Calibration transfer between SWNIR Si PDA instruments

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Introduction

Silicon photodiode array (PDA) detectors find use in high speed, low cost applications that require use of the Herschel region of the spectrum. Photodiode spectrometers vary in both photometric response and wavelength accuracy, such that while matching of instrument optics minimises differences between units, software correction is required in the calibration transfer process. The current study documents procedures for the porting of models between instruments, in context of assessment of intact fruit, i.e. high moisture (non storable) produce.

Results

The performance of models created on one unit and used in prediction of spectra collected on another unit was impacted both in terms of bias corrected RMSEP (SEP) and bias (Table 1).

Unit E, which used an older Zeiss MMS 1 spectrometer, suffered a poor pixel-wavelength assignment. Wavelength recalibration improved model performance on this but not other units.

The calibration transfer method with best results was PDS, based on a transfer set of the same variety of fruit.

Model updating and global models was successful, with use of more PLS factors (except unit E).

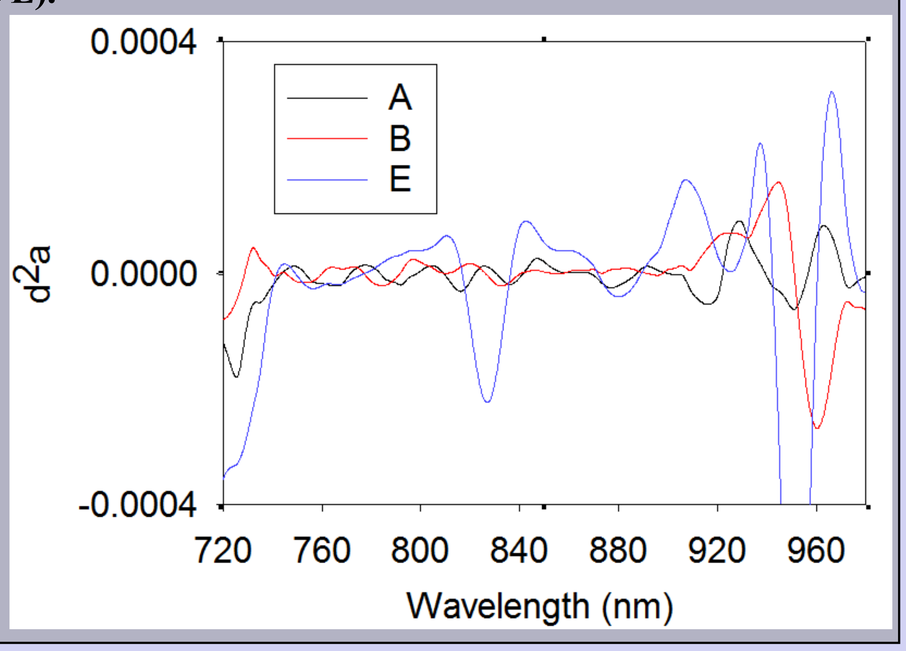

Figure 2. Difference D2Abs spectra (slave minus master)

Materials and Methods

ABS 2D spectra were acquired of mango fruit using six F-750 instruments (which use an interactance optical geometry), then fruit were destructively sampled for oven dry matter (%DM). Separate populations (harvest dates) were used for calibration (n=232, μ=13.7, σ=1.6 %DM), transfer (n=100, μ=14.4, σ=1.3 %DM), and validation (n=100, μ=13.8, σ=1.5 %DM). An apple set was also used in transfer (n=80). A partial least squares regression model for fruit dry matter (%DM) developed on the master unit was used with the unaltered and transformed spectra of the slave units, using the transfer methods of piecewise direct standardisation (PDS)[1], the difference spectrum adjustment (DSA)[2], as well as use of wavelength recalibration, global models (cal set spectra from all units) and model updating (MU, master unit spectra with slave unit transfer set spectra).

Pixel-to-wavelength assignments for the 695 – 1014 nm range were generated using a fourth order polynomial fit to wavelength peaks of spectra of polypropylene and mango fruit[3].

All calculations were performed using MATLab R2014a (MathWorks Inc., Natick, MA, USA) with PLS toolbox 7.3 (Eigenvector Research Inc., Wenatchee, WA, USA).

Figure 1. The F-750 (Felix Instruments) collects spectra between 340 and 1050 nm at ca. 3.3 nm steps and 10 nm FWHM resolution, using a Zeiss MMS 1 NIR enhanced spectrometer module.

	Master	A	B	C	D	E	Master	A	B	C	D	E
				R^2						Bias		
Direct	0.90	0.78	0.53	0.90	0.36	0.57	0.01	1.94	-0.26	-2.81	-1.68	-17.64
DSA	0.90	0.78	0.53	0.90	0.36	0.57	0.01	-0.37	-0.57	0.22	-0.63	0.03
Wave ADJ + DSA	0.90	0.82	0.51	0.86	0.56	0.82	0.01	0.18	-0.27	0.38	-0.17	0.01
PDS	0.90	0.87	0.84	0.89	0.88	0.91	0.01	0.01	0.09	0.14	0.20	-0.01
PDS(mango var 1 as transfer set)	0.90	N/A	0.82	0.88	0.85	0.89	0.01	N/A	0.04	-0.07	-0.09	-0.66
PDS (var 2 as transfer set)	0.90	N/A	0.41	0.82	0.86	0.92	0.01	N/A	0.40	-0.87	-0.03	-0.30
PDS (apple as transfer set)	0.90	0.89	0.83	0.88	0.87	0.65	0.01	-0.20	0.11	0.12	0.14	-1.20
Global	0.83	0.84	0.75	0.85	0.79	0.75	-0.03	0.30	0.42	-0.08	-0.13	0.38
Global (10 PCs)	0.90	0.89	0.85	0.92	0.86	0.79	0.02	-0.04	0.19	0.07	-0.16	0.37
Master model, global MU	0.86	0.86	0.82	0.88	0.85	0.77	0.14	0.14	0.36	-0.08	-0.07	0.43
Master model, global MU (10 PCs)	0.92	0.88	0.86	0.92	0.87	0.81	-0.03	-0.15	0.08	0.07	-0.30	0.23
Individual MU	0.91	0.86	0.83	0.89	0.84	0.87	-0.09	-0.42	-0.22	-0.05	-0.21	0.02
Individual MU - master predicted DM (no wet chem)	0.90	0.85	0.82	0.87	0.83	0.86	0.01	-0.22	-0.07	0.10	-0.07	0.12
Individual models using predicted DM (no wet chem)	0.89	0.85	0.82	0.84	0.84	0.81	-0.01	0.14	0.14	0.07	-0.03	-0.24

Table 1. DM prediction statistics for a model transferred (using various methods) from a F-750 unit master to slaves A, B, C, D and E.

Conclusion

Best results (R^2 and bias) were obtained using PDS using the same variety of fruit in calibration and transfer sets. This method is impractical due to seasonal availability of fruit. PDS using apple spectra can be achieved year round. A global model across units or model updating, including with use of reference values as estimated by the master unit can be utilised in field situations.

References

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