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Enhancing Transferability of Near-Infrared Spectral Models for Soluble Solids Content Prediction across Different Fruits

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Abstract: Near-infrared (NIR) spectroscopy is widely used for non-destructive detection of fruit quality, but the transferability of NIR models between different fruits is still a challenge. This study investigates the transferability of NIR models from strawberry to grape and apple using two case studies. A total of 94 strawberry, 80 grape, and 125 apple samples were measured for their soluble solids content (SSC) and NIR spectra. Partial least squares (PLS) regression was used to establish a model for predicting strawberry SSC, with an acceptable root mean square error of prediction (RMSEP) and correlation coefficient (R) of 0.53 °Brix and 0.91, respectively. Directly applying the strawberry model to grape and apple spectra significantly degrades the performance, increasing the RMSEP up to 3.47 and 16.40, respectively. Spectral preprocessing can improve the predictions for all three fruits, but the bias cannot be eliminated. Global modeling produces a generalized model, but the prediction for strawberry degrades. Calibration transfer with SS-PFCE and PLS correction, which are calibration methods without standard samples, was found to be an effective way to improve the prediction of grape and apple spectra using the strawberry model. Therefore, calibration transfer may be a feasible way for improving the transferability of NIR models for multiple fruits.

Keywords: near-infrared spectroscopy; fruit quality; multivariate calibration; calibration transfer; soluble solids content

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1. Introduction

Near-infrared (NIR) spectroscopy is a powerful analytical technique that enables rapid and non-destructive measurement of the chemical and physical properties of samples based on their spectral data [1–3]. NIR spectroscopy works by shining light in the near-infrared range (typically 700–2500 nm) onto a sample and measuring the amount of light that is absorbed or reflected by the sample. The resulting spectrum provides information about the sample's molecular composition and physical properties, such as moisture content, protein content, fat content, and more. Its advantages over other analytical methods include easy sample preparation, environmental friendliness, and the ability to provide online or in situ measurements. These advantages make NIR spectroscopy a popular tool that has been widely applied in various fields, such as food [4–6], pharmaceuticals [7], and agriculture [8–10].

Fruit quality evaluation is one of the most important and challenging tasks for NIR spectroscopy, as fruits are complex biological systems that contain a diverse range of components, such as sugars, acids, vitamins, minerals, water content, and firmness [11–13]. The total amount of solid substances that can be dissolved in water, comprising sugars, acids, vitamins, minerals, and other components, is referred to as soluble solids content (SSC) [14–16]. Fruit quality is a crucially important factor that is indicated by the SSC through the process of photosynthesis, plants convert sunlight, carbon dioxide, and water into sugar substances such as glucose and fructose which are subsequently stored in the

fruit. Consequently, the SSC of fruits is reflective of attributes such as ripeness, sweetness, texture, and overall quality. Monitoring and evaluating the quality attributes of fruits in a rapid and accurate way is essential for human health and nutrition. Chemometric methods, including multiple linear regression (MLR), principal component regression (PCR), partial least squares (PLS), artificial neural network (ANN), and support vector regression (SVR), as well as the techniques developed in recent years, are widely studied for multivariate calibration of NIR spectra [17–19]. However, the quality of a multivariate calibration model depends on a series of factors, e.g., the nature of the samples, the quality of the calibration data, the spectral variables used in the model, and even the technique of the modeling. Therefore, great efforts have been made for building a robust model, including studies on the methods for spectral preprocessing [20,21], outlier detection [22], variable selection [23,24] and the techniques of modeling [25]. With these methods, practical models with good predictability and reliability can be built in most applications. NIR spectroscopy provides a powerful tool for fruit non-destructive detection by measuring the spectra of fruit samples and applying multivariate calibration models to predict their quality parameters. Compared to conventional methods, NIR spectroscopy avoids sample destruction or contamination, reduces analysis time and cost, and covers a large sample area.

However, one of the main problems with using NIR spectroscopy for fruit detection is the difficulty in generalizing and transferring models between different fruits [4,26]. Each fruit type has to be modeled separately, as different fruits have different spectral characteristics due to their diverse compositions, structures, and shapes. Spectral variations caused by these factors may degrade the performance of calibration models or make them invalid for another kind of fruit. This requires a large amount of reference data collection and model establishment for each fruit type, which limits the practical application of NIR spectroscopy for fruit detection.

To address this problem, researchers have commonly resorted to three strategies: spectral preprocessing [27], global modeling [28,29], and calibration transfer without standard [30,31]. Spectral preprocessing methods aim to reduce noise and variation in the spectra and enhance relevant information for prediction, for example, Savitzky-Golay (SG) smoothing, standard normal variate (SNV), and continuous wavelet transform (CWT) [27,32]. While these methods do not require any information about the sample distribution to be transferred, they may sometimes produce unfavorable results. Global modeling methods, on the other hand, try to build a single model that can cover different fruits by using a large and diverse dataset. This approach commonly produces acceptable results for all fruits, but may degrade the already established model. Moreover, global modeling necessitates some spectral and reference values to be modeled for each fruit. Calibration transfer without standard methods attempts to correct the prediction bias when the model built for one fruit is applied to another, such as semi-supervised parameter-free calibration enhancement (SS-PFCE) [33] and PLS correction [34]. Similar to global modeling, these methods have comparable data requirements, but provide a more advanced modeling approach to update the model for each type of fruit with a few new corresponding measurements. It is important to note, however, that these techniques may not be as accurate or precise as using reference standards. Calibration transfer without standards should only be used when it is not possible to use reference standards, and the resulting data should be carefully evaluated to ensure that the accuracy and precision are acceptable for the intended use.

