most widely used such technique for leaf water content estimates (Curran et al., 2001; Huber et al., 2008; Stimson et al., 2005; Wang et al., 2009), enables individual reflectance absorption features to be compared from a common baseline (normalizing the reflectance spectra). CR highlights and identifies absorption features of interest (Huang et al., 2004). CR-transformed spectra can be used as input to determine water content using multivariate methods such as PLSR. In addition, the use of indices derived from the spectrum where the CR transformation has taken place yields accurate univariate models for predicting water content (Pu et al., 2003).

Our objective was to determine the suitability of field spectroscopy for estimating water content in three commercial vineyards using different wavelength ranges, spectral transformations (VI, CR and non-transformation) and regressions methods (OLSR and PLSR).

2. Materials and methods

2.1. Study site and experimental layout

The research was conducted with three different varieties of grape (Mencía, Tempranillo and Merlot) in three vineyards belonging to the Ribas del Cúa Winery – located in Cacabelos (León, Spain) with in the Bierzo Protected Designation of Origin (PDO) – in plots centered at latitude 42°36′28″ N and longitude 6°42′24″W (WGS84). All the vines shared the following characteristics: planting year (1997), training system (bilateral cordon, vertical shoot-positioning with two pairs of wires), rootstock (1103 Paulsen) and row spacing (1.1 m × 2.8 m). At the study site annual rainfall was 322 mm and average temperature was 12.2 °C in 2012. Sampling vines were selected by choosing one line in ten and one vine in twenty in each line. Leaf sampling followed a regular grid pattern of 20 m × 29 m corresponding to 14 vines/ha approximately. Field data collection was carried out on 16 and 17 July 2012, on days that corresponded physiologically to the growth phase between berry set and veraison that is the recommended time for these measurements (Santos and Kaye, 2009).

2.2. Workflow

The methodology involved three main steps: data acquisition (leaf collection, spectral measurements and leaf weighing), spectral data processing (pre-processing and spectral transformation) and statistical analyses (fitting and validation models) (Fig. 1). Spectral data measurement was made immediately after leaf collection. The spectral data workflow consisted of capturing and pre-processing the spectral measurements to obtain the mean spectral signatures and to identify the CR features. Three different transformations were made to obtain the CR spectrum, CR-derived indices and VI. PLSR and OLSR were used to estimate EWT from the spectral data and the suitability of the regression models was assessed by cross-validation.

2.3. Non-spectral data

Selected for the measurements were three shoots per vine, on the southeastern (shoot 1), central (shoot 2) and northwestern (shoot 3) parts of the vine, and selected for each shoot was the