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Achieving robustness to temperature change of a NIR model for apple soluble solids content

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Abstract

The temperature difference of fruit itself will affect its near infrared spectrum and the accuracy of its soluble solids content (SSC) prediction model. To eliminate the influence of apple temperature difference on the SSC model, a diffuse transmission dynamic online detection device was used to collect the spectral data of apples at different temperatures, and four methods were used to establish partial least squares correction models: global correction, orthogonal signal processing, generalized least squares weighting and external parameter orthogonal (EPO). The results show that the temperature has a strong influence on the diffuse transmission spectrum of apples. The 20 °C model can get a satisfactory prediction result when the temperature is constant, and there will be great errors when detecting samples at other temperatures. The effect of temperature must be corrected to establish a more general model. These methods all improve the accuracy of the model, with the EPO method giving the best results; the prediction set correlation coefficient is 0.947, the root mean square error of prediction is 0.489%, and the prediction bias is 0.009%. The research results are of great significance to the practical application of SSC prediction of fruits in sorting workshops or orchards.

Keywords: Apple; near-infrared spectroscopy; soluble solids content; temperature correction.

Introduction

Apples are rich in nutrients, replenishing a wide range of vitamins and minerals required by the human body, and their fruit trees are the first fruit tree species in China in terms of planted area and production (Bai *et al.*, 2011). Soluble solids content (SSC) in apples is one of the most important indicators of fruit nutrition and affects the taste and flavor of apples (Li *et al.*, 2016; Zhang *et al.*, 2019). However, for SSC in apples, traditional physical and chemical testing methods are often based on destructive sampling, which is time-consuming and laborious, and cannot quickly sort large quantities of fruit and meet the needs of quality inspection departments for on-site sampling and quality tracking during the growing season.

Visual–near infrared spectroscopy (Vis-NIRS) is a fast, simple, and non-destructive method that has been widely used for rapid internal quality inspection of fruits and vegetables (Gongal *et al.*, 2015; Sun *et al.*, 2020). NIR spectroscopy contains not only the structural and functional characteristics of the sample molecules, but also information on the hydrogen bonding between and within molecules, and the molecular bonding and vibrational modes can be affected by external factors such as temperature (Wülfert *et al.*, 1998; Shan *et al.*, 2015). On the one hand, temperature changes will cause changes in the internal molecular forces of the sample, which will be reflected in changes in spectral vibrations (Liu *et al.*, 2015); on the other hand, temperature changes will also cause changes in the bending and stretching vibrations of the water molecules of the sample, and the absorption bands and intensities of the O–H groups of the water molecules will be changed (Xu *et al.*, 2017). With the development of instrumentation science and technology, testing instruments have moved into production sites (Yao *et al.*, 2013; Wang *et al.*, 2018), such as online fruit quality grading and monitoring of fruit growth characteristics in orchards. When the instrumentation is moved from the laboratory, where the temperature is precisely controlled, to the production site, the fruit temperature varies considerably and if the internal quality of the fruit is tested using a model developed under specific temperature conditions, the results will be less than satisfactory, a problem that can limit the application of the model to a large extent. Therefore, it is necessary to research the temperature effects and correction methods of NIR spectroscopy models for the detection of internal quality indicators of apples, to establish detection models with high accuracy, good stability, and temperature adaptability.

The main temperature correction methods include the global temperature correction modeling method (Wülfert *et al.*, 2000), the exclusion of temperature sensitive bands method (Centner *et al.*, 1996), the spectral correction method (Sun and Fan, 2020), the formula correction method (Kang *et al.*, 2011), and the multi-step modeling

