Two standard-free approaches to correct for external influences on near-infrared spectra to make models widely applicable

Puneet Mishra, Jean Michel Roger, Douglas N. Rutledge and Ernst Woltering

Postharvest Biology and Technology, Volume 170, December 2020, 111326

Abstract

In near-infrared (NIR) spectroscopy of fresh fruit often the external influences due to differences in physical, chemical and environmental conditions lead to model failure. Correction methods are required where standard samples are measured covering all different conditions and then remodeling is performed. However, in the real-world, it is often difficult to measure standard samples. To deal with this, two different approaches to correct for external influences without standard sample measurements i.e., dynamic orthogonalization projection (DOP) and domain adaption (DA), are presented, and for the first time are applied to NIR spectroscopy of fresh fruit. Four different case studies, chosen based on their importance and their frequency of occurrences in the NIR spectroscopy domain, were used for the demonstration. The first case was an adaption to maintain the predictive performance of a model when used on a spectra from a second similar instrument. The second case was the correction of the temperature effects due to sensor heating. The third and fourth cases were about maintaining the model performance for multi-season fruit quality prediction models for mangos and for apples. In all of the cases, the aim was to solve the challenges without resorting to new measurement of standards. The results showed that for all the cases, both DOP and DA improved model performances. Up to 31% increase in $R^2_{p,}$ and 98% and 66% reduction in prediction bias and root mean squared error (RMSE) of prediction were noted, respectively. The main benefit of the DOP and DA techniques in NIR spectroscopy is the limited need for standard measurements, providing general-purpose tools to complement the NIR spectroscopy and make the models scalable, transferable, and reusable.