FRUITNIR-GUI: A graphical user interface for correcting external influences in multi-batch near infrared experiments related to fruit quality prediction

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Postharvest Biology and Technology, Volume 175, May 2021, 111414

Abstract

Near infrared (NIR) spectroscopy is widely used for non-destructive prediction of fruit traits. Common traits such as dry matter (DM) and soluble solids contents (SSC) can be predicted with reliable accuracy. However, the main problem with NIR spectroscopy is that a model developed on one batch may not perform very well when tested on other batches. Reasons for that are the physical, chemical and environmental differences between the experiments performed in different batches. To deal with these issues, approaches such as variables selection, dynamic orthogonal projection (DOP) and transfer component analysis (TCA) can be used. However, the techniques are known but it is rarely possible for a new user or non-specialist to implement them in the practical situations. To overcome this limitation, for the first time, a graphical user interface-based toolbox (FRUITNIR-GUI) for basic chemometric data processing (regression and variable selection) is developed and presented. The GUI allows performing model adaption and maintenance in the context of multi-batch NIR spectroscopic experiments related to fruit. Furthermore, a case-study demonstrating its effectiveness in correcting for seasonality when predicting DM in apples is presented. The toolbox provides a push-button approach to build chemometric models of varying complexity for the characterization of fruit quality. Moreover, approaches such as variable selection and batch correction with DOP and TCA can improve the model performances on new batches. FRUITNIR-GUI can be freely downloaded at https://github.com/puneetmishra2/FRUITNIR and run using the password “welovenirs” (without quotation marks).