Effect of Spectra Correction on Water Content Prediction of Red Guava Fruit Using UV-Visible-Near Infrared Spectroscopy

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Abstract. Water content of red guava (*Psidium guajava* L.) can be used as an indicator of fruit texture. Determination of water content using uv-visible-near infrared spectroscopy is a non-destructive method. The research was conducted from June to September 2018 at Horticulture Laboratory, Faculty of Agriculture, Universitas Padjadjaran. The samples were 100 fresh red guava fruits. Samples were divided into 3 groups, then stored for 0 day, 4 days, and 8 days. NirVana AG410 spectrometer from 300 to 1065 nm was performed for absorbance spectra acquisition. Absorbance data were pre-treated using spectra correction methods including orthogonal signal correction (OSC) and standard normal variate (SNV). Model development was done by partial least squares (PLS) for the calibration model and full cross-validation for the validation model. The purpose of this research was to determine the best spectra correction to develop calibration model for predicting water content of red guava fruit. The result showed that the best spectra correction was OSC based on the value of coefficient of determination (R^2), root mean squares error of calibration (RMSEC), root mean squares error of cross-validation (RMSECV) and ratio of performance to deviation (RPD). OSC displayed R^2 of calibration (0.97) and validation (0.91), RMSEC (0.006), RMSECV (0.005) and RPD (3.29). This study concluded that spectra correction of OSC was able to develop the calibration model with the most reliable and accurate model for predicting water content of red guava fruit.

Keywords: absorbance data, fruit quality, NirVana AG410, respiration, spectra correction.

1 Introduction

Red guava is one of the climacteric fruits. Respiration rate of fruit increases during maturation. The maturity stage is related to shelf life and quality fruit. Water content is an indicator of fruit texture. Ripe fruit has a higher water content than unripe fruit. The water content of red guava fruit ranged from 87.55-88.23% [1]. Water content is the amount of water contained in the fruit. Water content determines the texture, taste and appearance of the fruit. Water content changes during storage. Red guava fruit that stored for 0 day, 4 days and 8 days showed the decrease of firmness and the increase of water content [2].

The value of water content can be measured quantitatively. Determination of water content is usually done by invasive and non-invasive technique. Basically, invasive technique causes damaged fruit and disadvantage for farmers. Therefore, the non-invasive technique is considered eco-friendly, fast and accurate for predicting fruit quality. One of the invasive techniques that can be used is uv-visible-near infrared spectroscopy. This technique has been informed to measure the water content of sapodilla [3], avocado [4], passion fruit [5] and dragon fruit [6]. Besides, uv-vis-spectroscopy is usable to discriminate fruit species from other species [7]. The wavelengths ranged from 312-1050 nm was reported to predict sapodilla quality attributes such as total soluble solids, firmness, and surface color [8].

Uv-visible-near infrared spectroscopy produced data interpreted in spectra. The collected spectra data is processed using multivariate analysis. This analysis is able to process the data with a lot of variables to find relationship between two or more variables. The type of multivariate analysis that is widely used is partial least squares (PLS). The purpose of data processing with PLS is to develop the calibration model including the predictor variable (X) and the response variable (Y). The calibration model is the correlation between spectra as the predictor variable and reference data

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as the response variable. The accuracy of the calibration model can be verified with validation. Generally, PLS is used to prevent multicollinearity.

The data taken by uv-visible-near infrared spectroscopy sometimes still include noises. The presence of other light entering the detector, shaking during scanning and the presence of other chemicals such as fruit waxing caused noises. Physical or chemical interference during scanning induced noise [9]. Noises can reduce the accuracy of the calibration model, but the spectra data can be processed using spectra correction. It is useful to reduce noise of spectra data in order to acquire the proper regression value [10]. Orthogonal signal correction (OSC) and standard normal variate (SNV) could be performed to correct the spectra data. Both methods have been commonly used to improve the accuracy of fruit quality evaluation, including coffee [11], persimmon [12], oil palm fruit [13] and apple [14]. Based on this explanation, the purpose of this research was to determine the best spectra correction to develop calibration model to predict the water content of red guava fruit.

2 Materials and Method

2.1 Red guava fruit samples

Red guava fruits were collected from Sumedang, West Java, Indonesia. A total of 100 samples were transported to Horticulture Laboratory, Agriculture Faculty, Universitas Padjadjaran. All samples were harvested at the same maturity level. The samples were sorted, numbered and stored for 0 day, 4 days and 8 days at room temperature (±28^{0}C). The samples were placed on 4 plastic baskets divided into 25 samples per basket.

2.2 Spectra measurement

Spectra aquisition of red guava fruit was done using NirVana AG410 spectrometer with wavelengths from 300 to 1065 nm. The detector of spectrometer measured the reflectance of the reflected light from the sample. Red guava fruit was irradiated 6 times, including top (near stalk), middle, and bottom on two different sides. Spectra data were averaged for each sample.

