Construction and analysis of the near-infrared prediction model of Figs' brix

Yunhu Wang[1], Chengzhong Wang[1], Rui Sun[1, a, *], Lei Sun[2]

[1]Qilu University of Technology (Shandong Academy of Science), Jinan, 250353, China

[2]Shandong Forestry Research Institute, Economic forest station, Jinan, 250014, China

[a]sunruisr@yeah.net

*Corresponding author

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Abstract: In order to solve the problem that the quality of hand-picked figs is difficult to be classified and graded, near-infrared spectral diffuse reflection detection technology is adopted. The prediction model of brix was established respectively, and PLS and PCR modeling effects were compared and analyzed. The results showed that PLS modeling was better than PCR. Among them, the brix model was the best. The technical method of this study provides a reasonable reference for the quality classification and grading of hand-picked mature figs.

1. Introduction

Figs belongs to the genus Ficus Linn in Moracea e, is one of the earliest human improved cultivation of fruit tree species, planted widely around the world. At present, the main producing areas are concentrated in the Mediterranean countries. [1] The fruit has attracted increasing attention because of its round color and sweet taste. Figs not only has delicious taste, but also has rich nutritional value and medicinal value. They have good effects on anti-oxidation, anti-cancer, anti-aging, chronic enteritis and other diseases.

In recent years, near-infrared spectroscopy is developing rapidly. Combined with stoichiometry, rapid nondestructive testing of samples can be realized. It has been applied in petrochemical, pharmaceutical, agricultural and food fields and plays an important role in agricultural production, which makes it possible to realize non-destructive quality testing and intelligent grading of figs [2]. Because each sample has its unique near infrared spectrum, and similar samples have similar spectral characteristics. Therefore, samples with similar near infrared spectra have similar chemical and physical properties, but so far, few experiments have studied figs by combining soluble solids and texture indexes with near-infrared spectroscopy.

The main purpose of this experiment is to use the near-infrared analysis technology to study the feasibility of determining the maturity and high-quality intelligent grading of figs rapidly and nondestructively by the near-infrared model of brix. Partial least square method and principal component regression method were adopted, and multiple comparisons were made in spectral pretreatment to verify and evaluate each model, so as to achieve efficient classification of figs.

2. Material and method

2.1 Figs sample

Figs used in this experiment were picked from Binzhou figs planting base in Shandong province in October 2017, green husk variety. When selecting fruit without mechanical damage, the sample should be preserved and send for inspection immediately after picking. At room temperature, the sample was determined by near-infrared spectroscopy, and the full-band (900-1700nm) spectral scanning was performed on the maximum diameter of the near-infrared spectrometer.

2.2 Determination of figs Brix

The handheld Brix meter ATAGO pal-1 was used for determination of Brix. The instrument has

a wide measuring range (Brix 0.0 to 53.0%) and is suitable for almost any fruit juice, food and beverage measurement. Make three parallel measurements, and record the values.

2.3 The obtaining of near-infrared spectroscopy

In the laboratory of total shading at room temperature (~20℃), figs samples were determined by near-infrared spectroscopy. Using Marine optics NIRQuest512, QR400-7-vis-nir fiber, WS-1 diffuse reflection standard, HL-2000-hp halogen tungsten light source, covering the wavelength range of 900-1700 nm. Figs were measured by diffuse reflection spectrophotometry. The blank correction was carried out before the measurement. The integral time was 123.3ms, the average frequency was 5 times, and the smoothness was 3.When measuring, take a point of Yin and Yang on the equator line of figs for spectral scanning.

2.4 The data processing

All figs spectral data came from The Unscrambler X 10.4 software and built a mathematical model of nir analysis, then the samples involved in the modeling were predicted, and the abnormal samples with significantly large sample prediction error were removed [4].Out a total of 90 data, according to the proportion of 2:1, correction of random classification is divided into set (60) and the validation set (30), in the whole spectral range (900-1700 nm), used for calibrating smooth, vector normalization (SNV), multiple scatter correction (MSC), first-order derivative and second-order derivative and so on conducting single or conjoint preprocessing to eliminate background noise and baseline drift and uneven scattering, and reduce the influence of external factors. The model was established based on principal component regression (PCR) and partial least square (PLS).PCR is designed to analyze multivariate collinearity problems, and PLS is widely used due to its advantages of simplicity and robustness, small computation and high prediction accuracy. Select the optimal model for verification and evaluation.

