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Research on prediction for ripeness of apples by means of NIR-spectroscopy

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ABSTRACT

Prediction for ripeness of apple had an important significance to determine the optimum harvest time and the accurate classification of apple. Soluble solids content (SSC) and firmness, as important internal physical and chemical indicators of apple, were important parameters of the evaluation of the ripeness degree of apple. Since Near infrared spectral analysis technology was a fast and non-destructive method to determine the internal quality of apple, different pretreatment methods and modeling methods were studied in this paper, and the best combined method was chosen as the modeling method of SSC and firmness. The result showed partial least squares (PLS) was the best modeling methods both to SSC and firmness. The modeling correlation coefficient, calibration standard deviation, the prediction correlation coefficient and predicted standard deviation of SSC were: 0.9093, 0.6145, 0.9622 and 0.4104, respectively. The modeling correlation coefficient, calibration standard deviation, the prediction correlation coefficient and predicted standard deviation of firmness were: 0.8463, 0.3825, 0.8268 and 0.2919, respectively. The ripeness degree could be evaluated by SSC and firmness which was detected by NIR spectral analysis. At last, the evaluation software for the ripeness of apple which was based on matlab GUI was designed.

KEYWORDS

NIR spectral analysis;
SSC;
Firmness;
PLS;
Ripeness.

INTRODUCTION

With the improvement of people's lives, the requirements on fruit quality are also increasing. When consumers are in the purchase of fruit, are not only satisfied with the size, color, shape and other appearance qualities, but taste and nutrition of fruit is their ultimate goal. The ripeness of the fruit is the main factor to determine the internal quality of fruit, and directly determines its taste and acceptability of consumers' demands. Only when the ripeness of fruit is understood do famer can pick fruit selectively and consumers can choose fruit what taste they want. Therefore it is considerable important to detect and control the ripeness degree of fruit.

Traditional testing for the ripeness of fruit makes use of sugar content instrument, firmness instrument to detect the internal qualities which are related to ripeness-indicators of fruit. These tests are destructive detection method, and it is not only destroys fruit tissue in the detection process, but also can't detect a large number of fruit one by one, which is not suitable for modern fruit production. Near infrared spectroscopy (NIR) is a nondestructive testing technology which uses the optical characteristics of fruit. Currently, many scholars, engaged in the research on ripeness and nondestructive testing for the internal quality of fruit, use near-infrared spectroscopy as the best method.

This paper explored the relationship between spectra of apple and their internal qualities -SSC and firmness based on near-infrared spectroscopy technology, and established the prediction models of SSC and firmness. SSC values and firmness values obtained by near-infrared spectroscopy were used to evaluate the ripeness degree of apple.

MATERIALS AND METHODS

Experimental materials

Red fuji Apples as the experimental samples were procured from the local fruit market. There was no obvious external defect on the surface of apples and the color was uniform. Every apple was marked before the experiment, and then be placed in the laboratory for 12 hours to make the temperature of apple consistent with the environment temperature.

Near-infrared spectroscopy analysis

Spectra of apple were acquired by the MATRIX-1 type Fourier transform infrared spectrograph, the range of wavelength was 120000~4000cm^{-1}, the number of the sampling points was 1037, and 16 times scans were averaged. Four points of every sample which were equidistant and near the equator were selected to be measured, as much as possible to avoid the obvious surface defects, and the average spectrum of the four points as the final spectrum of the sample. The original spectra of all samples were showed in Figure 1.

SSC and firmness analysis

SSC of apple was measured by PAL-1 digital refractometer, the 4 point measured by spectrograph of each apple were picked as the measurement positions, the unit was % Brix, and the average value of the four results was taken as the final value of the sample. Firmness was measured by GY-1 fruit firmness instrument. Firstly, the peel of the measurement position was removed, and then the instrument was inserted to the pulp uniformly with the depth of 10mm, the unit was N/cm^2, similarly the average value of the four results was taken as the final value of the sample.

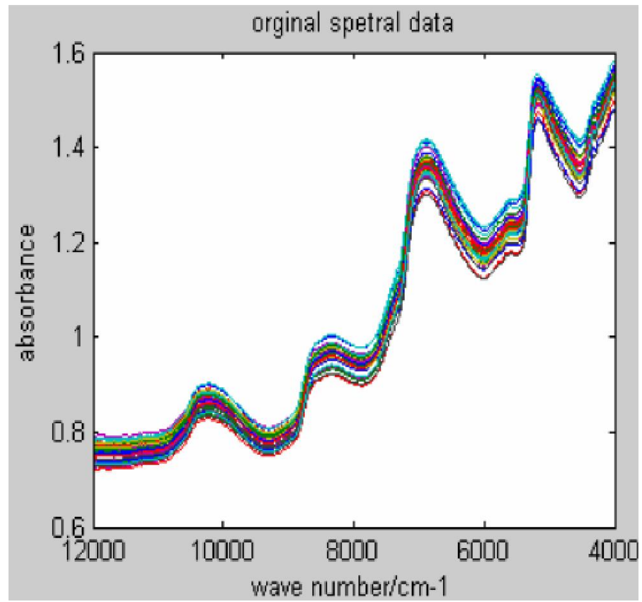

Figure 1 : Original spectra of apples

Data processing: Spectral data was processed by using matlab software. The original reflectance spectra were processed with filtering, smoothing and correction processing by matlab, to remove noise and enhance the effective of the spectral information. The pretreatment methods included Savitzky-Golay smoothing convolution (SG), spectral differentiation, additional scatter correction (MSC) and so on. Spectra obtained in this experiment were recorded of the absorbance at each wavelength: log 1/R, R is the ratio of reflected light intensity and incident light intensity. Prediction model was built by linear regression, multiple linear regression and partial least squares method which were commonly used as modeling algorithm, and standard deviation and correlation coefficient were the main indicators to evaluate the accuracy of the model. To eliminate the abnormal samples before the establishment of the model, Chauvenet criterion was chosen as the method of removing the abnormal samples. In accordance with the content gradient method, the samples were divided into 30 modeling set

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and 9 prediction set. The statistics of modeling set and prediction set was shown in TABLE 1.

TABLE 1 : Statistics of modeling set and prediction set of apples

index		num	max	min	mean	SD
SSC	modeling set	30	17.00	11.10	14.20	1.49
	Prediction set	9	16.40	12.50	14.28	1.35
firm-ness	modeling set	30	8.00	5.24	6.91	0.70
	prediction set	9	7.82	6.99	7.27	0.30

(SD: standard deviation)

RESULTS AND DISCUSSION

Effect of pretreatment methods on the models

Different pretreatment methods had a great impact on building and predictive ability of model, and their results were also different. Therefore choosing the best pretreatment method was very important before building the model. This paper compared several pretreatment methods and their combinations on the models in TABLE 2 and TABLE 3. According to various indicators evaluating the models, it was found that the result of SSC modeling was best with MSC pretreatment method. But the overall results of firmness were worse than SSC, and it was found that the result of firmness modeling was best without any pretreatment. So it showed that the spectra can be pretreated to eliminate some of the unwanted spectral information, but it also could amplify some noise, reduce the effectiveness of the spectra information, and make the results of modeling with pretreatment worse than the modeling based on original spectra. The results of different pretreatment methods on the model of SSC and firmness were shown in TABLE 2 and TABLE 3, respectively.

TABLE 2 : Result of different pretreatment methods on the model of SSC of apples

pretreatment method	main factor of PLS	calibration set		validation set	
		Rc	RMSEC	Rp	RMSEP
none（orginal spectra）	8	0.9631	0.3972	0.9591	0.4702
MSC	6	0.9093	0.6145	0.9622	0.4104
SG	6	0.8587	0.7571	0.8934	0.4104
first order differential	4	0.9690	0.3640	0.8720	0.6952
first order differential +SG	5	0.9797	0.2958	0.8995	0.6525
MSC+ first order differential +SG	2	0.8398	0.8019	0.8445	1.2834
second order differential	4	0.9961	0.1303	0.5532	1.1077
second order differential +SG	5	0.9900	0.3083	0.4102	1.2418
MSC+ second order differential +SG	2	0.7312	1.0078	0.3303	1.2834
MSC +SG	6	0.9039	0.6318	0.9608	0.4680

(Rc: correlation coefficient of Calibration set, RMSEC:The standard deviation of Calibration set, Rp: correlation coefficient of Validation set, RMSEP: The standard deviation of Validation set)

TABLE 3 : Result of different pretreatment methods on the model of firmness of apples

pretreatment method	Main Factor of PLS	calibration set		validation set	
		Rc	RMSEC	Rp	RMSEP
none（orginal spectra）	2	0.8463	0.3825	0.8268	0.2919
MSC	2	0.8073	0.4237	0.7666	0.3208
SG	2	0.8458	0.3830	0.8249	0.2938
first order differential	5	0.9956	0.0671	0.7449	0.3080
first order differential +SG	2	0.8323	0.3986	0.7155	0.3302
MSC+ first order differential +SG	4	0.9725	0.1671	0.6921	0.3551
second order differential	2	0.9077	0.3830	0.7676	0.2938
second order differential +SG	5	0.9930	0.0849	0.7464	0.3701
MSC+ second order differential +SG	4	0.9921	0.0900	0.7571	0.2927
MSC +SG	2	0.8075	0.4235	0.7684	0.3216

The model of SSC

It was found that the result of SSC model was best with MSC pretreatment method. The result of SSC was as follows: the correlation coefficient of the modeling set was R=0.9093, the standard deviation was RMSEC=0.6145, the correlation coefficient of the prediction set was Rp=0.9622, the standard deviation was RMSEP=0.4104. NIR was feasible to predict SSC of apple. The relationship between measured values and predicted values of calibration set and prediction set was shown in Figure 2 and Figure 3, respectively.

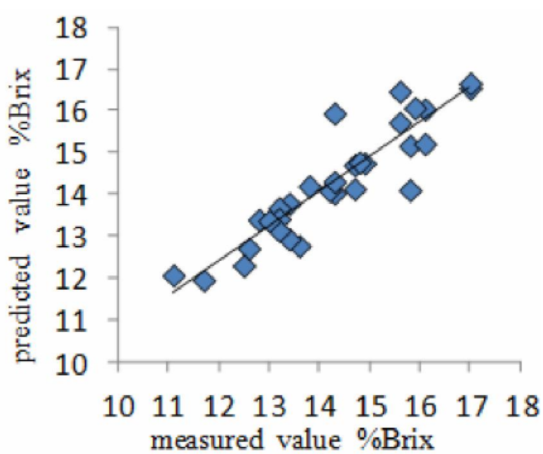

Figure 2 : The relationship of measured and predicted value of calibration set of SSC

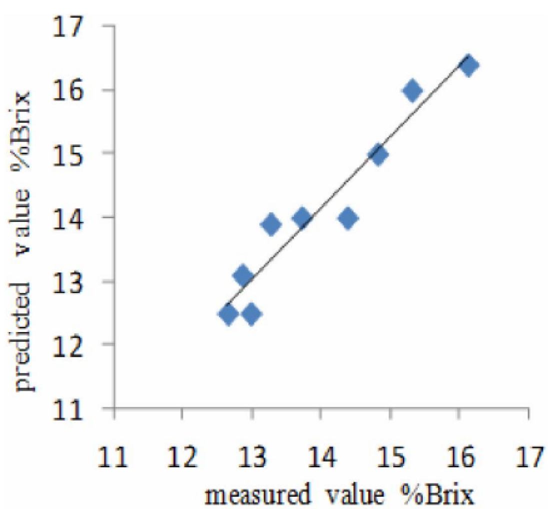

Figure 3 : The relationship of measured and predicted value of validation set of SSC

The model of firmness

The model of firmness was built by using different methods, including simple linear regression, multiple linear regression and partial least squares (PLS). Correlation coefficient method was selected to determine the wavelength point when using modeling method of simple linear regression and multiple linear regression. The results were shown in TABLE 4.

TABLE 4 : Results of different modeling methods on firmness

modeling method	clibration set		vlidation set	
	Rc	RMSEC	Rp	RMSEP
simple linear regression	0.8574	0.3695	0.8073	0.3238
multiple linear regression	0.8718	0.3518	0.7874	0.3676
PLS	0.8463	0.3825	0.8268	0.2919

As seen from TABLE 4, the results of PLS modeling method were superior to the other two. The relationship between measured values and predicted values of calibration set and prediction set based on PLS modeling method was shown in Figure 4 and Figure 5, respectively.