In this paper, the feasibility of transferring NIR spectral models from one kind of fruit to another is investigated through two case studies: strawberry-to-grape transfer and strawberry-to-apple transfer. PLS regression is used as a baseline method to build NIR models for predicting the SSC of strawberries from their NIR spectra. The performance of the strawberry model on original datasets with grape and apple datasets is compared using root mean square error of prediction (RMSEP) as an evaluation metric. Some methods that can improve the transferability of NIR models between fruits, such as spectral preprocessing methods (including CWT, SG smoothing, and SNV), global model, and calibration transfer

without standards (PLS correction, SS-PFCE), are also explored. The advantages and disadvantages of these methods are discussed, and some suggestions for future research directions are provided.

2. Materials and Methods

2.1. Fruit Sample Preparation and NIR Spectra Measurement

In this study, we collected samples of three different fruits: 94 strawberry, 80 grape, and 125 apple samples. These fruits were obtained from a local market and were chosen based on their availability and variety. All fruits were stored at room temperature (around 20 °C) and a humidity of 40% in the laboratory for approximately 2 h before measuring their spectra directly from the equatorial region without any additional treatment.

The NIR spectra of the fruit samples were measured using a handheld near-infrared spectrometer MicroNIR 1700 (Viavi, Santa Rosa, CA, USA). Each individual spectrum was the average of 50 scans with an integration time of 15 ms. The spectrum includes 125 wavelength variables with a resolution of 6.2740 nm over the wavelength range of 900–1669 nm. To reduce measurement noise, the spectra were averaged over three replicates. A certified reflection standard (Labsphere, North Sutton, NA, USA) was used to measure the reference spectrum. The measurements were performed at a room temperature of 20 °C and a humidity of about 40%.

2.2. Soluble Solids Content Measurement

After measuring the NIR spectra of the fruit, the SSC of the fruit samples was measured immediately using a refractometer (Zhejiang Topu Yunnong Technology Co., Ltd., Hangzhou, China). The instrument was calibrated to zero using distilled water before each measurement. For each fruit sample, the refractometer was placed on the cut surface of the fruit, and a drop of juice was extracted using a handheld juicer. The juice was then filtered by filter paper and applied to the prism of the refractometer, and the SSC value was recorded in degrees Brix (°Brix). Table 1 summarizes the sample detection information, including the SSC range and the number of samples for each fruit category.

Table 1. Sample information.

Fruits	SSC Range (°Brix)	Number of Samples
Strawberry	6.40–13.20	94
Grape	6.15–18.20	80
Apple	9.35–17.55	125

2.3. Calibration

NIR models for predicting the SSC of strawberry samples were developed using PLS regression. PLS regression is a statistical approach utilized to model the correlation between a set of independent variables, known as predictors, and dependent variables, known as responses. The PLS technique is especially beneficial when there is a high correlation among the predictors, and many predictors exist, making the construction of a conventional regression model challenging. In PLS, latent variables, also referred to as factors, are derived from the original data to represent the predictors and responses as linear combinations. These factors are selected to account for the maximum variance observed in both the predictors and responses.

Before establishing the PLS model, the data set should be divided into calibration set and validation set. A calibration set and a validation set were created for the strawberry samples with a split ratio of 7:3 to build and assess models, respectively. Additionally, transfer sets were created for grape and apple, with 20 samples each, to transfer the strawberry model, while the remaining samples were used for validation. Preprocessing methods, including SG smoothing, SNV, and CWT, were applied to the NIR spectra, and the optimal number of latent variables (*n*LV) was determined using 10-fold cross-validation

based on the root mean square error of cross-validation (RMSECV). The final PLS model was constructed using the optimal *n*LV and the preprocessed spectra. The model performance was evaluated using the root mean square error and correlation coefficient in the calibration and validation sets (RMSEC, RMSEP, Rc, and Rp). Independent sets of grape and apple samples were utilized to test the generalization performance of the strawberry model on other fruits.

2.4. Global Modeling

A global modeling strategy was used on the combined dataset of the calibration set of strawberry and the transfer sets of grape and apple samples to investigate the feasibility of building a versatile model that performs better for all fruits. PLS algorithms were used to establish the global model, and 10-fold cross-validation was used to determine the optimal *n*LV. The performance of the global model was evaluated on the validation set of both strawberry, grape and apple, resulting in the corresponding RMSEP and Rp.

2.5. Calibration Transfer

Calibration transfer without standards was performed to investigate the feasibility of transferring the NIR models from one fruit to another using two distinct methods: PLS correction [34] and SS-PFCE [33]. These methods are able to transfer a model developed for one fruit (in this case, strawberry) to accommodate the spectra of other fruits (grape and apple) with only a few spectra and reference values, thereby minimizing the need for extensive calibration efforts for each individual fruit.