2.3 Destructive analysis

Water content of fruit was measured using gravimetric method [15]. The measurement was done by drying the samples using the oven. Each sample was sliced and dried at temperature of 80^0 C. Water content (%) is described by following equation:

water content (%): x 100% (1)

where:

W_1 : Fresh weight of the sample,

W_2 : Dried weight of the sample

2.4 Data analysis

NirVana AG410 spectrometer was performed to measure the spectra data (reflectance). The data were moved to the computer and interpreted by ISIS (Integrated Software for Imagers and Spectrometers). Reflectance data were transformed into absorbance data (log 1/R). Spectra data was pre-processed using spectra corrections, including OSC and SNV. Principle of OSC is eliminating predictor variable that unrelated with the response variable [16]. SNV works by removing scatter effects from spectrum and creating individual spectrum. Function of SNV correction is erasing multiplicative interferences from scatter effects on spectrum data [17]. Data analysis was run using software Unscrambler 10.4. Calibration model was built using PLS method.

Multivariate analysis is a series of data processing with a large number of samples and variables. PLS is prediction analysis by analyzing the predictor variables and response variables simultaneously [18]. The problem of multicollinearity as overlapping data can be minimized by PLS [19]. The regression model, can be written as follows:

Ratio performance to deviation (RPD) is the comparison between standard deviation from actual data and RMSECV from cross validation set. The RPD value can be used as one of the determinants of the accuracy of the NIR application model. the formula for calculating RPD is written below:

$$RPD = \frac{SD}{RMSECV} \quad (2)$$

where:

SD : value of standard deviation of reference data,

RMSECV : value of root mean squares error in cross validation set.

3 Results and discussion

The storage of red guava fruit was intended to obtain variation in water content data. Water content of red guava fruit ranged from 76.71% – 85.8%. Wide range of water content data was expected to increase the value of prediction accuracy.

Table 1. Summary of water content data of guava red fruits

value	0 day	4 days	8 days
Min	76.71%	77.7%	77.51%
Max	84.81%	85.8%	85.74%
Mean	81.52%	81.1%	82.60%
Stdev	1.82%	1.80%	2.00%

Table 1 showed minimum, maximum, and standard deviation of measured water content of red guava fruit on different storage. Minimum value of 0 day storage was 76.71%, 4 days storage was 77.7% and 8 days storage was 77.51%. Maximum value of 0, 4, and 8 days storage were 84.81%, 85.8%, and 85.74%, respectively. Averaged values of 0, 4, and 8 days storage were 81.52%, 81.1%, and 82.60%, respectively. Transpiration is the evaporation process in the agricultural product. This process involves the changes in insoluble propectin into soluble pectin, hence the pectin degraded into polygalactonate acid and then produced water [20]. The standard deviation states the level of deviation of individual data to the average value. This value used to describe variety of data. Storage of 0, 4 and 8 days resulted standard deviation of 1.82%, 1.80% and 2.00%, respectively.

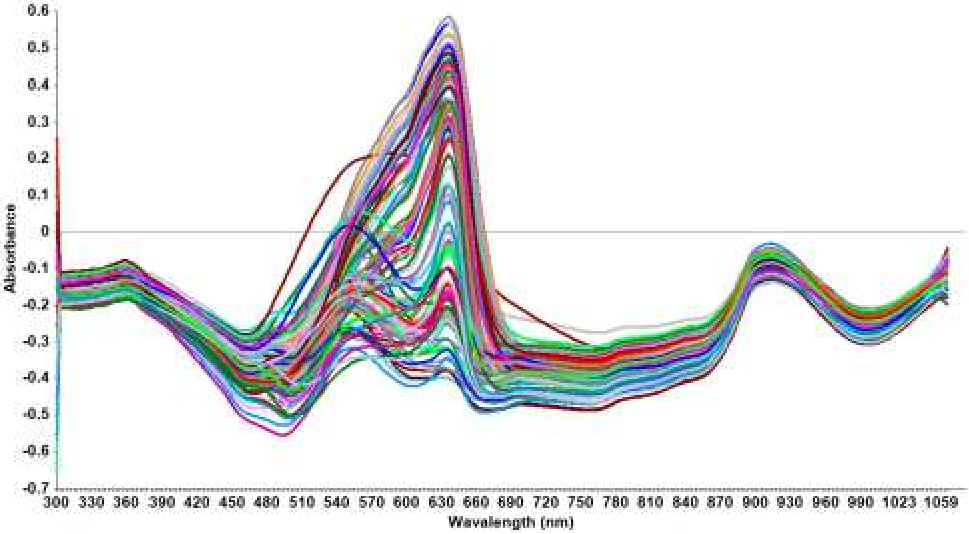

Figure 1. Absorbance spectra of red guava fruit

Figure 1 displayed original spectra of red guava fruit from 300-1065 nm. Scanning using uv-visible-near infrared spectroscopy created peaks and valleys. The highest peak was at wavelength of 636 nm with value of 0.58 while the lowest valley was at wavelength of 492 with value of -0.55. Peaks and valleys indicate the detected quality attributes of samples. Original absorbance spectra presented noises at wavelengths ranged from.483-861 nm. Spectra correction was expected to eliminate the noises. The light contamination and vibration during spectra acquisition cause noises. Besides, noises could be caused by frequency and energy that are not correspond to the sample [21]

