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Robustness improvement of NIR-based determination of soluble solids in apple fruit by local calibration

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ABSTRACT

Nondestructive determination of soluble solids content (SSC) has been used in the fruit industry by using near infrared (NIR) spectroscopy. The robustness of prediction models, which is of great importance in practical application, remains a challenge because of the variability of fruit samples associated with different maturity stages and storage status. Local calibration was investigated in this study as means of improving prediction robustness. As robustness is often reduced by extrapolation, we assessed the robustness by the accuracy of predicting extrapolation samples (samples outside the range of the calibration set). Local calibration was effective in improving the robustness of models compared with global calibration. It is proposed that local calibration optimizes the composition of calibration subset by selecting the samples of same level of starch fractions for each sample to be predicted, and thus provides better robustness due to the homogeneity.

1. Introduction

Sweetness is an important taste index, as it directly influences the evaluation of apple by consumers. Sweetness, which is approximately quantified by the soluble solids content (SSC), can be nondestructively determined by near infrared (NIR) spectroscopy. As one of the most appropriate techniques for rapid assessment of the internal quality of fruits (Xie et al., 2016), NIR spectroscopy exploits the theory that the internal composition and structure of samples affect the wavelengths of their absorption energies, yielding different spectral characteristics. Considering that signals can be weak and overlapping, and given the complexity of NIR spectra, the success of NIR-based measurements largely relies on mathematical models that quantify the relationship between the spectra and the targeted properties. The selection of samples for the calibration set critically affects the final calibration performance (Berzaghi et al., 2000). In current NIR models for predicting the SSC of fruit (either by on-line sorting systems or portable instruments), the calibration set is typically constructed from many samples covering a large spectral variability, namely, global calibration.

Although global calibration improves the robustness of the prediction to a certain extent (Bobelyn et al., 2010; Louw and Theron, 2010; Parika et al., 2016), it has several limitations. Firstly, with the enlarged variability of calibration set, the accuracy of prediction usually decreases (Shenk et al., 1997). This is because the heterogeneity, resulting from the large variability of calibration set, increases the risk of non-linearity, and thus makes the original model less appropriate. Secondly, it is not robust against extrapolation samples. Theoretically, a multivariate regression model works well only when the samples to be predicted fall in the range of calibration set. An ideally perfect model therefore is the one that include all possible sources of variation that can be encountered in future predictions in the calibration set; however, this is almost impossible in real world (Balabin and Lomakina, 2011), especially when evaluating agricultural products. A good calibration method applicable in practice should have the ability to work under extrapolation conditions (Barman et al., 2010; Balabin and Lomakina, 2011; Balabin and Smirnov, 2012).

An alternative to global calibration is to use a local approach, which is capable of dealing with the non-linearity problem as can support vector machine (SVM) or artificial neural network (ANN). The essential idea of local calibration is to identify, within the calibration set, a subset of samples those are spectrally similar with the one to be predicted, and build a model specifically for the sample (Fearn and Davies, 2003). The approaches include comparison analysis using restructured near infrared and constituent data (CARNAC) (Davies et al., 1988), local weighted regression (LWR) (Næs et al., 1990; Næs and Isaksson, 1992) and LOCAL (Shenk et al., 1997; Barton et al., 2000; Berzaghi et al., 2000). These approaches differ by their similarity definitions and ways of building the local model. CARNAC uses a method combing Fast Fourier Transformed spectra and reference values. LWR select similar

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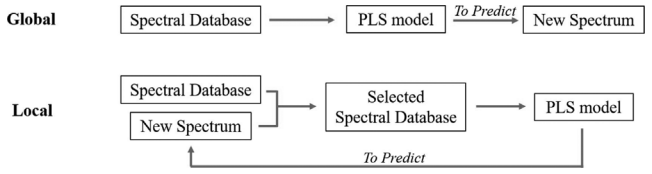

Fig. 1. Flowchart comparison of global calibration and local calibration. PLS: partial least squares.

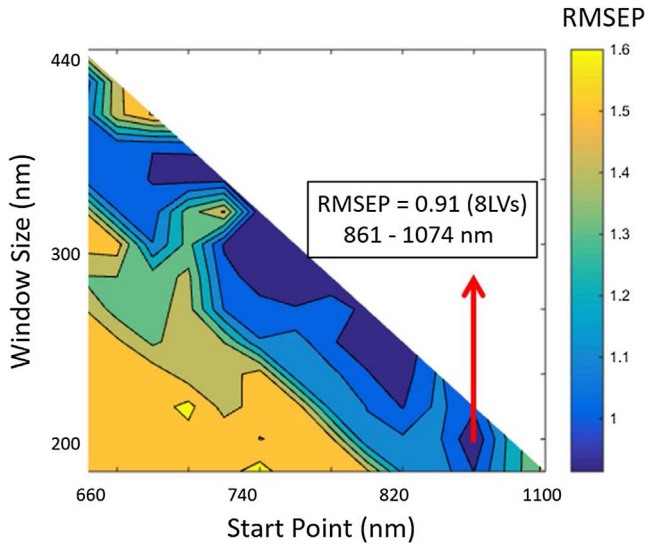

Fig. 2. Result of wavelength selection by CSMWPLS. The selected range was 861–1074 nm, where the RMSEP was minimized. RMSEP: root mean square error of prediction; LVs: latent variables. (For interpretation of the references to colour in text, the reader is referred to the web version of this article).