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method using temperature information (Peirs *et al*., 2003). The global temperature correction modeling method uses sample spectra containing temperature variations to build a quantitative analysis model (Sun *et al*., 2018). This method is simple and widely used, but the accuracy of the model relies heavily on the number and representativeness of the calibration set data and needs to cover as many samples as possible with a wide range of temperature variation. The method of removing temperature-sensitive bands uses wavelength selection methods, such as Simulated Annealing (SA; Bao *et al*., 2012), Successive Projections Algorithm (SPA; Peng *et al*., 2014) and Genetic Algorithm (GA; Bouveresse and Massart, 1996) to remove bands that are sensitive to temperature changes, but the removed bands may contain both temperature and concentration information, thus reducing the precision of the model. The formula correction method and the multi-step modeling method using temperature information introduce secondary errors due to temperature intermediate variables, indirect modeling, etc. Spectral correction methods that correct the temperature-varying spectra to those at standard temperatures, such as Piecewise Direct Standardization (PDS; Barboza and Poppi, 2003), generalized least squares weighting (GLSW; Chen *et al*., 2004), orthogonal signal processing (OSC; Fu *et al*., 2012), Individual Contribution Standardization (ICS; Roger *et al*., 2003) and external parameter orthogonal (EPO; Martens *et al*., 2003), can effectively reduce the effect of temperature on model accuracy.

There are no general rules to determine which method to use in which situation, but rather the choice is based on the specific problem. This study aims to develop a more general model for NIR apple SSC detection under temperature variation. Due to the large temperature differences between the fruit in the sorting plant and the orchard, it is necessary to research the temperature effects and calibration methods of NIR spectroscopy detection models for internal apple quality indicators to establish detection models with high accuracy, good stability, and temperature adaptability. In this study, single temperature models, global calibration, and OSC, EPO, and GLSW methods were used to build calibration models and to compare the predicted outcomes.

Materials and Methods

Materials

In this study, 500 apples were purchased from an orchard in Yantai City (China) in October 2022 and stored in a cool and ventilated room using red Fuji apples as the subject. All samples were cleaned and numbered. The samples were divided into eight groups by number and collection temperature and the overall statistics are shown in Table 1. Group 1 of 360 samples, with spectra taken at 20 °C, was used to build the 20 °C model. The spectra of samples from groups 2–7 were collected at 5, 10, 15, 20, 25, and 30 °C as the validation set. The spectra of 20 samples in group 8 were collected at six temperatures, which were used to design the temperature difference matrix. The sample temperature was controlled using a cryostat DM-0040 (Heng Min Instrument, Yancheng, China).

VIS/NIR spectral acquisition

The experiments were conducted using a self-developed diffuse transmission dynamic online inspection device to collect apple spectral data (Liu *et al*., 2021), as shown in Figure 1. The device mainly has a light source, spectrometer, and tray. The light source is six 12-V, 100-W tungsten halogen lamps distributed around both sides of the sample; the QE65000 spectrometer from OceanOptics (Dunedin, FL, USA) is a short-wave near-infrared spectrometer with a wavelength range of 350–1150 nm; the inner ring of the fruit cup is equipped with a soft plastic shading ring, which can effectively suppress stray light through indicators such as the shape and weight of the fruit; when collecting the spectra dynamically online, the fruit cup moves forward with the drive chain and is irradiated by the light source, while the spectrometer collects the spectral information.

The sample temperature was controlled using the cryostat DM-0040, which has a temperature range of 0–90 °C and an accuracy of ±0.1°C. The refrigeration uses a fully enclosed compressor and condenser. The sample was placed in a plastic bag to prevent water from being absorbed into the sample. Set the temperature and place the sample in. Groups 1–7 samples were placed in a water bath at 20, 5, 10, 15, 20, 25, and 30 °C to maintain a constant temperature. Group 8 sample spectra were measured at six different temperatures: t={5, 10, 15, 20, 25, 30} °C. The samples were subjected to a water bath at t=5°C and immersed for 30 min. The apples were then measured one by one with the detection device as soon as possible to avoid temperature changes. They were then placed back into the water bath, whose temperature was raised by 5 °C; this was repeated for each temperature step. Only one spectrum was taken for each sample to avoid changes in sample temperature during the measurements.