The PLS correction method [34] was employed to correct the bias of the strawberry model when applied to grape and apple samples. This approach is based on the assumption of a linear relationship between the spectral difference and the prediction error of the primary model, which is developed using spectra from a large calibration set of strawberry. Specifically, the PLS model of strawberry, represented by $\begin{bmatrix} b_0 \\ \mathbf{b} \end{bmatrix}$, was used to predict the spectra of the transfer set of grape or apple, denoted as $\mathbf{X}$, using Equation (1),

$$\hat{\mathbf{y}} = [\mathbf{1X}] \begin{bmatrix} b_0 \\ \mathbf{b} \end{bmatrix} \tag{1}$$

where $\mathbf{1}$ denotes a vector consisting of a column of numbers 1 of sample size on the standard set, and b_0 and $\mathbf{b}$ are the intercept and coefficients of the model, respectively.

The prediction error of grape or apple spectra with direct usage of the strawberry model, represented by $\mathbf{e}$, was obtained as Equation (2),

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} \tag{2}$$

Subsequently, the prediction error of grape or apple spectra was regarded as the dependent variable, and the spectra in the corresponding transfer set as the independent variable, to establish the correction models, $\begin{bmatrix} b_0^* \\ \mathbf{b}^* \end{bmatrix}$, using PLS algorithm, as shown in Equation (3),

$$\mathbf{e} = [\mathbf{1X}] \begin{bmatrix} b_0^* \\ \mathbf{b}^* \end{bmatrix} + \mathbf{r} \tag{3}$$

where, $\mathbf{r}$ denotes the fitting residual of the correction model.

During the prediction process with PLS correction, the strawberry model was initially used to predict the spectra of grape or apple, resulting in a biased prediction. Next, the corresponding correction models were used to obtain the estimated prediction error of the direct usage of the strawberry model on other fruits. Finally, the accurate prediction of grape and apple was achieved through the addition of biased prediction and the estimated prediction error.

In contrast to the aforementioned PLS correction strategy, the SS-PFCE method [33] proposes a different approach to achieve the transferability of prediction models across different fruit types. This method employs a few spectra of new fruits with reference values, in order to directly adjust the PLS model originally developed for strawberry to accommodate grape and apple spectra.

To implement this method, the strawberry model $\begin{bmatrix} b_0 \\ \mathbf{b} \end{bmatrix}$ was utilized as the initial values, and the spectra ($\mathbf{X}$) and the reference values ($\mathbf{y}$) in the standard sets of grape and apple were fed into Equation (4) to obtain the transferred model $\begin{bmatrix} b_{0,s} \\ \mathbf{b}_s \end{bmatrix}$.

$$\min_{b_{0,s},\, \mathbf{b}_s} \left(\left\| \mathrm{y} - [\mathbf{1X}] \begin{bmatrix} b_{0,s} \\ \mathbf{b}_s \end{bmatrix} \right\|^2 \right) \tag{4}$$

$$\text{s. t. } \mathrm{corr}(\mathbf{b}_s, \mathbf{b}_m) > r_{th}$$

where $\mathrm{corr}(\mathbf{b}_s, \mathbf{b}_m) > r_{th}$ represents that during the establishment of a transferred model, the correlation coefficients of model coefficients, excluding the intercept term, must not exceed a predefined threshold of 0.98, as recommended by [33]. This constraint ensures that the transferred model is not overfitted to the training data and maintains a reasonable level of generalizability to new data. With a global optimization algorithm, sequential quadratic programming, we could obtain the adjusted strawberry model for grape and apple.

During the prediction process, the spectra of grape and apple could be directly with the corresponding adjusted models obtained through SS-FPCE. The decrease in RMSEP and increase in Rp of grape and apple spectra with the strawberry model before and after calibration transfer were used to evaluate the feasibility of transferring prediction models across different fruit types.

In this work, all calculations, including spectra preprocessing (CWT, SG smoothing, and SNV algorithms), PLS modeling, and calibration transfer (PLS correction and SS-PFCE algorithms) were carried out by self-editing programs in MATLAB (Ver. R2022a: The MathWorks, USA).

3. Results and Discussion

3.1. Calibration Results

The raw NIR spectra of strawberry, grape, and apple are presented in Figure 1. The spectra exhibit high absorption in the range of 1300–1500 nm, which is likely caused by the water content in the fruits. The bands between 930 and 1000 nm and in the wavelength range of 1400–1500 nm can be assigned to the 1st and 2nd overtones of O-H vibrations. Meanwhile, the bands between 1100 and 1200 nm can be assigned to the 2nd overtones of C-H vibrations. Furthermore, it is apparent that the spectra of the three fruits have varying shapes and intensities. Specifically, the grape spectra exhibit the most fluctuating background, while the apple spectra display the smallest. These differences in spectral characteristics may be attributed to the diverse shapes and compositions of the measured fruits, which could potentially impede the transferability of models across fruits.

A PLS model using 15 latent variables was developed on the raw spectra of strawberries to predict SSC. The model showed good performance on the validation set with an RMSEP of 0.53 °Brix and Rp of 0.91 (Table 2). However, the same model applied to grapes and apples resulted in less accurate predictions, with RMSE values of 3.47 and 16.40, respectively, which were 6.5 and 30.9 times higher than those on strawberry data. The R values of grape and apple also decreased to 0.84 and 0.01, respectively. The PLS model for strawberries cannot be applied to grapes and apples directly.