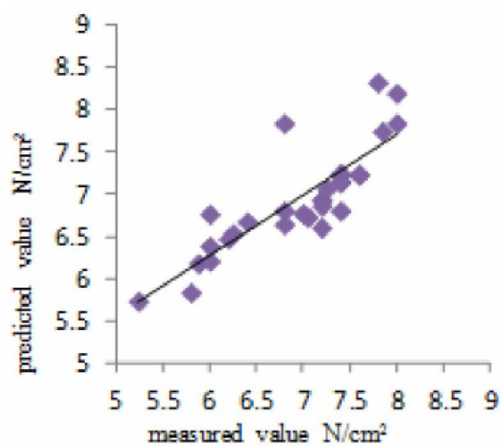

Figure 4 : The relationship of measured and predicted value of calibration set of firmness

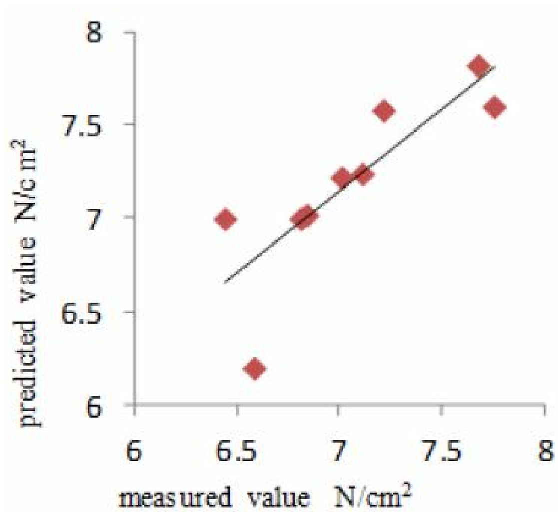

Figure 5 : The relationship of measured and predicted value of validation set of firmness

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Ripeness degree of apples: After getting the value of SSC and firmness of apple, through the national standard GB / T 10651-2008 "Apples", physical and chemical indicators of maturity requirements (firmness $\geq$7kgf/cm^2, soluble solids $\geq$ 13%), marked the apple reaching maturity 1, and immature 0. The comparison result of predictive maturity and measured maturity was shown in TABLE 5, and the percentage of correct classification for the ripeness degree of apple was 74%.

TABLE 5 : Classification of ripeness degree of apples

NO.	Measured maturity	Predicted maturity	NO.	Measured maturity	Predicted maturity
1	0	0	21	1	1
2	0	0	22	1	1
3	1	1	23	1	0
4	0	0	24	0	0
5	1	0	25	0	0
6	1	0	26	0	0
7	1	0	27	1	1
8	1	1	28	0	0
9	0	1	29	1	1
10	1	1	30	0	0
11	1	1	31	0	0
12	0	0	32	1	0
13	0	0	33	0	0
14	1	1	35	0	0
15	0	0	35	1	1
16	1	0	36	1	0
17	1	0	37	1	0
18	0	0	38	1	1
19	0	0	39	1	1
20	1	1			

Apple ripeness software: Apple ripeness software included two parts: spectral data preprocessing and prediction for apple ripeness. The screen of the software was designed by matlab GUI. There were three screens: one main screen and two minor screens. The software could read the file of spectral data, display the graph of spectra, preprocess spectral data, storage the data and predict the value of SSC, firmness and ripeness degree of apple.

CONCLUSION

Although the result of model of firmness was worse than SSC, there was some human error when using instrument resulting in some deviations of the data, the results also showed that NIR spectral analysis was feasible to predict SSC and firmness. Because the prediction for the ripeness of apple depended on the prediction for SSC and firmness of apple, to improve the classification accuracy of ripeness degree of apple, it was necessary to improve the accuracy of the model of SSC and firmness. In this study, the single experimental material lead to the model of narrow applicability, so it is necessary to increase the apple type to expand the application scope of the model; Since the limited number of samples, the number can be increased in the future, and constantly improve the model's reliability; The design of the modeling method is limited, in the future more modeling methods could be studied to improve the accuracy of the model.

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