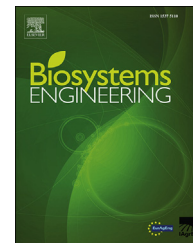




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Leaf water content estimation by functional linear regression of field spectroscopy data

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Grapevine water status is critical as it affects fruit quality and yield. We assessed the potential of field hyperspectral data in estimating leaf water content (C_w) (expressed as equivalent water thickness) in four commercial vineyards of *Vitis vinifera* L. reflecting four grape varieties (Mencía, Cabernet Sauvignon, Merlot and Tempranillo). Two regression models were evaluated and compared: ordinary least squares regression (OLSR) and functional linear regression (FLR). OLSR was used to fit C_w and vegetation indices, whereas FLR considered reflectance in four spectral ranges centred at the 960, 1190, 1465 and 2035 nm wavelengths. The best parameters for the FLR model were determined using cross-validation. Both models were compared using the coefficient of determination (R^2) and percentage root mean squared error (%RMSE). FLR using continuous stretches of the spectrum as input produced more suitable C_w models than the vegetation indices, considering both the fit and degree of adjustment and the interpretation of the model. The best model was obtained using FLR in the range centred at 1465 nm ($R^2 = 0.70$ and % RMSE = 8.485). The results depended on grape variety but also suggested that leaf C_w can be predicted on the basis of spectral signature.

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1. Introduction

Water plays an important role in plant physiology, as it conditions yield and quality of crops such as grapes (*Vitis vinifera* L.). Water stress induces stomata closure to reduce transpiration, which, in turn, also reduces photosynthesis and carbon assimilation. The management of water deficits by controlling grapevine vigour and improving grape maturity could be an efficient strategy for producing a high-quality wine (Chaves et al., 2010). Water content estimation is, therefore, an important issue in managing vineyards.

Several techniques are available for water content estimation in crops. The main ground-based method used in viticulture is leaf water potential, which requires measurement of sap pressure in the xylem (Scholander, Hammel, Bradstreet, & Hemmingsen, 1965). However, this is a destructive and laborious method for estimating water content, especially as variations in water potential are often related to soil type (Chone, Van Leeuwen, Dubordieu, & Gaudillère, 2001). Thus, although it provides the most accurate assessments of plant water status, it is not feasible for estimates involving large areas (Oumar & Mutanga, 2010).

Since water has some absorption maxima in the infrared region of the spectrum centred at the 970, 1200, 1440 and 1950 nm wavelengths (Palmer & Williams, 1974), it is possible to assess plant water status using non-destructive remote sensing technologies. These are faster than the water potential method, and so offer a cost/time ratio advantage; moreover, spatial patterns of water plant content can also be detected by imagery (Moshou, Pantazi, Kateris, & Gravalos, 2014; Xue & Su, 2017).

The use of remote sensing to monitor crop growth and development is attracting interest from researchers and commercial organisations alike. This interest is primarily driven by opportunities for cost-effective generation of spatial data capable of supporting precision agriculture (Hall, Lamb, Holzapfel, & Louis, 2002). To date, limited use has been made of this technology in the grape and wine sector, whether for research or commercial monitoring purposes. This article describes the key principles of remote sensing, reviews the current status of remote sensing in viticulture and discusses remote sensing's potential as an integrated management tool for vineyards. Sims and Gamon (2003) classified remote sensing methods as follows: (1) vegetation index calculation using mathematical formulae for reflectance at several wavelengths; (2) continuum removal (CR) of the spectral signature and analysis of depth and area in the dip below the continuum; and (3) water content fitting to spectral reflectance over a range of two wavelengths mainly centred on the water absorption maxima.

Spectroscopic determination of leaf water content has been explored by Cheng, Rivard, and Sánchez-Azofeifa (2011) and Ustin, Riaño, and Hunt (2012), while a number of studies have analysed vine water status estimation using remote sensing. Strever (2005) assessed water stress in vines by field spectroscopy, finding important differences depending on vine vigour and concluding that the spectral reflectance of higher vigour and lower vigour vines was related to leaf water content and pigment, respectively. Serrano, González-Flor,

and Gorchs (2010) studied the feasibility of using field spectral measurement to estimate vine water status at both leaf and canopy levels, reporting strong correlations for the water index (WI) and stomatal conductance (g_s), with coefficient of determination (R^2) values over 0.80. Note, however, that this result was obtained for potted plants subjected to varying degrees of water availability. In the field they demonstrated a correlation between predawn water potential and the normalized difference vegetation index (NDVI), achieving $R^2 = 0.57$. Serrano, González-Flor, and Gorchs (2012) related berry yield and quality with hyperspectral reflectance indices at canopy level, estimating berry yield by NDVI and WI ($R = 0.57$ and $R = 0.61$, respectively), and suggesting that total soluble acidity and the total soluble solids/total soluble acidity ratio might be estimated by WI when vineyards were experiencing moderate to severe water deficits.

Field spectroscopy is an effective technique for assessing the canopy density of vines. Dobrowski, Ustin, and Wolpert (2002) observed strong correlations between leaf area per metre of canopy and narrow vegetation indices, achieving R^2 values of 0.87, 0.92 and 0.79 for the ratio vegetation index (RVI), NDVI and perpendicular vegetation index (PVI), respectively. These authors recommended RVI for vineyard remote sensing applications, since it is more linearly related to canopy density and contains the same information as the NDVI. Similar results were found for imagery at vineyard level: the RVI was linearly correlated (R^2 values of between 0.68 and 0.88) with pruning weight for growing seasons (Dobrowski, Ustin, & Wolpert, 2003). Dobrowski, Pushnik, Zarco-Tejada, and Ustin (2005) linked vine physiological status and photosynthetic functioning with reflectance fluorescence indices (RFIs) calculated in the red-edge spectral region at canopy level. They indicated that RFIs were more suitable than the photochemical reflectance index (PRI) and NDVI indices for tracking photosynthetic status and plant stress, especially for rapid changes in vine status.

The use of sensors in applications to grapevines is complicated by the fact that a vineyard has a temporally and spatially changing environment that affects light interactions with leaves and grapes (Strever, Bezuidenhout, Zorer, Moffat, & Hunter, 2012). Nevertheless, the literature cited above would support the usefulness of passive reflectance measurements in monitoring vine physiological status, so remote sensing methods for estimating water content merit further study.

A different approach to tackling the problem of water content estimation from reflectance is based on considering spectral signatures as continuous curves instead of discrete values. A review of potential applications of this kind of functional data analysis to chemometrics is provided by Aguilera, Escabias, Mariano, Valderrama, and Aguilera-Morillo (2013) and by Saeys, Keteleare, and Darius (2008). In exemplifying the use of functional models, Saeys et al. (2008) concluded that functional data analysis is comparable to partial least squares regression (PLSR) in terms of predictive ability. Reiss and Ogden (2007) introduced functional versions of principal component regression and PLSR to NIR spectral analyses of both real and simulated data, concluding that functional models offer advantages over non-functional approaches. Dias, García, Ludwig, and Saraiva (2015) also used functional data techniques to calibrate and predict NIR spectral data. Ordóñez, Martínez, Matías, Reyes, and

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