samples in the principal components space. LOCAL uses the correlation between the spectrum of the sample to be predicted and that of each sample in database. Furthermore, Gogé et al. (2012) combined two spectral compression methods (Principal Component Analysis or Fast Fourier Transformation) with two distinct distance metrics (Mahalanobis distance or correlation coefficient) to optimize the criteria for sample selection, and concluded that the index based on the correlation coefficient with FFT compression led to best results for the prediction of soil constituents. Allegrini et al. (2016) proposed two novel algorithms, namely, Local Calibration by Percentile Selection (LCPS) and Local Calibration by Customized Radii Selection (LCCRS), which use Mahalanobis distance to select similar samples in PLS scores space, and automatize the decision about the number of samples used to build each local model. A comparison between global calibration and local calibration is illustrated in Fig. 1.

The most prominent effect of local calibration is the improved prediction accuracy compared with global calibration. Sánchez et al. (2012) applied the LOCAL algorithm to a MEMS handheld NIR instrument for quality evaluation of strawberries. They found that the application of a LOCAL algorithm improved the ability of models to predict SSC, titratable acidity, and firmness, and concluded that the LOCAL algorithm was appropriate for use in routine quality predictions in intact strawberries in the field and in cold storage. Similar results were also found for apple (Dardenne et al., 2000), grape (Dambergs et al., 2006), and nectarine (Sánchez et al., 2011). Fernández-Ahumada et al. (2013) compared the performances of the CARNAC, LWR and LOCAL methods in NIR predictions of compound feed ingredients. The three local methods considerably reduced the prediction error from that of global calibration.

Most studies comparing local calibration and global calibration have focused on prediction accuracy, but not robustness. In the case of NIR-based determination of SSC in fruit, the prediction model is usually required to be adjusted or re-built because of the variability of the samples associated with factors such as different maturity stages, different cropping patterns, and different storage status. Therefore, a robust calibration strategy capable of coping with such problems is required. In this work, we evaluate whether local calibration confers higher robustness than global calibration. Given that the extrapolation problem seriously degrades the robustness in practical applications (Balabin and Lomakina, 2011; Balabin and Smirnov, 2012), we take the accuracy of predicting extrapolation samples (samples outside the range of the calibration set) as the robustness measure. In SSC predictions, the extrapolation problem arises in both the Y-space and the X-space. In the former, the Brix values of test samples lie outside the calibration range; in the latter, the spectra of test samples exhibit different characteristics to the calibration set. Such difference can be introduced by the change of season (Parika et al., 2016), origin, shelf-life (Bobelyn et al., 2010) and maturity stage (Martins et al., 2016). A model with weak performance on extrapolation problems is insufficiently robust, and thus not useful in practice. This is the first attempt to study the extrapolation problem in NIR-based SSC prediction, which is the major reason degrading the robustness in practical applications. Local calibration is tried for potential improvement.

2. Materials and method

2.1. Apple samples

The success of local calibration depends to a large extent on the range of spectral library. To obtain data with a relatively wide range of variation, 'Fuji' apples were harvested at five maturity stages of two different cropping patterns (pre-harvest fruit bagging and non-bagging), and the samples were divided into two groups (harvest-time and post-storage) for further data collection. The five maturity stages were 165, 172, 179, 186, and 193 days after full bloom (DAFB). As each stage corresponds to a different physiological development phase of the fruit, the samples span a broad range of physicochemical properties. Hereafter, samples of the five maturity stages are referred to as "m1", "m2", "m3", "m4", and "m5", respectively. Data of the harvest-time samples were collected immediately after harvest, while data of post-storage samples were collected after storage at 2 °C for 6 months. Consequently, we prepared 20 combinations of samples (five levels of maturity, two cropping patterns, and two storage statuses). After collecting the data of 24 samples for each combination, we generated 480 samples with presumably variable SSC values and spectral characteristics.

2.2. Data collection

To avoid the influence of temperature, the fruit samples were equilibrated overnight (> 16 h) at 20 °C before collecting their spectra. For spectral and SSC data collection, each apple was pre-marked at two opposite locations on its equator. The NIR spectra were collected in interactance mode in a Fourier transfer (FT)–NIR spectrometer (Thermo Electron Corp., Madison, WI, USA) equipped with a Si detector. Each spectrum was recorded as log (1/R) (R = reflectance) in the 15,000–9000 cm^{-1} (667–1111 nm) range with a resolution of 16 cm^{-1} by averaging 64 scans. Immediately after spectral collection, the juice was squeezed from the pulp at the sites from which the NIR spectra were taken, and the SSC was measured with an Atago Pallete Series Model PR101 digital refractometer (Atago Co. Ltd., Tokyo, Japan).

2.3. Calibration and prediction set partitioning

To estimate the robustness of the tested models, the extrapolation samples were partitioned as the prediction set. The partitioning was performed as follows: