Prediction of water content and soluble solids content of ‘manalagi’ apples using near infrared spectroscopy

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Abstract. The purpose of the research was to predict quality attributes of ‘manalagi’ apples using near infrared spectroscopy (NIRS). The desired quality attributes were water content and soluble solids content. Spectra data collection was performed at wavelength of 702 to 1065 nm using a Nirvana AG410 spectrometer. The original spectra were enhanced using orthogonal signal correction (OSC). The regression approaches used in the study were partial least squares regression (PLSR) and principal component regression (PCR). The results showed that water content prediction acquired coefficient of determination in calibration set (R²cal) of 0.81, coefficient of determination in prediction set (R²pred) of 0.61, root mean squares error of calibration set (RMSEC) of 0.009, root mean squares of prediction set (RMSEP) of 0.020, and ratio performance to deviation (RPD) of 1.62, while soluble solids content prediction displayed R²cal, R²pred, RMSEC, RMSEP, and RPD of 0.79, 0.85, 0.474, 0.420, and 2.69, respectively. These findings indicated that near infrared spectroscopy could be used as an alternative technique to predict water content and soluble solids content of ‘manalagi’ apples.

1. Introduction

Indonesia is a tropical country that is suitable for planting various horticultural crops. One of the types of horticultural plants that can be cultivated is fruits. The lowlands and highlands are suitable growing environments for various types of fruits. One of the fruit plants that are widely cultivated is the apple. The apple commodity that is greatly developed in Indonesia, especially in the city of Malang is Manalagi apples, which have a reddish green skin color with white flesh.

The assessment of the quality of apples during harvesting by farmers is usually done by looking at the size, shape and color of the fruit. ‘Manalagi’ apples have a sweeter taste than other apples, so the level of sweetness is the main parameter of the quality of apples. In addition to its sweet taste, apples contain many kinds of vitamins which are also good for health.

The quality of apples generally changes after harvesting. The process of distributing commodities from the time of harvesting to the final consumers takes a lot of time. Quality monitoring is needed to ensure that consumers get products that have good quality. Water content is the key to fruit freshness. Apple fruit quality parameters in the form of sweetness and water content cannot be assessed based on the visual appearance. Conventional determination of water content and soluble solids content (SSC) is usually performed by destructing the fruit.
Destructive determination is more difficult to do because it will cause fruit damage. Non-destructive methods can be used as an alternative choice to predict fruit quality parameters. New technology in a non-destructive way has been widely applied to detect post-harvest fruit quality. One of the non-destructive technologies that can be used is near infrared (NIR) spectroscopy. The advantage of this method is that it can evaluate various quality parameters without causing fruit damage. This technique can be used to measure the quality of vegetables and fruits [1]–[8].

There are some linear regression methods used to process data from NIR spectroscopy, including partial least squares regression (PLSR) and principal component regression (PCR). PLS is a predictive step method by processing various independent and dependent variables simultaneously and PCR is a predictive step method by focusing on one variable, namely the independent variable [9]. The two regression methods are often used to process data from NIR. The purpose of this study was to examine the use of NIR spectroscopy to predict water content and soluble solids content (SSC) of ‘manalagi’ apples.

2. Materials and methods

Apple samples

Samples of apple variety ‘manalagi’ were harvested as many as 150 pieces from an apple orchard located in Malang, Indonesia. A total of 150 samples were divided into 2 groups, namely the calibration set (100 samples) and the prediction set (50 samples). The fruit was harvested and brought to the laboratory for testing. Analysis of water content and SSC was carried out at the Horticulture Laboratory, Faculty of Agriculture, Universitas Padjadjaran.

2.1 Spectra acquisition

Spectra data were collected using a NirVana AG410 spectrometer. The wavelength used in this study is 702-1065 nm which includes the near infrared region. Data acquisition was carried out at 6 points per sample which was then averaged.

2.2 Measurement of water content and soluble solids content

Determination of water content in apple samples was done by drying method using an oven at a temperature of 60°C. The fruit was cut into small pieces and put in aluminum foil and dried in the oven. The dry weight of the sample was weighed until it was constant. SSC measurements were carried out with a refractometer so that the %Brix value was obtained which indicated the level of sweetness of the sample. The sample solution was dripped 3 times into the refractometer detector and the average value of each sample was taken.