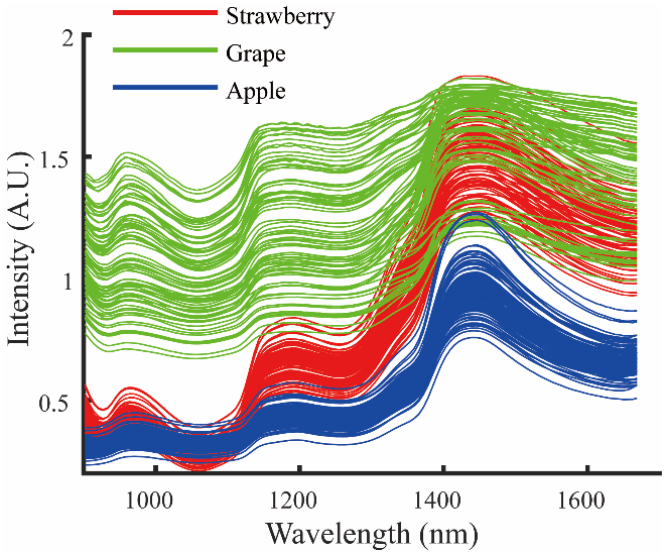


Figure 1. NIR spectra of strawberry, grape, and apple.

Table 2. Strawberry models established with different spectral preprocessing methods and the application to different fruits.

Preprocessing Methods	*n*LV	Calibration		Validation	
		RMSEC (°Brix)	Rc	RMSEP (°Brix)	Rp
None					
Strawberry	15	0.32	0.95	0.53	0.91
Grape	-	-	-	3.47	0.84
Apple	-	-	-	16.40	0.01
CWT					
Strawberry	19	0.30	0.96	0.41	0.95
Grape	-	-	-	2.40	0.74
Apple	-	-	-	4.90	0.12
SG Smooth					
Strawberry	12	0.54	0.86	0.78	0.80
Grape	-	-	-	2.94	0.67
Apple	-	-	-	25.44	0.28
SNV					
Strawberry	19	0.18	0.99	0.41	0.95
Grape	-	-	-	6.48	0.34
Apple	-	-	-	14.45	0.11

Due to the fact that NIR spectra frequently contain interferences of background information, drift, and noise, the raw NIR spectra were subjected to spectral preprocessing. To improve the accuracy of the model, spectral preprocessing techniques including CWT, SG smooth, and SNV were applied, resulting in a more accurate model for strawberries. The best model, which used CWT, had an RMSEP of 0.41 °Brix and an R value of 0.95, representing a decrease of 7.8% and an increase of 4.2%. Additionally, the generalization of the model to grapes and apples showed remarkable improvement, with a decrease in RMSEP to 2.41 and 4.90, respectively, corresponding to 5.9 and 11.9 times the RMSEP on the strawberry data. Therefore, CWT was selected as the spectral preprocessing method for the following analysis.

The NIR spectra of three different fruits with CWT preprocessing are shown in Figure 2A. Compared with the raw spectra (Figure 1), the intensity distribution differences between the three fruits were significantly smaller. Differences were only observed in the spectra at 1100–1500 nm, which represent the absorption of the 1st overtone of the -OH

group. This difference may be due to variations in water content among the different fruits. Overall, the background fluctuations of the spectra were significantly reduced after CWT preprocessing, which is likely the main reason for the improvement in the generalization of the strawberry model to different fruits.

