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Chemometric modelling of apple quality with **spectroscopy**

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Introduction

Near infrared (NIR) spectroscopy offers the prospect of quality evaluation of intact fruit. Standard laboratory testing involves destructive assessment of parameters such as sugar and dry matter (DM). DM is considered a reliable indicator of quality and storage potential in apples. There is a relationship between DM content at harvest and fruit sugar levels after storage. The aims of the experiment were:

•To construct calibration models for the non-destructive prediction of quality in 'Elshof' apples

•To evaluate the performance of these models depending on the preprocessing methods used

Materials and Methods

150 'Elshof' apples grown in the orchards of Aarhus University were analysed at harvest in October 2011. Two reflectance spectra were obtained from each fruit using an AgriQuant FT-NIR Analyser fitted with an InGaAs detector covering a spectral range of 4,000-11,000cm^{-1}. Two samples were removed from each fruit for DM and sugar analysis at the same equatorial location on the fruit as the spectra.

Fig. 1 Taking spectra on an apple between two measuring lines

Spectra outside the range of the detector were removed due to excessive noise. Destructive measurements and spectra were averaged to give a dataset based on each fruit. The instrument automatically transformed the spectra from reflectance (R) to absorbance (log 1/R).

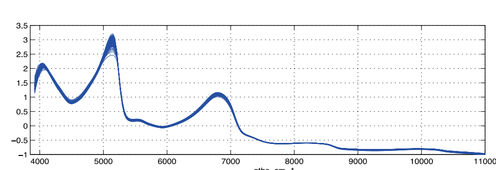

Fig. 2 Typical InGaAs apple spectra after SNV pre-processing

PLS regression modelling, using both quality and spectral data, was performed. The spectra were pre-processed to improve prediction modelling with Standard normal variate (SNV) or Multiplicative scatter correction (MSC). All models were validated using 2-segmented cross-validation.

Results

The spectra have three distinct absorbance peaks - including water at 6986 and 5128cm^{-1} and carbohydrate at 4302cm-1. These peaks are composed of multiple overtone and combination bands. Baseline correction and pre-processing improved prediction modelling for both parameters. In contrast to sugar, DM prediction was enhanced by including more latent variables (LV) in the model – 12 for DM compared to an optimum of 7 for sugar.

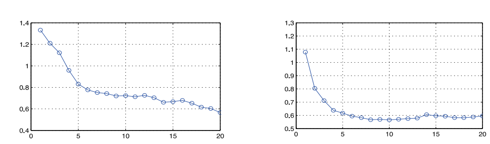

Fig. 3 RMSECV versus nLV plots for DM (left) and sugar

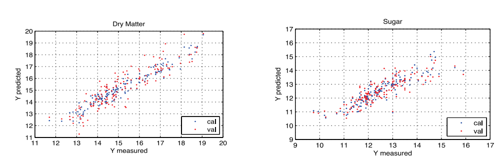

Fig. 4 Predicted versus measured plots for DM and sugar

MSC pre-processing produced better models for DM whilst SNV was sufficient for sugar prediction.

Pre-processing	R^2	RMSECV	nLV
MSC	0.8	0.73	12

Pre-processing	R^2	RMSECV	nLV
SNV	0.7	0.6	7

Fig. 5 Prediction model statistics for DM (top) and sugar

Conclusion

The success of NIR spectroscopy in predicting apple quality depends on the accuracy of the calibration models. The results show a correlation between DM or sugar and the spectra but the R^2 values are not strong enough and the RMSECVs are too high to allow accurate quality prediction.

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