

Title Calibration transfer between miniature photodiode array-based spectrometers in the near infrared assessment of mandarin soluble solids content

Author C.V. Greensill and K.B. Walsh

Citation J. Near Infrared Spectrosc. 10, 27-35 (2002)

Keywords calibration transfer; NIR spectroscopy; direct standardization; DS; piecewise direct standardisation; PDS; double window PDS; DWPDS; finite impulse filter; FIR; orthogonal signal correction; OSC; wavelet transforms; chemometrics

Abstract

The transfer of predictive models among photodiode array based, short wave near infrared spectrometers using the same illumination/detection optical geometry has been attempted using various chemometric techniques, including slope and bias correction (SBC), direct standardization (DS), piecewise direct standardization (PDS), double window PDS (DWPDS), orthogonal signal correction (OSC), finite impulse transform (FIR) and wavelet transform (WT). Additionally, an interpolation and photometric response correction method, a wavelength selection method and a model updating method were assessed. Calibration transfer was attempted across two populations of mandarin fruit. Model performance was compared in terms of root mean squared error of prediction (*RMSEP*), using Fearn's significance testing, for calibration transfer (standardization) between pairs of spectrometers from a group of four spectrometers. For example, when a calibration model (Root Mean Square Error of Cross-Validation [$RMSECV = 0.26\%$ soluble solid content (SSC)], developed on one spectrometer, was used with spectral data collected on another spectrometer, a poor prediction resulted ($RMSEP = 2.5\%$ SSC). A modified WT method performed significantly better (e.g. $RMSEP = 0.25\%$ SSC) than all other standardization methods (10 of 12 cases), and almost on a par with model updating (MU) (nine cases with no significant difference, one case and two cases significantly better for WT and MU, respectively).