CLASSIFICATION OF BITTER AND SWEET ALMONDS USING NIR MINIATURIZED INSTRUMENTS

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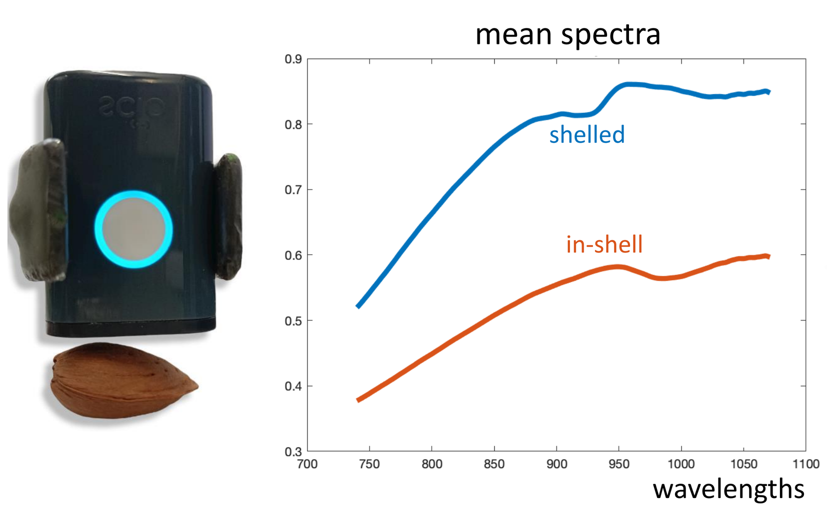
INTRODUCTION

Miniaturized NIR instruments have gained more interest in recent years despite the lack of proper analytical strategies to obtain reliable results with their use. In this work, we have studied different sources of variability to characterize the performance of two portable low-cost NIR devices (SCiO and NeoSpectra) by measuring sweet and bitter almonds (shelled and in-shell measurements). Measurement error covariance and correlation matrices were calculated and then visually inspected to find the optimal preprocessing technique and to check if this strategy results in an improvement in the construction of classification models to distinguish sweet and bitter almonds.

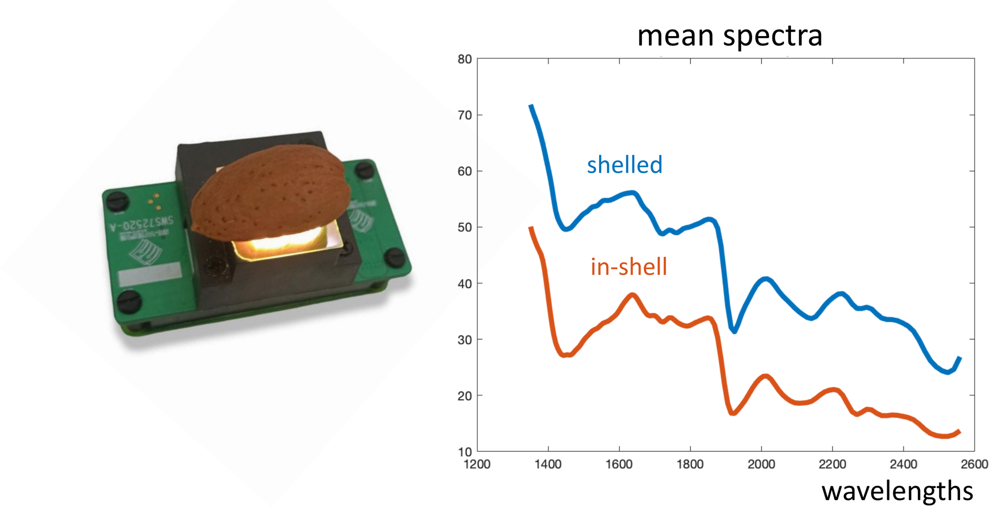
INSTRUMENTATION AND EXPERIMENTAL WORK

SCiO (Consumer Physics)



- 740-1070 nm (331 λ)
- Dispersive element
- Osram broadband IR led
- Photodiode array
- Contact to 1 cm-distance measurements

NeoSpectra (Si-Ware)



- 1350-2558 nm (134 λ)
- Monolithic MEMS Michelson interferometer
- Three tungsten halogen lamps
- Single InGaAs photodetector
- Contact measurements

ECMs

The error covariance and correlation matrices were calculated experimentally using Matlab through the measurement of 15 spectra (3 experimental replicates with 5 instrumental replicates each) for each almond and then average covariances were pooled over the entire almond samples. A total of 247 almonds were analyzed of which 130 were sweet almonds, and 117 were bitter almonds. Almonds were measured in shelled and in-shell forms.