3. Results and discussion

Table 1 shows the maximum, minimum, mean and standard deviation of the correction set and verification set of Figs Brix samples. The sample verification set is similar to the calibration set and within the calibration and range, so it can be used to establish Figs near-infrared model. Figs Brix reflects the taste of the flesh.

Table 1. Fruit quality analysis of Figs fruit sample correction set and verification set

Parameters	maximum	minimum	mean	standard deviation
	correction set verification set	correction set verification set	correction set verification set	correction set verification set
Brix	23.70 23.50	11.50 11.40	17.20 16.40	3.71 3.63

FIG. 1 shows the spectrum of Figs' Brix parameters after different pretreatments. At first, the sugar spectrum showed a considerable baseline drift, and the derivative pretreated the spectrum better. After pretreatment, the spectral absorption peak of Brix was more obvious, and the difference between bands was also larger, while the spectrum of texture all showed dense absorption peak.

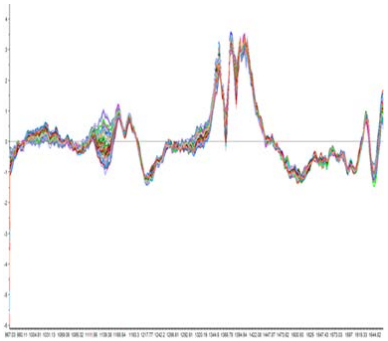

Figure 1. Picture1 Brix (first derivative+snv)

Table 2 illustrates the influence of different pretreatment methods on the performance of figs. Different pretreatment methods were compared according to the determination coefficient (R), corrected root mean square error (RMSEC) and verified root mean square error (RMSEP).It can be seen that the optimal pretreatment method of sugar content is the first-order derivative +SNV, and the derivative and SNV have better effects in various pretreatment methods, which may be related to the main problems of baseline shift, drift and other background interference in the spectrum.

Table 2. Figs Brix parameter modeling statistical results

	Spectral pretreatment method	The modeling method	Rc^2	RMSEC	Rp^2	RMSEP
	first-order derivative+SNV	PLSR	0.94	0.95	0.95	0.86
Brix	first-order derivative+ smoothing+SNV	PLSR	0.96	0.79	0.97	0.65
	Second-order derivative + smoothing+MSC	PLSR	0.97	0.68	0.98	0.66
	First-order derivative+SNV	PCR	0.83	1.64	0.82	1.76
	first-order derivative+ smoothing+SNV	PCR	0.80	1.80	0.79	1.96
	Second-order derivative+ smoothing+MSC	PCR	0.70	2.19	0.70	2.33

Table 3 shows the Sep/Sec value, Bias and residual prediction deviation (RPD=SD/RMSEP) of the optimal model for brix prediction parameters, and Sep/Sec should be less than or equal to 1.2.It can be seen from the table that SEP/SEC values of all parameters are less than 1.2, indicating that the accuracy of the model meets the requirements; Figs brix Bias was -0.012;RPD is 6.83; it indicates that the near-infrared model of sugar parameters can be used for daily detection and has good prediction accuracy. According to the study of Maria Luisa Amodio et al., the TSS R2 of strawberry was 0.85; the RPD is 4.36, and the model has a good effect. The value of brix PLS model is better than that of the two.

Table 3. Statistics of figs' optimal model for predicting parameters

Parameter	Spectral pretreatment method	SEP	SEC	SEP/SEC	Bias	SD	RPD
Brix	First-order derivative+SMV	0.62	0.65	0.95	0.024	4.24	6.83

4. Conclusion

The internal brix of figs was analyzed by nir diffuse reflectance spectroscopy, using different spectral pretreatment methods, and the model is established based on two different modeling methods. Various data show that the saccharinity of figs has a certain correlation with near-infrared diffuse reflectance spectra. In the experiment, the model was evaluated by correlation coefficient (R^2), root mean square error (RMSEP), relative analysis error (RPD) and other indicators. The results show that it is feasible to establish the near infrared model to predict the quality and maturity of figs.

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