

Metadata about the data set of “Determining optimum wavelengths for leaf water content estimation from reflectance: a distance correlation approach” (by Celestino Ordóñez, Manuel Oviedo de la Fuente, Javier Roca-Pardiñas, José Ramón Rodríguez-Pérez)

The work was conducted with four different varieties of grape (Cabernet Sauvignon, Mencía, Merlot and Tempranillo) in four vineyards in the village of Cacabelos (León, Spain) that belong to the Bierzo Protected Designation of Origin. All the vineyards shared the same characteristics: row spacing, training system, rootstock and planting year. A total of 162 vines were selected for leaf measurements (47 Cabernet Sauvignon, 45 Mencía, 27 Merlot and 43, Tempranillo vines). Field data collection was carried out on days between berry set and veraison that is the time recommended by Santos and Kaye (2009).

A FieldSpec 4 portable spectroradiometer (Analytical Spectral Devices, Inc., Boulder, CO, USA) was used for collecting the leaf reflectance data. This spectroradiometer captures spectral data at wavelengths in visible, near infrared and short-wavelength infrared (the wavelengths ranged from 860 nm to 2500 nm). Additionally, a plant probe was used (in order to minimize measurement errors associated with stray light). This device consists of a grip to locate the fibre optic cable input to the spectroradiometer, a quartz halogen bulb, and a quartz window to press the probe against the surface of the leaf (Lau et al 2003)

Three mature leaves per vine were measured. The upper face of the leaf was measured three times at three different points (avoiding veins, holes and leafspots) and the mean reflectance value for each leaf was saved. Each measured leaf was cut off immediately placed in a sealable plastic bag and stored in an insulated cooler. Leaf water content was calculated by the equivalent water thickness (EWT), that is the water weight (difference between fresh and dry weight of the leaf) divided by the leaf area.

The spectral reflectance values were pre-processed after modeling. Continuum Removal (CR) transformation of the spectra data was used to identify the water absorption features in the leaf spectrum (Kokaly and Clark, 1999). This transformation normalizes reflectance values to a common baseline and it requires identifying the ranges of wavelengths to calculate the CR.

References:

A.O. Santos and O. Kaye. Grapevine leaf water potential based upon near infrared spectroscopy. *Scientia Agricola*, 66:287-292, 2009.

R. F. Kokaly and R.N. Clark. Spectroscopic determination of leaf biochemistry using band-depth analysis of absorption features and stepwise multiple linear regression. *Remote Sensing of Environment*, 67:267-287, 1999.

I.C. Lau, T.J. Cudahy, G. Heinson, A.J. Mauger, and P.R. James. Practical applications of hyperspectral remote sensing in regolith research. *Advances in Regolith*, 66:249-253, 2003.

Data files: DataSet_CHEMOLAB_2017.xlsx and DataSet_CHEMOLAB_2017.ods

The both files contains the same information but in two formats: MS Excel (*.xlsx) and OpenDocument (.ods).

The vine variety (Variety) and leaf identifier (Leaf_id) is denoted.

The reflectance values are organized by wavelength (e.g.: the column “853_nm” shows the reflectance value for the wavelength 853 nm).

Sheet "EWT_data": Leaf water content (equivalent water thickness -EWT) of each leaf.
Units: kg m⁻².

Sheet "Raw_spectral_data": reflectance values measured in the field.

Sheet "CR_spectral_data": all reflectance values transformed by Continuum Removal.

Sheet "CR_spectral_data_Z1": reflectance values of zone 1(Z1: from 860 nm to 1065 nm) transformed by Continuum Removal.

Sheet "CR_spectral_data_Z2": reflectance values of zone 2(Z2: from 1114 nm to 1265 nm) transformed by Continuum Removal.

Sheet "CR_spectral_data_Z3": reflectance values of zone 3(Z3: from 1265 nm to 1668 nm) transformed by Continuum Removal.

Sheet "CR_spectral_data_Z4": reflectance values of zone 4(Z4: from 1830 nm to 2240 nm) transformed by Continuum Removal.