Preprocessing methods evaluated

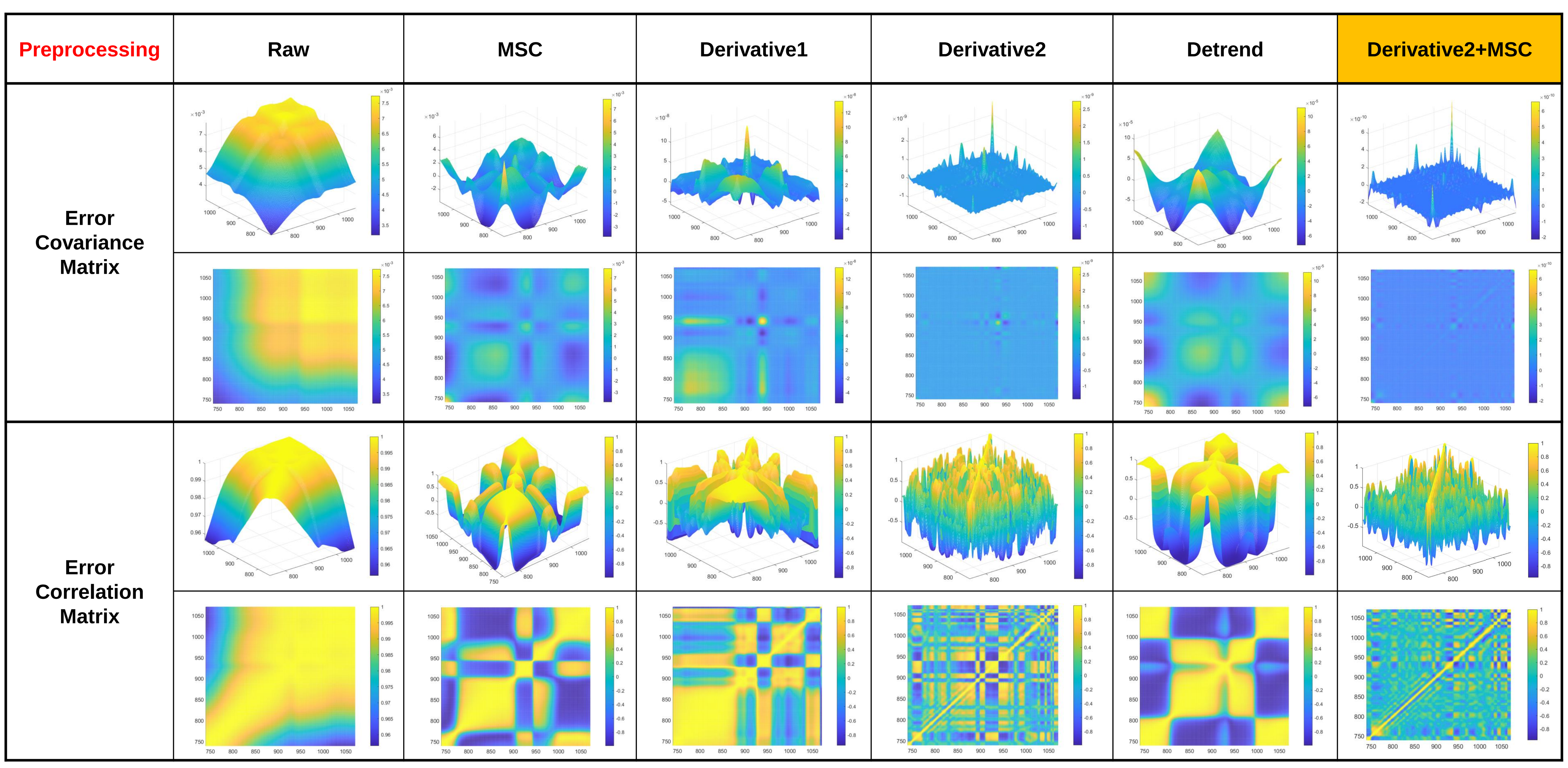
Different spectral pre-processing methods were tested: multiplicative scatter correction (MSC), standard normal variate (SNV), detrend, first and second Savitzky–Golay derivatives with a different number of smoothing points. Data were always mean-centered.

