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Research Paper

Effect of spectrum measurement position variation on the robustness of NIR spectroscopy models for soluble solids content of apple

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In this paper, the influence of variation of spectrum measurement position on the near-infrared (NIR) spectroscopy analysis of soluble solids content (SSC) of apple was studied. The spectra were collected around stem, equator and calyx positions for each apple. Partial least squares (PLS) was used to develop compensation models of SSC for each measurement position separately (local position models) and for the full data set containing all positions (global position model). The results indicated that the influence of measurement position on the spectra affected the prediction accuracy of SSC. Compared with the local position models, the global position model was well suited to control the prediction accuracy of the calibration model for SSC with respect to the variation of spectrum measurement position. Next, competitive adaptive reweighted sampling (CARS) was used for the robust global position model to select the most effective wavelengths (EWs). It indicated that the global model established with effective wavelengths (EWs-global position model) achieved more promising results, with r_p and RMSEP values for three measurement positions being 0.977, 0.977, 0.955 and 0.409, 0.386, 0.486 °Brix, respectively. Moreover, the local position models based on these effective variables (EWs-local position models) were more accurate than the models built with full range spectrum. The overall results indicated that the EWs-global position model could make the variation of spectrum measurement position a negligible interference for SSC prediction.

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1. Introduction

Apple is an important and widespread agricultural commodity on global produce market (Mendoza, Lu, & Cen, 2014). Apple is also a good source of antioxidant components, such as ascorbic acid and polyphenolic, which exert protective effects against various degenerative diseases (Giovanelli, Sinelli, Beghi, Guidetti, & Casiraghi, 2014). Soluble solids content (SSC) is one of the most important internal properties that influence the consumer purchasing decision on fresh apple fruit (Lu, 2004). It is also a key parameter in assessing apple maturity and determining harvest time (Peng & Lu, 2008). Consequently, non-destructive and rapid detection of SSC of apple is of great value in determining optimal harvest time and meeting the ever-increasing consumer demands for consistent, high quality fruit.

The use of NIR spectroscopy to measure internal quality attributes of fresh fruit has been investigated extensively during the last decade (Nicolaï et al., 2007) because the technique allows non-destructive analysis of food products, requires little or no sample preparation, generates no waste and allows several constituents to be evaluated at the same time (Oliveira, Bureau, Renard, Pereira-Netto, & Castilhos, 2014). NIR radiation can be absorbed by fundamental vibrations of C–H, O–H and N–H molecular bonds in compounds. The recorded NIR spectroscopy contains both physical and chemical information of the radiated samples (Cabassi, Cavalli, Fuccella, & Gallina, 2015). The technique, coupled with an appropriate predictive model which could be established by various statistical methods, such as multiple linear regression (MLR), principle component regression (PCR) and particle least square (PLS), has been successfully applied for non-destructive SSC assessment of apple (Ventura, de Jager, de Putter, & Roelofs, 1998; Liu & Ying, 2005; Xiaobo, Jiewen, Xingyi, & Yanxiao, 2007; Fan, Zha, Du, & Gao, 2009; Mendoza et al., 2014).

In order to get more stable and robust NIR calibration models of apple SSC for practical implementation, the effect of biological variability (cultivar, season, shelf-life and origin) (Peirs, Tirry, Verlinden, Darius, & Nicolaï, 2003b; Bobelyn et al., 2010) and fruit temperature (Peirs, Scheerlinck, & Nicolaï, 2003a) on the spectra and robustness of NIR models for SSC of apple has been studied. It was found that the biological variability and temperature fluctuation affected the NIR spectra and the accuracy of the models increased considerably when more variability was included in the calibration data set. In addition, Chauchard, Roger, and Bellon-Maurel (2004) developed a methodology based on variable selection (wavelength selection) to reduce the effect of the apple fruit temperature on SSC prediction. The MLR variable selection was performed with a customised stepwise procedure and PLSR model variables were selected using the genetic algorithm (GA) technique. This study demonstrated that the stepwise MLR was the most efficient method to reduce the effect of fruit temperature, when compared with GA-PLSR or external parameter orthogonalisation (EPO)-PLSR which was a preprocessing method aimed at removing from the spectra space the part mostly influenced by temperature variations (Roger, Chauchard, & Bellon-Maurel, 2003). The effect of spectrometer temperature on the robustness of the apple SSC calibration model was studied by Sánchez, Lurol, Roger, and Bellon-Maurel (2003), and they found that the relationship between prediction result and spectrometer temperature was described by a linear function within the considered temperature range.

With the development of NIR technology, much attention has been paid to the design of portable instruments and on-line monitoring of SSC during commercial applications. A portable instrument could be used to detect the distribution of SSC over the whole surface within an individual fruit sample, which could better evaluate the quality attribute for fruit on trees or apple fruits after postharvest storage. For on-line detection, the position facing the detection probe within the fruit sample is random because of the size of the fruit or the transmission of the fruit tray. As the NIR technique only assesses a small portion of the each individual product unit, the spatial variability of spectrum measurement position should be taken into account for developing a robust calibration model for both portable instrument and on-line detection system. The effect of spectrum measurement position on the spectra acquired from five different locations on each apple around the equator was studied by one-way analysis of variance (ANOVA) by Liu (2006). It was found that there was no obvious difference between these spectra at absorption peaks of 10,176, 8313, 6860, 5172 and 4321 cm^{-1} wave number and that the effect of measurement position around the equator on SSC prediction was negligible. Fu (2008) analysed the difference of spectra acquired from different positions of pear. The results of ANOVA of average absorbance and root mean square noise for spectra obtained from three latitudes and three longitudes (nine points) on each pear fruit shown that the differences of spectra from different latitudes were much more than the difference of spectra from different longitudes. As a result, the spatial variability of spectrum measurement, especially along the distal (stem)-proximal (calyx) axis within an individual fruit may affect the accuracy of NIR calibration models.

However, the calibration models in the literatures about apple SSC prediction were almost all developed with the spectra acquired from equatorial position. The accuracy of these calibration models might be affected when they were used to predict the SSC in other positions on the apple, which makes these models difficult to apply in an industrial environment because of the lack of robustness. Therefore, it is necessary to study the effect of variation of spectrum measurement position on the SSC detection of apple. The objective of this study was to assess the influence of spectrum measurement position on the NIR spectroscopy analysis of SSC of apples. Additionally, we have designed compensation methods to offset the influence.

2. Materials and methods

2.1. Samples

A total of 130 ‘Fuji’ apples (Malus × domestica Borkh. ‘Fuji’) were purchased from the local fruit market in Beijing. All samples were individually washed and numbered and then