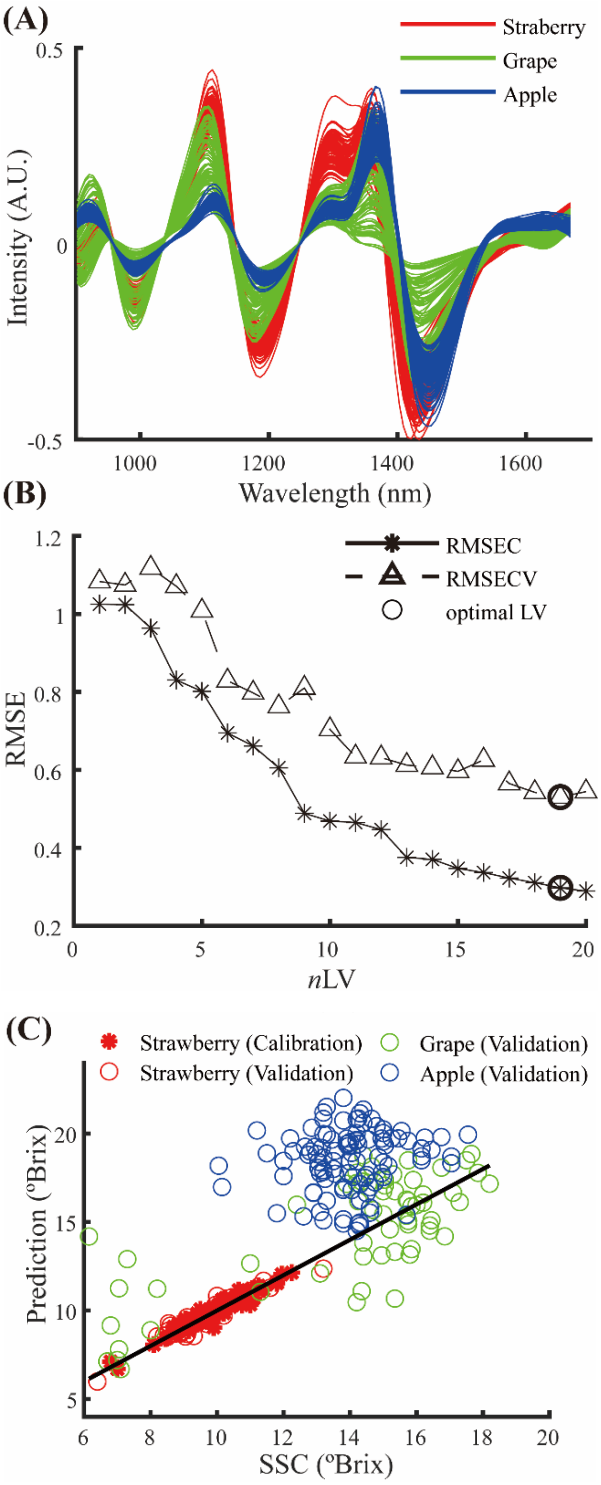


Figure 2. NIR spectra of three different fruits preprocessed with CWT (**A**). Cross-validation results for established PLS model for strawberry (**B**). Prediction of the strawberry model when applied to different fruits (**C**).

Figure 2B displays the variation of RMSEC and RMSECV with different *n*LV. Initially, both RMSEC and RMSECV were observed to be relatively high. However, as the *n*LV increased, the RMSEC and RMSECV gradually decreased. The RMSECV reached its minimum value (0.53 °Brix) at *n*LV = 19. The model developed with this optimal LV showed good prediction results for strawberry, as evidenced by the close agreement between the predicted and reference values of both the calibration and prediction sets shown in Figure 2C. However, for grape and apple, the predictions were far worse than those for strawberry, especially for SSC in apple, which were both overpredicted.

3.2. Global Modeling

To improve the accuracy of calibration models for grape and apple, a global model was developed using PLS with CWT preprocessing on a large calibration set that included the calibration set for strawberry and the transfer set for grape and apple. The optimal number of LVs was determined to be 13 using cross-validation, and the PLS model was established. Figure 3 compares the PLS models for strawberry only and the global model. While the global model and the PLS model for strawberry have similar trends, the relative intensity of the global model is smaller than that of the PLS model for strawberry.

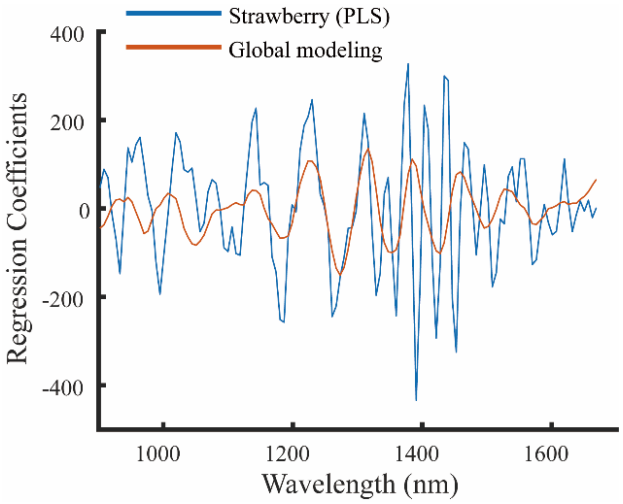


Figure 3. Comparison of PLS model for strawberry and the global model.

Figure 4 shows the prediction of the global model applied to the three different fruits. In comparison to the PLS model for strawberry, the global model performed significantly better when applied to grape and apple spectra, with RMSEP decreasing to 1.55 and 1.28, respectively. These values were only 3.8 and 3.1 times higher than the RMSEP of the strawberry model on the strawberry validation set. The Rp also improved, increasing to 20% and 264% for grape and apple, respectively. However, the performance of the global model decreased when applied to the validation set of strawberry, with RMSEP and Rp decreasing to 0.66 °Brix and 0.86 °Brix, respectively, in comparison to a 61% increase and a 9% increase for the PLS model for strawberry (Table 3). Therefore, the global model is a versatile model that is suitable for all three fruits, but it may not be the most optimal model for the fruit with the largest training dataset, which in this case is strawberry.

Table 3. Prediction of global model on three different fruits.

Prediction Set	RMSEP (°Brix)	Rp
Strawberry	0.66	0.86
Grape	1.55	0.89
Apple	1.28	0.45

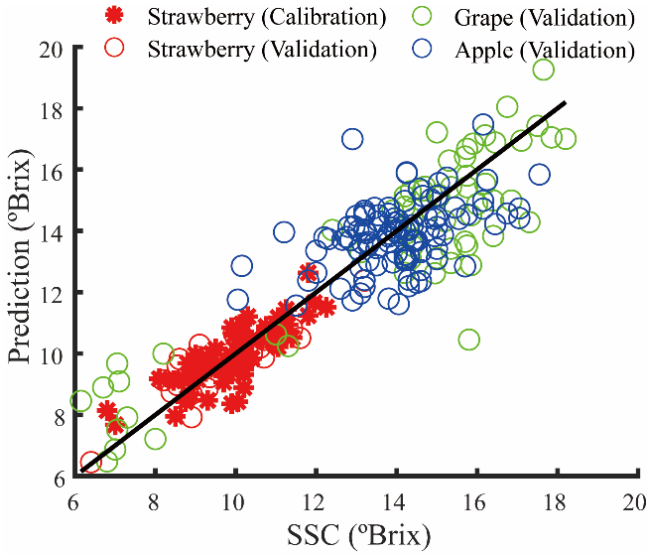


Figure 4. Prediction of global model when applied to three different fruits.