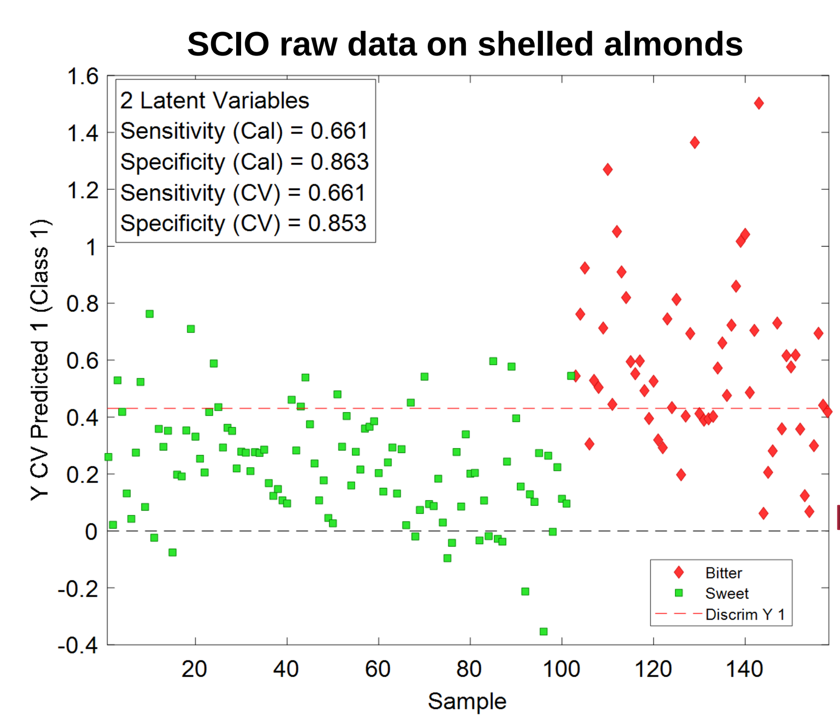
Validation of PLS-DA models

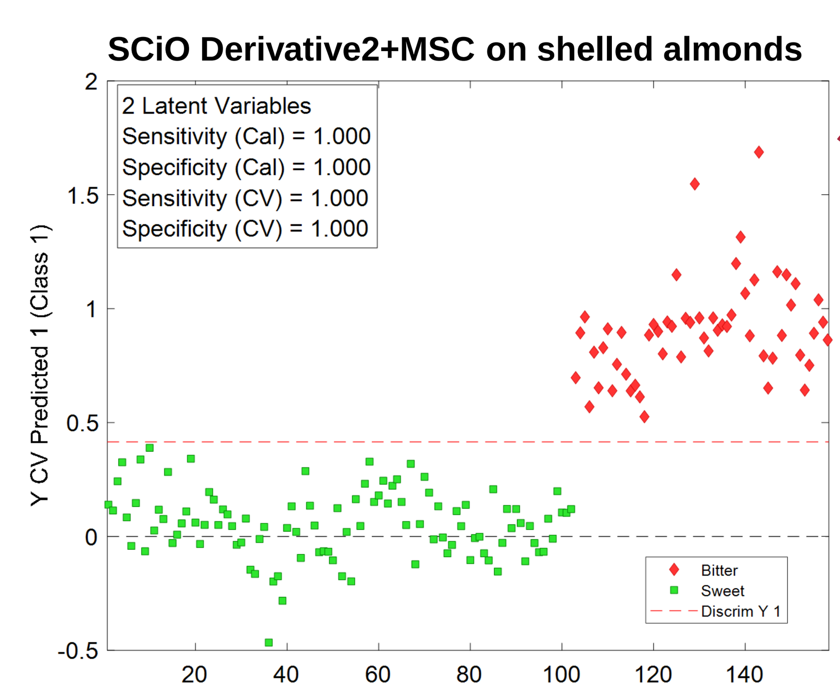
Venetian blinds with different data splits was used for cross-validation. For the prediction models, separate training sets and test sets were used. The PLS Toolbox running on Matlab was used for calculations.

RESULTS AND DISCUSSION

- ❖ The following figures correspond to SCiO measurements, which produces the best results, on shelled almonds. NeoSpectra gives different results depending on the analytical session used and these calculations are in progress.
- ❖ Preprocessing techniques that resulted in flat and smooth surfaces known as independent and identically distributed errors (*iid*) without any structure of errors, were found to be the optimal preprocessing as shown in the figures below.







PLS-DA	Sensitivity	Specificity	Accuracy	RMSEP	RMSECV	LVs
SCiO	1.00	1.00	1.00	0.20	0.19	2
NeoSpectra	0.78	0.58	0.68	0.54	0.34	3

- ❖ For the classification with SCiO, 2nd-degree derivative combined with MSC produced optimal preprocessing.

- ❖ SCiO produced good classification models while NeoSpectra produced less accurate models.

CONCLUSIONS

- ✓ Error covariance and correlation matrices can be used to identify in a visual way the optimal preprocessing for multivariate data analysis in miniaturized NIR instruments.
- ✓ The identification of the optimal preprocessing allowed us to develop optimal classification models.
- ✓ Bitter almonds can be classified from sweet almonds as in-shell and shelled forms using portable low-cost NIR instruments after selecting optimal preprocessing. SCiO measurements provide the best classification models.

REFERENCES

[1] B. Giussani, G. Gorla, J. Riu, Crit. Rev. Anal. Chem. (2022) DOI: 10.1080/10408347.2022.2047607.
[2] G. Gorla, A. Taiana, R. Boqué, P. Bani, O. Gachiuta, B. Giussani, Anal. Chim. Acta, 1211 (2022) 339900.
[3] Leger, M. N.; Vega-Montoto, L.; Wentzell, P. D. Chemometr. Intell. Lab. Syst. 2005, 77 (1), 181–205. DOI: 10.1016.2004.09.017.

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