Spectral amplification in multivariate calibration of near infrared spectrophotometer

Marc Meurens

Université Catholique de Louvain - Croix du Sud, 2 (8), B-1348 Louvain-la-Neuve, Belgium.
E-mail: meurens@bnut.ucl.ac.be.

Introduction

Spectral amplification (AMPLI) is the name of the new method of near infrared (NIR) calibration based on a combination of automatic stepwise multiple linear regression (MLR) and partial least squares regression (PLS). The performances of this mixed method shown at the shoot-out competition of the International Diffuse Reflectance Conference of Chambersburg (IDRC) in August 1998 are presented here to illustrate the advantages of the wavelength selection and the amplification of the selected spectral data in the PLS multivariate calibration of an NIR spectrometer.

Material and methods

The vis-NIR spectra of 140 samples of wet and dry fescue grass were sent, by Professor W.F. McClure (North Carolina State University, Raleigh, NC, USA), to each participant of the shoot-out, in order to prepare a presentation of the best data treatment in this special session of the IDRC-98. The composition of the samples has been communicated, notably, in percentages (%) of water and nitrogen.

For the spectral amplification (AMPLI), first a wavelength selection was done by automatic stepwise multiple regression (MLR) with the NSAS software 3.30 of NIRSystems (Silver Spring, MD, USA). Afterwards, the selected spectral data were multiplied by amplification coefficients so that they

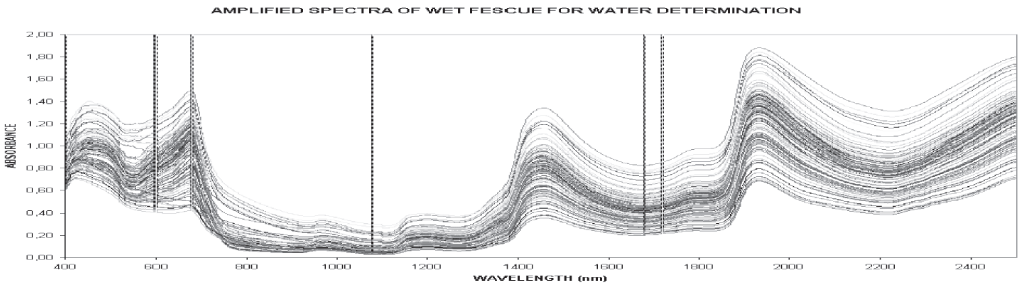

Figure 1. The vis-NIR spectra of the 140 wet fescue grass samples are displayed indicating the selected wavelength where the spectral data were mutiplied by amplification coefficients to improve the PLS calibration model for the water determination.

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dominated all the other spectral data in the partial least squares (PLS) calibration using the software package Unscrambler 5.5 (CAMO, Oslo, Norway). Seventy samples were used in the calibration set and 70 samples were used in the validation set.

Results and discussion

The spectra of the 140 samples of wet and dry fescue grass are presented below (Figures 1 and 2) indicating the wavelengths selected, first by MLR and afterwards amplified by PLS for the prediction of water and nitrogen on a validation set of 70 samples.

The advantage of precision, due to the selection and the amplification of a limited number of spectral data (at seven wavelengths for water and eight wavelengths for nitrogen), is obvious in the comparison of the NIR predictions between the PLS, MLR and AMPLI calibration models for the water determination on wet fescue grass (Figure 3) and for the nitrogen determination on dry fescue grass (Figure 4). For the determination of water on wet grass, the standard error of prediction (*SEP*) is re-

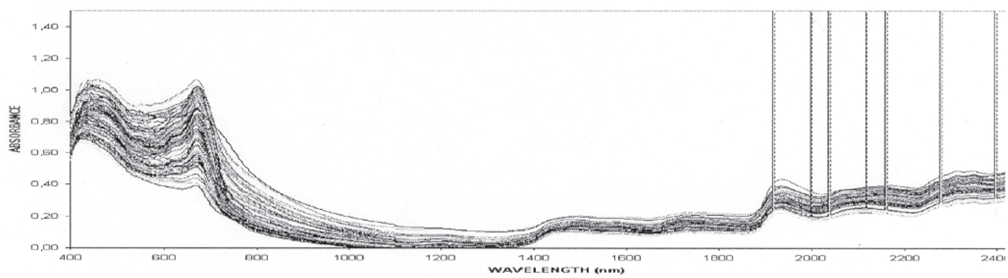

Figure 2. The vis-NIR spectra of the 140 dry fescue grass samples are displayed indicating the selected wavelengths where the spectral data were mutiplied by amplification coefficients to improve the PLS calibration model for the nitrogen determination.

