Jokin Ezenarro

Universitat Rovira i Virgili (Spain)

Research fields and interests

Jokin Ezenarro is a postdoctoral researcher in chemometrics and analytical chemistry, currently based at the Department of Food Science at the University of Copenhagen. His work focuses on the development of methods for spectroscopic applications, with particular emphasis on dataset validation strategies, measurement error quantification, and the optimisation of preprocessing techniques. He has experience working with both benchtop and miniaturised NIR instruments and has applied his methodologies across a range of food applications.

From noise to information: quantifying spectral measurement errors to guide preprocessing in NIR spectroscopy

J. Ezenarro, D. Schorn-García, O. Busto, R. Boqué

Miniaturised near-infrared (NIR) spectrometers are transforming the applications of spectroscopy in analytical chemistry, enabling portable, fast, and low-cost measurements. However, differences in instrument architecture, evolving manufacturing processes, ambient temperature and light, and other phenomena introduce measurement errors that can significantly impact model robustness and transferability, especially in data-driven classification or regression tasks.

We present a systematic strategy to characterise and manage measurement errors in miniaturised NIR instruments, using two case studies: (i) the classification of sweet and bitter almonds using three low-cost portable devices, and (ii) the prediction of cannabinoid content across 15 NIR spectrometers of the same model and their virtual counterparts. In both cases, error covariance and correlation matrices were constructed from spectral replicates to uncover underlying error structures (such as heteroscedasticity, error correlations, signal-dependent noise, and device-specific biases) that directly influence the effectiveness of chemometric modelling.

To aid preprocessing selection, we introduce the Integral Error Correlation Index (IECI): a novel metric that quantifies the degree of correlation in measurement errors, offering an objective criterion for the screening of preprocessing methods. Results demonstrate that lower IECI values are associated with more homoscedastic, independent errors and, therefore, yield simpler, more accurate PLS models. For example, selecting preprocessing strategies guided by IECI led to classification accuracies up to 98% in the almond study and significantly improved prediction precision in cannabinoid quantification. This approach represents a step forward in evidence-based preprocessing and instrument evaluation. It supports more reliable multivariate models and facilitates the broader adoption of portable NIR devices in food authentication.