3.3. Calibration Transfer without Standards

To further improve the prediction of grape and apple, two calibration transfer methods without standards were utilized. With the previously established PLS model for strawberry and the transfer set of grape and apple, models for grape and apple were obtained by SS-PFCE, as depicted in Figure 5. The grape and apple models obtained by SS-PFCE showed a similar shape and intensity to the strawberry model, although slight differences were observed across the spectral range upon closer inspection. When the transferred models were applied to the corresponding spectra in the validation sets, the prediction of all three fruits was close to the reference values, as shown in Figure 6A. Notably, the prediction of apple was significantly improved compared to the global model, with a decrease in RMSEP from 1.41 °Brix to 1.28 °Brix (Table 4). PLS correction was also used to train correction models for both grape and apple, and the obtained results were comparable to those obtained with SS-FPCE (Figure 6B). Overall, the results suggest that SS-PFCE and PLS correction can be effective calibration transfer methods for improving the prediction accuracy of fruit quality attributes.

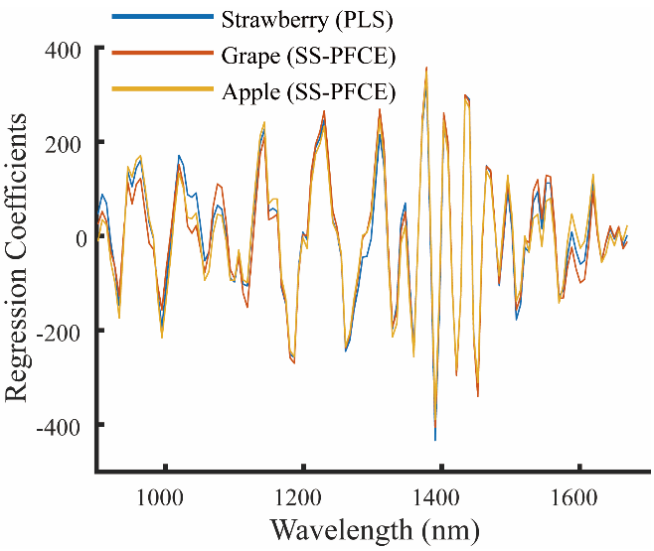


Figure 5. Comparison of PLS model for strawberry and the transferred models for grape and apple.

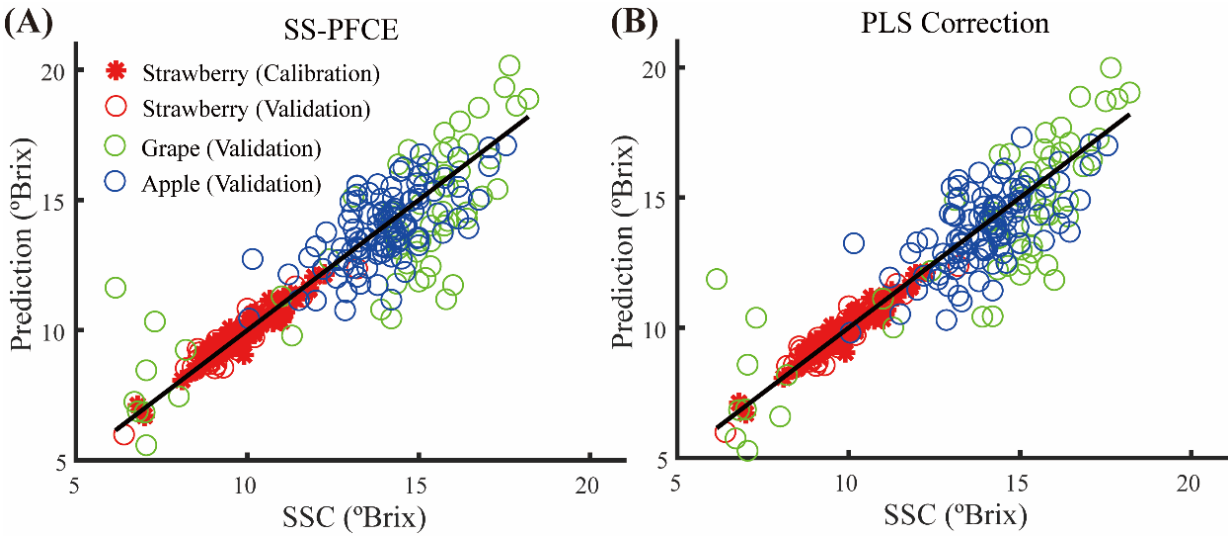


Figure 6. Prediction of transferred models by SS-PFCE (**A**) and PLS correction (**B**).

Table 4. Prediction of the strawberry model without and with calibration transfer.

Model	Prediction Set	RMSEP (°Brix)	Rp
Strawberry	Strawberry	0.41	0.95
Strawberry	Grape	2.40	0.74
Strawberry	Apple	4.90	0.12
SS-PFCE	Grape	1.99	0.84
SS-PFCE	Apple	1.14	0.65
PLS Correction	Grape	1.77	0.87
PLS Correction	Apple	1.22	0.64

4. Conclusions

In conclusion, this study investigated the feasibility of transferring NIR spectral models from one type of fruit to another. The results showed that the transferability of NIR models between fruits is challenging due to the spectral variations caused by various factors such as temperature change, humidity change, instrument drift, sample heterogeneity, and background noise. However, several methods, including spectral preprocessing, global modeling, and calibration transfer without standard, can improve the transferability of NIR models between fruits.