2.3 Data analysis

The results of spectral data acquisition and laboratory analysis (water content and SSC) were then processed using The Unscrambler 10 software for calibration modeling. Each quality parameter was processed using two different methods, namely the partial least square regression (PLSR) and principal component regression (PCR) methods. The results of statistical evaluation used for calibration and prediction of the two methods are coefficient of determination (R²), root mean square errors of calibration (RMSEC), root mean square errors of prediction (RMSEP) and ratio performance to deviation (RPD).

3. Results and discussion

Figure 1. shows the spectra data for ‘manalagi apples’. The spectra contain information about the chemical composition information contained in apple samples recorded at a wavelength of 702-1065 nm (near infrared). Spectra data carry information from organic matter and can be used for interpretation of chemical content data. The NIR spectrum is responsible for products involving C-H,
N-H, S-H and O-H molecular bonding responses [8], [10]. The high and low peaks indicate that the wavelength plays a role in the detection of chemical compounds.

![Near infrared spectra of ‘manalagi’ apples.](image)

Table 1. Results of regression analysis on water content and soluble solids content of ‘manalagi’ apples.

| Regression method | Quality attributes | Spectra preprocessing | PC | \( R^2_{\text{cal}} \) | RMSEC | \( R^2_{\text{pred}} \) | RMSEP | RPD |
|-------------------|--------------------|-----------------------|----|-----------------|------|-----------------|------|-----|
| PLSR              | Water content      | Original              | 8  | 0.78            | 0.009| 0.61            | 0.020| 1.62|
|                   |                    | OSC                   | 3  | 0.81            | 0.009| 0.61            | 0.020| 1.62|
|                   | SSC                | Original              | 7  | 0.80            | 0.460| 0.84            | 0.440| 2.54|
|                   |                    | OSC                   | 1  | 0.79            | 0.474| 0.85            | 0.420| 2.69|
| PCR               | Water content      | Original              | 6  | 0.64            | 0.012| 0.55            | 0.021| 1.51|
|                   |                    | OSC                   | 1  | 0.67            | 0.012| 0.54            | 0.021| 1.50|
|                   | SSC                | Original              | 8  | 0.78            | 0.480| 0.83            | 0.452| 2.50|
|                   |                    | OSC                   | 1  | 0.79            | 0.474| 0.85            | 0.420| 2.69|

PLSR: partial least squares regression, PCR: principal component regression, SSC: soluble solids content, OSC: orthogonal signal correction, PC: principal component, \( R^2_{\text{cal}} \): coefficient of determination in calibration set, RMSEC: root mean squares error of calibration, \( R^2_{\text{pred}} \): coefficient of determination in prediction set, RMSEP: root mean squares error of prediction, RPD: ratio performance to deviation.

Table 1 displays the results of the regression analysis on the two observed quality parameters. The best calibration model on water content was obtained from the combination of PLSR and OSC with values of \( R^2_{\text{cal}} \), RMSEC, \( R^2_{\text{pred}} \), RMSEP, and RPD respectively 0.81, 0.009, 0.61, 0.020, and 1.62. In SSC estimation, the best calibration model was obtained from the combination of PLSR + OSC and PCR + OSC, both of which showed the same good model performance with values of \( R^2_{\text{cal}} \) (0.79), RMSEC (0.474), \( R^2_{\text{pred}} \) (0.85), RMSEP (0.420), and RPD (2.69). The results of the statistical analysis show that the resulting model is reliable to be used to predict new unknown samples [11]. The OSC spectra correction method is able to improve the accuracy of the model compared to the original spectra. This is supported by the results of research on the prediction of SSC and water content in
melons using visible/near infrared spectroscopy which concluded that the OSC spectra correction method showed the best results [12-15].

Figure 2. Scatter plot of calibration model for water content.

Figure 3. Scatter plot of calibration model for soluble solids content.

Figure 2 and Figure 3 show scatter plots for the calibration model on the water content and SSC. The scatter plot describes the relationship between laboratory analysis results and NIRS predictions. In both quality parameters, the distribution of data is recorded to be close to the regression line indicating a strong relationship between laboratory data and NIRS predictions. This strengthens the results of statistical analysis which shows the value of the coefficient of determination is quite high on both quality parameters.

4. Conclusions
The results showed that near infrared spectroscopy can predict the water content and soluble solids content of ‘manalagi’ apples with a high degree of accuracy. This is indicated by the $R^2_{\text{cal}}$ and RPD values of 0.81 and 1.62 for the water content parameter, while for the soluble solids content the values obtained were 0.79 and 2.69. These statistical data confirmed that near infrared spectroscopy was able to be used as an alternative technique to predict the water content and soluble solids content of ‘manalagi’ apples.
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