Table 2. Summary of calibration and validation model using different spectra correction methods

Spectra	Factor	Calibration		Validation		RPD
		R^2	RMSEC	R^2	RMSECV	
Absorbance	21	0.97	0.002	0.87	0.006	2.85
OSC	13	0.97	0.002	0.91	0.005	3.39
SNV	17	0.83	0.007	0.50	0.014	1.41

Table 2 showed calibration and validation data such as R^2, RMSEC, RMSEP, factor and RPD. The results displayed that OSC spectra correction gave the best prediction accuracy among 2 others spectra. OSC yielded smallest factor value, RMSEC, and RMSECV. Besides, OSC also acquired the highest calibration R^2, validation, and RPD. Calibration analysis that produces R>0.71 (R2>0.5) is an effective model and feasible to predict independent samples (William 2007). OSC spectra correction is useful to minimize factor of regression analysis. Factor of original absorbance presented the value of 21, while the corrected spectra using OSC method denoted the factor value of 13. This revealed that OSC is effective to reduce the factor. Low factor value indicates the low interference of spectra. The use of OSC gave lowest factor than original absorbance and SNV spectra for predicting water content of cocoa beans, lower factor value provides better prediction [22].

The accuracy of model could also be explained by coefficient of determination value. It explained by the value ranged from 0-1. Closer to the 1, the better prediction accuracy of the model has. All three spectra showed coefficient determination value close to 1.

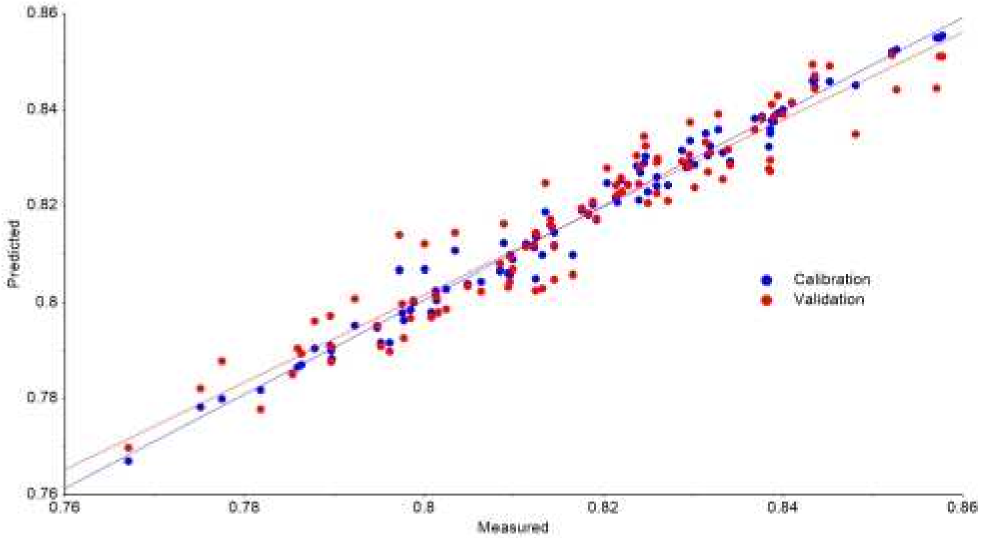

Figure 2. Scatter plot for water content red guava fruit with OSC

Calibration model of water content was develop using PLS and non-iterative partila least squares (NIPAL) algorithm. Figure 2 displayed the scatter plot of calibration model and validation of OSC corrected spectra. Distribution data of calibration and validation showed close to the regression line, it resulted high coefficient of determination. The regression was made from spectra data as predictor variable and destructive water content data as respon variable. Validation was processed using cross-validation method with 20 segments.

RPD value is also an indicator to check the accuracy of model. OSC corrected spectra gave value that affects the calibration scatter plot. RPD above 3 presents excellent angle of regression line (slope closes to 1) [23]. Calibration model of OSC corrected spectra produced RPD above 3, which means the calibration model is reliable, while original absorbance and SNV showed RPD value below 3. RPD value <1.5 indicates the calibration model is unusable, ranged from 1.5-1.9 denotes the model is able to distinguish the variation between sample, whereas 2.0-2.9 explains that the model is good, and RPD above 3 means the model is excellent [24].

Conclusions

The best spectra correction was OSC method based on the value of R^2, RMSEC, RMSECV, RPD, and factor. OSC displayed R^2 of calibration (0.97) and validation (0.91), RMSEC (0.006), RMSECV (0.005) and RPD (3.29). This study concluded that spectra correction of OSC was able to develop the calibration model with the most reliable and accurate model for predicting water content of red guava fruit.

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