The two case studies conducted in this study, namely strawberry-to-grape transfer and strawberry-to-apple transfer, demonstrated that the performance of NIR models built for one fruit type could be degraded when applied to another fruit type. The comparison of various methods showed that global modeling approaches generally have acceptable results for all fruits but degrade the performance of already established models. Calibration transfer without standard methods, such as semi-supervised parameter-free calibration enhancement and PLS correction, can correct the prediction bias when the model built for one fruit is applied to another with similar data requirements as global modeling.

This study provides valuable insights for improving the practical application of NIR spectroscopy in fruit detection by investigating the feasibility of transferring NIR spectral models between fruits. The strong penetrating power of NIR spectroscopy makes it suitable for analyzing the quality of thin-skinned fruits, including apples, strawberries, pears, and other similar fruits. This non-destructive and efficient technology can effectively assess fruit quality, which is of great importance to fruit industry stakeholders. Future research should explore more effective approaches to improving the transferability of NIR models between fruits, such as incorporating more diverse reference datasets, developing more

robust calibration transfer methods, and exploring the use of artificial intelligence and machine learning techniques.

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Conflicts of Interest: The authors declare no conflict of interest.

References

1. Pasquini, C. Near infrared spectroscopy: A mature analytical technique with new perspectives—A review. *Anal. Chim. Acta* **2018**, *1026*, 8–36. [CrossRef] [PubMed]
2. Gan, F.; Luo, J. Simple dilated convolutional neural network for quantitative modeling based on near infrared spectroscopy techniques. *Chemom. Intell. Lab. Syst.* **2023**, *232*, 104710. [CrossRef]
3. Mishra, P.; Rutledge, D.N.; Roger, J.M.; Wali, K.; Khan, H.A. Chemometric pre-processing can negatively affect the performance of near-infrared spectroscopy models for fruit quality prediction. *Talanta* **2021**, *229*, 122303. [CrossRef] [PubMed]
4. Sohaib Ali Shah, S.; Zeb, A.; Qureshi, W.S.; Arslan, M.; Ullah Malik, A.; Alasmary, W.; Alanazi, E. Towards fruit maturity estimation using NIR spectroscopy. *Infrared Phys. Technol.* **2020**, *111*, 103479. [CrossRef]
5. Li, X.; Zhang, L.; Zhang, Y.; Wang, D.; Wang, X.; Yu, L.; Zhang, W.; Li, P. Review of NIR spectroscopy methods for nondestructive quality analysis of oilseeds and edible oils. *Trends Food Sci. Technol.* **2020**, *101*, 172–181. [CrossRef]
6. Roberts, J.J.; Cozzolino, D. An overview on the application of chemometrics in food science and technology—An approach to quantitative data analysis. *Food Anal. Methods* **2016**, *9*, 3258–3267. [CrossRef]
7. Yan, H.; Ma, Y.; Han, B.X. Rapid detection of the component contents in caryophylli flos by a handheld near infrared spectrometer based on digital light processing technology. *J. Near Infrared Spectrosc.* **2018**, *26*, 389–397. [CrossRef]
8. Zhang, J.; Guo, C.; Cui, X.Y.; Cai, W.S.; Shao, X.G. A two-level strategy for standardization of near infrared spectra by multi-level simultaneous component analysis. *Anal. Chim. Acta* **2019**, *1050*, 25–31. [CrossRef]
9. Cortés, V.; Blasco, J.; Aleixos, N.; Cubero, S.; Talens, P. Monitoring strategies for quality control of agricultural products using visible and near-infrared spectroscopy: A review. *Trends Food Sci. Technol.* **2019**, *85*, 138–148. [CrossRef]
10. He, Y.; Xiao, Q.; Bai, X.; Zhou, L.; Liu, F.; Zhang, C. Recent progress of nondestructive techniques for fruits damage inspection: A review. *Crit. Rev. Food Sci. Nutr.* **2022**, *62*, 5476–5494. [CrossRef]
11. Fan, S.; Li, J.; Xia, Y.; Tian, X.; Guo, Z.; Huang, W. Long-term evaluation of soluble solids content of apples with biological variability by using near-infrared spectroscopy and calibration transfer method. *Postharvest Biol. Technol.* **2019**, *151*, 79–87. [CrossRef]
12. Yan, H.; Xu, Y.; Siesler, H.W.; Han, B.X.; Zhang, G.Z. Hand-held near-infrared spectroscopy for authentication of fengdous and quantitative analysis of mulberry fruits. *Front. Plant Sci.* **2019**, *10*, 1548. [CrossRef] [PubMed]
13. Anderson, N.T.; Walsh, K.B. The evolution of chemometrics coupled with near infrared spectroscopy for fruit quality evaluation. *J. Near Infrared Spectrosc.* **2022**, *30*, 3–17. [CrossRef]
14. Liu, S.; Huang, W.; Lin, L.; Fan, S. Effects of orientations and regions on performance of online soluble solids content prediction models based on near-infrared spectroscopy for peaches. *Foods* **2022**, *11*, 1502. [CrossRef] [PubMed]
15. Jie, D.; Xie, L.; Rao, X.; Ying, Y. Using visible and near infrared diffuse transmittance technique to predict soluble solids content of watermelon in an on-line detection system. *Postharvest Biol. Technol.* **2014**, *90*, 1–6. [CrossRef]
16. Pu, H.; Liu, D.; Wang, L.; Sun, D.-W. Soluble solids content and pH prediction and maturity discrimination of lychee fruits using visible and near infrared hyperspectral imaging. *Food Anal. Methods* **2016**, *9*, 235–244. [CrossRef]
17. Moros, J.; Garrigues, S.; Guardia, M.d.l. Vibrational spectroscopy provides a green tool for multi-component analysis. *TrAC Trends Anal. Chem.* **2010**, *29*, 578–591. [CrossRef]
18. Shao, X.G.; Bian, X.H.; Liu, J.; Zhang, M.; Cai, W.S. Multivariate calibration methods in near infrared spectroscopic analysis. *Anal. Methods* **2010**, *2*, 1662–1666. [CrossRef]
19. Boido, E.; Fariña, L.; Carrau, F.; Cozzolino, D.; Dellacassa, E. Application of near-infrared spectroscopy/artificial neural network to quantify glycosylated norisoprenoids in Tannat grapes. *Food Chem.* **2022**, *387*, 132927. [CrossRef]