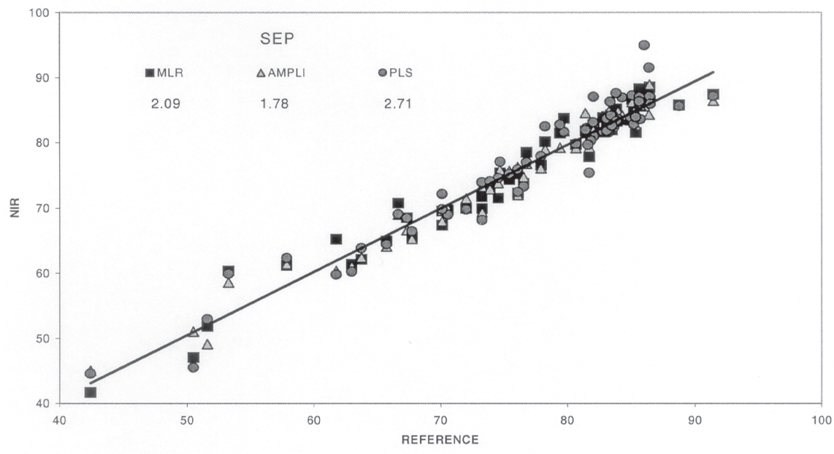

Figure 3. Validation plot of the PLS, MLR and AMPLI calibration models in the prediction of water content of the wet fescue grass samples.

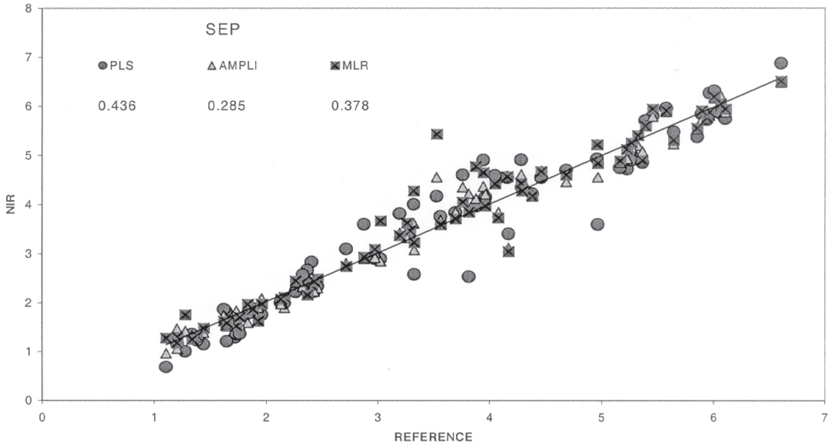

Figure 4. Validation plot of the PLS, MLR and AMPLI calibration models in prediction of nitrogen from the NIR spectra of dry fescue grass.

duced by 34% in the AMPLI model (*SEP* = 1.78) compared with the PLS model (*SEP* = 2.71) and by 15% in the AMPLI model (*SEP* = 1.78) compared with the MLR model (*SEP* = 2.09). For the determination of nitrogen on dry grass, the standard error of prediction is reduced by 35% in the AMPLI model (*SEP* = 0.285) compared with the PLS model (*SEP* = 0.436) and by 25% in the AMPLI model compared with the MLR model (*SEP* = 0.378).

Conclusion

The comparison of the NIR predictions between the classical multilinear calibration methods PLS, MLR and the new mixed calibration method AMPLI demonstrates clearly that it is possible to improve the precision of the PLS method using a few spectral data at selected wavelengths instead of all the spectrum and that it is also possible to improve the wavelength selection made by the MLR method using the PLS method to check the prediction robustness of the selected wavelength by cross-validation.