Table 1. Overall statistics for apple SSC (%)

Group	Number	Temperature (°C)	Mean (%)	SD (%)
1	360	20	11.9	1.6
2	20	5	12.3	1.3
3	20	10	11.8	1.3
4	20	15	11.8	1.5
5	20	20	11.5	1.2
6	20	25	12.3	1.2
7	20	30	11.7	1.8
8	20	5, 10, 15, 20, 25, 30	12.3	1.6

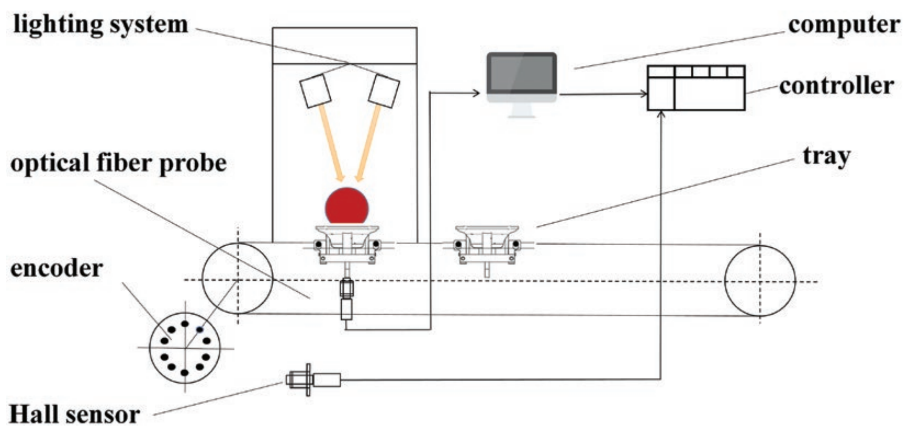

Figure 1. Fruit dynamic online sorting equipment.

Measurement of the soluble solids content of the samples

The SSC of apple samples was measured by a PAL-1 refraction digital sugar meter (ATAGO, Tokyo, Japan) with automatic temperature compensation. After collecting the NIR spectra of the samples, the SSC of the apples was collected at 20 °C. Cut 1-cm thick slices along the equator scanned by Vis-NIR of apples, then divided them into four equal parts squeezed for juice, and took the average value as SSC.

Data processing and analysis

The collected apple spectra and SSC data were imported into MATLAB and Unscrambler software to build a partial least squares (PLS) model of apple SSC. The precision of the model was estimated using the prediction set correlation coefficient (R_p), root mean square error of prediction (RMSEP), and prediction bias (Pred Bias). To remove the effect of temperature on SSC model of apple, global model, OSC, EPO, and GLSW were used to establish PLS model.

The PLS method is currently the most widely used quantitative algorithm (Mateos-Aparicio, 2011). The PLS analysis process analyses the information in the sample component concentration data and the NIR spectral data simultaneously to maximize the extraction of the information with the greatest correlation between the two and performs regression analysis. The global calibration means that a representative number of samples are selected from each sample set at each temperature to build a global calibration model that takes into account all external variations and then uses this model to make predictions (Kuda-Malwathumullage and Small, 2014). The OSC algorithm allows the standardization of spectral data under different external conditions and is used to eliminate incoherent information in the spectral matrix and the concentration matrix, thus building a more general multivariate calibration model (Acharya *et al.*, 2014). The EPO algorithm is a method to reduce the dimension of external interference parameters. This method projects the sample spectrum into the orthogonal space of the interfering variables, thus filtering out the interfering information (Ge *et al.*, 2020). The GLSW algorithm creates a matrix for filtering by analyzing the differences in the X variables corresponding to similar y variables, thus eliminating the information on the changes in the X matrix caused by external variables (Haroon *et al.*, 2020).

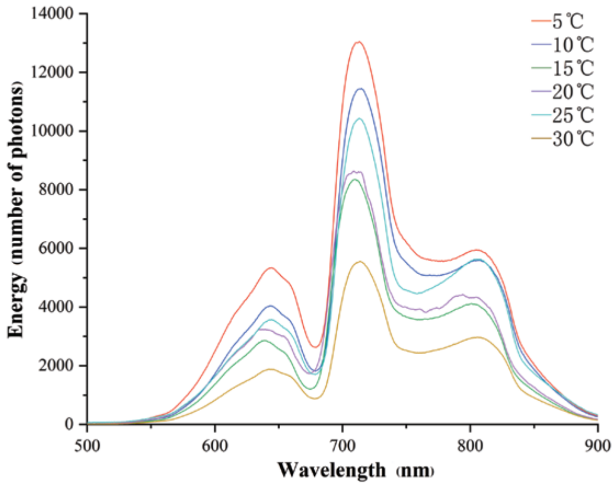

Figure 2. Spectra of apples at different temperatures.