20. Ma, C.; Shao, X.G. Continuous Wavelet Transform applied to removing the fluctuating background in near-Infrared spectra. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 907–911. [CrossRef]
21. Rady, A.; Fischer, J.; Reeves, S.; Logan, B.; James Watson, N. The effect of light intensity, sensor height, and spectral pre-processing methods when using NIR spectroscopy to identify different allergen-containing powdered foods. *Sensors* **2019**, *20*, 230. [CrossRef] [PubMed]
22. Bian, X.H.; Cai, W.S.; Shao, X.G.; Chen, D.; Grant, E.R. Detecting influential observations by cluster analysis and Monte Carlo cross-validation. *Analyst* **2010**, *135*, 2841–2847. [CrossRef] [PubMed]
23. Xu, H.; Liu, Z.; Cai, W.S.; Shao, X.G. A wavelength selection method based on randomization test for near-infrared spectral analysis. *Chemom. Intell. Lab. Syst.* **2009**, *97*, 189–193. [CrossRef]
24. Yun, Y.H.; Bin, J.; Liu, D.L.; Xu, L.; Yan, T.L.; Cao, D.S.; Xu, Q.S. A hybrid variable selection strategy based on continuous shrinkage of variable space in multivariate calibration. *Anal. Chim. Acta* **2019**, *1058*, 58–69. [CrossRef]
25. Shao, X.G.; Bian, X.H.; Cai, W.S. An improved boosting partial least squares method for near-infrared spectroscopic quantitative analysis. *Anal. Chim. Acta* **2010**, *666*, 32–37. [CrossRef]
26. Li, L.; Huang, W.; Wang, Z.; Liu, S.; He, X.; Fan, S. Calibration transfer between developed portable Vis/NIR devices for detection of soluble solids contents in apple. *Postharvest Biol. Technol.* **2022**, *183*, 111720. [CrossRef]
27. Rinnan, Å.; van den Berg, F.; Engelsen, S.B. Review of the most common pre-processing techniques for near-infrared spectra. *TrAC Trends Anal. Chem.* **2009**, *28*, 1201–1222. [CrossRef]
28. Workman, J.J. A review of calibration transfer practices and instrument differences in spectroscopy. *Appl. Spectrosc.* **2018**, *72*, 340–365. [CrossRef]
29. Wang, J.J.; Li, Z.F.; Wang, Y.; Liu, Y.; Cai, W.S.; Shao, X.G. A dual model strategy to transfer multivariate calibration models for near-infrared spectral analysis. *Spectrosc. Lett.* **2016**, *48*, 348–354. [CrossRef]
30. Mishra, P.; Nikzad-Langerodi, R.; Marini, F.; Roger, J.M.; Biancolillo, A.; Rutledge, D.N.; Lohumi, S. Are standard sample measurements still needed to transfer multivariate calibration models between near-infrared spectrometers? The answer is not always. *TrAC Trends Anal. Chem.* **2021**, *143*, 116331. [CrossRef]
31. Liu, Y.; Cai, W.S.; Shao, X.G. Linear model correction: A method for transferring a near-infrared multivariate calibration model without standard samples. *Spectrochim. Acta Part A* **2016**, *169*, 197–201. [CrossRef] [PubMed]
32. Cui, X.Y.; Yu, X.; Cai, W.S.; Shao, X.G. Water as a probe for serum–based diagnosis by temperature–dependent near–infrared spectroscopy. *Talanta* **2019**, *204*, 359–366. [CrossRef] [PubMed]
33. Zhang, J.; Li, B.; Hu, Y.; Zhou, L.; Wang, G.; Guo, G.; Zhang, Q.; Lei, S.; Zhang, A. A parameter-free framework for calibration enhancement of near-infrared spectroscopy based on correlation constraint. *Anal. Chim. Acta* **2021**, *1142*, 169–178. [CrossRef] [PubMed]
34. Li, X.; Cai, W.S.; Shao, X.G. Correcting multivariate calibration model for near infrared spectral analysis without using standard samples. *J. Near Infrared Spectrosc.* **2015**, *23*, 285–291. [CrossRef]

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