Results and Discussion

Apple spectra at different temperatures

Figure 2 shows the spectra of a particular apple at 5, 10, 15, 20, 25, and 30 °C. The peaks at 710 nm are mainly related to the doubling frequency stretching vibrations of the C–H and O–H bonds (McDevitt *et al.*, 2005), and the peaks at 805 nm are mainly related to the secondary doubling frequency absorption of the C–H and N–H bonds (Zhou *et al.*, 2012). It can be clearly seen that the spectral intensity of apples decreases with increasing temperature near 710 nm. There is little difference in spectral shape and trend of the same apple at different temperatures, but the spectral intensity will change. This indicates that the NIR spectra of the experimentally collected apple samples contain not only information related to the components of the samples themselves, but also information related to the temperature of the samples, resulting in a corresponding change in the spectra of the same samples when the temperature changes.

Effect of temperature on the prediction model

A partial least squares calibration model at 20 °C was developed using data from Group 1 samples. For the experimental samples of 360 apples, the Kennard–Stone (K-S) algorithm was used to classify the calibration and validation sets, with

240 calibration sets and 120 validation sets. To prevent over- or under-fitting of the model, the number of latent variables (LVs) was set from 1 to 20. Figure 3 shows that the results of the 20 ºC model have good correlation, with correlation coefficient of correction set (R_c) and R_p of 0.968 and 0.948, respectively, root mean square error of calibration (RMSEC) of 0.415%, and RMSEP of 0.494%. The difference between RMSEC and RMSEP is small, and the 20 °C model can obtain satisfactory prediction results at a constant temperature.

The 20 ºC model predicts the soluble solids content of samples at mixed temperature (samples from Group 2 to Group 7), and the results are shown in Figure 4. The R_p of the SSC prediction for the validation samples was 0.588 and the RMSEP was 1.181% and the Pred Bias was 0.123%, which shows that the prediction error of the model at 20 °C increased and the accuracy of the validation samples decreased. This is mainly because the temperature has a significant effect on the NIR spectra of apples resulting in a decrease in the prediction effectiveness of the single temperature model at 20 °C for the mixed temperature samples.

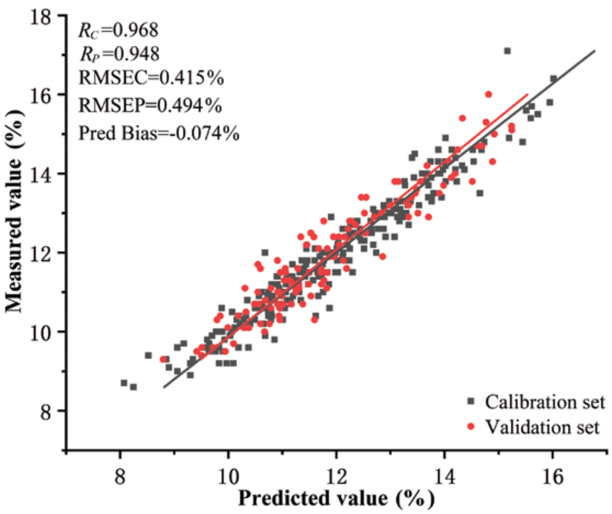

Figure 3. Scatter plot of single temperature model prediction results at 20 °C.

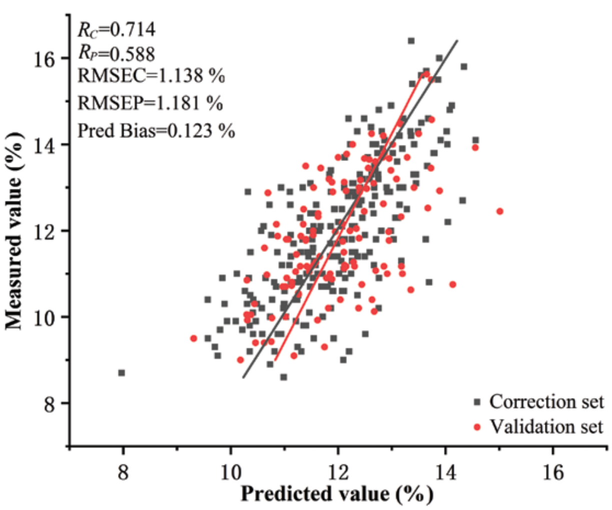

Figure 4. Scatter plot of SSC predictions for mixed temperature samples from a single temperature model at 20 °C.

Global calibration

The global calibration method uses sample spectra containing temperature changes to establish a quantitative analysis model. The K-S algorithm was used to select 10 samples from the validation set at each temperature to be added to the calibration set to build the global calibration model. The results are shown in Figure 5, with Rp increasing to 0.886, RMSEP decreasing to 0.673% and the Pred Bias was –0.036%. The global calibration model reduced the prediction error of the validation sample SSC to some extent. The global correction removes the effect of temperature on prediction to some extent. The global correction model is still less effective in predicting mixed temperature samples and further research is needed into other methods to remove the effect of temperature on the apple SSC model.

Orthogonal signal processing

The OSC algorithm can be used to eliminate irrelevant information in concentration matrix and spectral matrix. The results of the prediction of the SSC of the validation set samples using the developed OSC correction model are shown in Figure 6. The use of the OSC algorithm improved the correlation coefficient of the model to some extent and improved the precision of the correction model, with an R_p of 0.909, an RMSEP of 0.600%, and a Pred Bias of 0.005% for the SSC of the validation set samples. it can be seen that the OSC correction model has improved model performance compared to the original spectral model and the global calibration model.

Generalized least squares weighting

The GLSW algorithm requires adjustment of the weighting parameter α. It determines the strength of the weighted processing, with a general value of 0. 0001–1. A smaller value of the weight α corresponds to a stronger filtering effect. In this study, three kinds of temperature difference matrices D1, D2, and D3 (based on Group 8 data) were designed by subtracting the spectra obtained at the lowest temperature (5 ºC), the middle temperature (15 ºC) and the highest temperature (30 ºC) from the spectral data of Group 8. Using the temperature difference matrix D1 to correct the spectra of the samples, the model obtained the lowest RMSEP. As shown in Figure 7A, the best combination of parameters was α of 0.0001 and LV of 6. The prediction results are shown in Figure 7B, where the model correlation improved to 0.920, the RMSEP was reduced to 0.607%, and the Pred Bias was 0.156%.

External parameter orthogonalization

The goal of the EPO algorithm is to obtain a temperature-independent spectral matrix using the difference matrix (D). The parameter optimization process is similar to that of the GLSW algorithm. The lowest RMSEP was obtained using the D1 difference matrix, and from Figure 8A, the best combination of parameters was g of 20 and LV of 5. The prediction results are shown in Figure 8B, where the R_p as improved to 0.947, the RMSEP was reduced to 0.489%, and the Pred Bias was 0.009%.

Model comparison

The prediction results for the single temperature model, global correction model, OSC correction model, GLSW

Table 2. Prediction results of the PLSR model for soluble solids content using different temperature correction methods

Method	D	R_p	RMSEP (%)	Pred Bias (%)
Single temperature	—	0.588	1.181	0.123
Global correction	—	0.886	0.673	-0.036
OSC	—	0.909	0.600	**0.005**
EPO	**D1**	**0.947**	**0.489**	0.009
EPO	D2	0.899	0.651	0.020
EPO	D3	0.921	0.570	0.026
GLSW	D1	0.920	0.606	0.156
GLSW	D2	0.919	0.607	0.157
GLSW	D3	0.919	0.607	0.156

The model with bold font showed the best result.

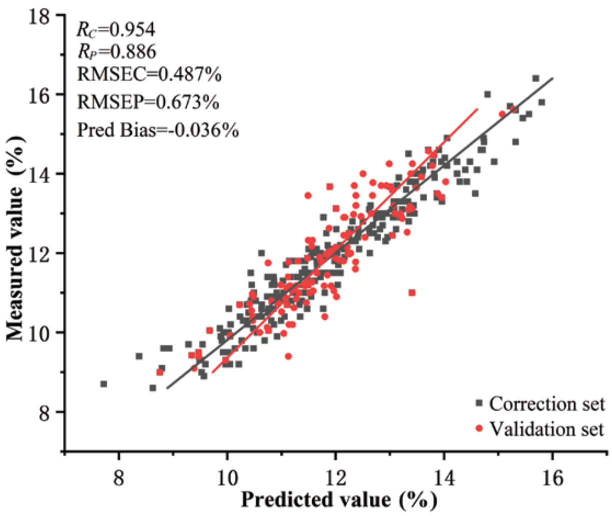

Figure 5. Scatter plot of global calibration prediction results.

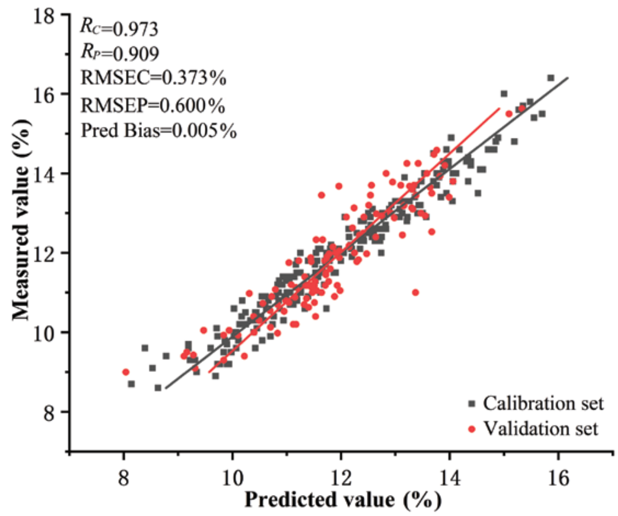

Figure 6. Scatter plot of predicted results from the OSC correction model.

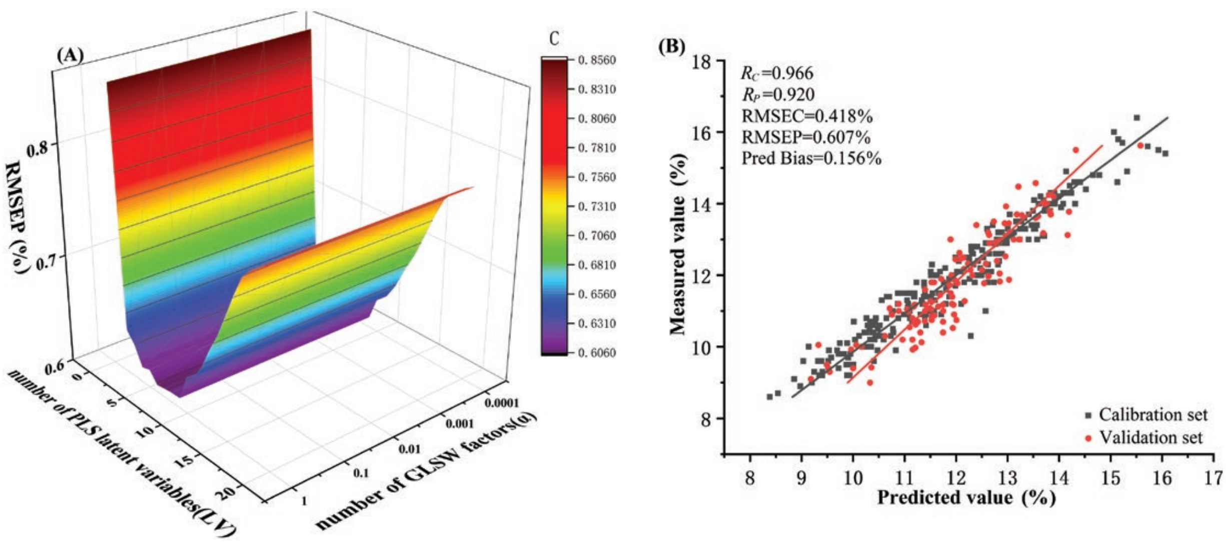

Figure 7. Prediction results of GLSW correction model. (A) Variation in RMSEP based on D1 difference matrix. (B) Scatter plot of GLSW correction model prediction results.

correction model and EPO correction model are shown in Table 2. The results show that global correction, OSC method, GLSW method, and EPO method all improve the prediction ability of the model, and the prediction error of the model with temperature correction is smaller than that of the model without correction. These temperature correction

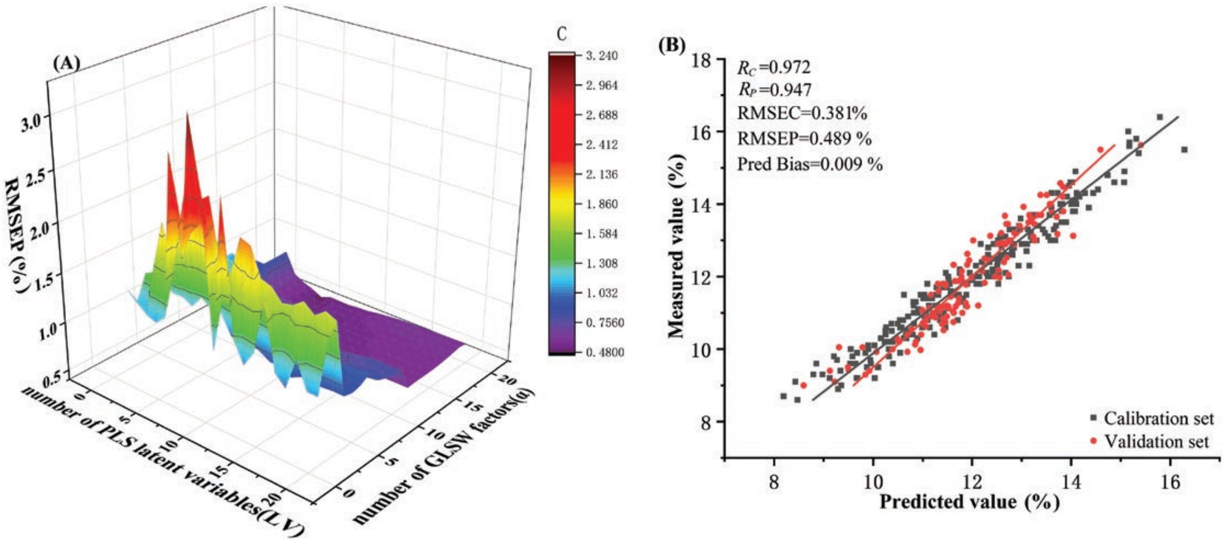

Figure 8. EPO correction model prediction results. (A) Plot of RMSEP variation based on D1 difference matrix. (B) Scatter plot of EPO correction model prediction results.

methods improve the adaptability of the model to temperature. Compared with other methods, EPO method obtains the best prediction results, R_p is 0.947, RMSEP is 0.489%, and Pred Bias is 0.009%, which indicates that its temperature correction ability is superior to global correction, OSC method and GLSW method.

Conclusions

In this study, the SSC prediction model of apple was established, and the effect of temperature on apple spectrum and model was analyzed. The results show that the temperature has a significant effect on apple spectra, which leads to a reduction in the accuracy of the model prediction and poor applicability of the model to temperature. To improve the robustness of the PLSR model to sample temperature, the performance of the model was improved by correcting for temperature effects using temperature correction methods such as EPO, GLSW, OSC, and global correction. The best results were obtained by using EPO method. The RMSEP of the model was 0.489%, R_p was 0.947, and the prediction deviation was 0.009%. The EPO method can correct the temperature well. The results have practical implications for the application of NIR spectroscopy in the prediction of fruit quality in environments such as production plants.

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Author Contributions

All authors have made equal contributions to this research work. All authors read and approved the final manuscript.

Conflict of Interest

The authors declare that they have no conflict of interest.

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