Jurnal Biodjati 4(1):89-95, May 2019

e-ISSN : 2541-4208
p-ISSN : 2548-1606

JURNAL BIODJATI

http://journal.uinsgd.ac.id/index.php/biodjati

NON-DESTRUCTIVE CLASSIFICATION OF FRUITS BASED ON UV-VIS-NIR SPECTROSCOPY AND PRINCIPAL COMPONENT ANALYSIS

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Received : March 21, 2019
Accepted : May 06, 2019

DOI: 10.15575/biodjati.v4i1.4389

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Abstract. *Fruits are one of the sources of nutrition needed for health. Fruit quality is generally assessed by physical and chemical properties. Measurement of fruit internal quality is usually done by destructive techniques. Ultraviolet, visible and near-infrared (UV-Vis-NIR) spectroscopy is a non-destructive technique to measure fruit quality. This technique can rapidly measure the fruit quality, the measured fruit still remains intact, and can be marketed. Besides, UV-Vis-NIR spectroscopy can also be used to classify fruits. The study aimed to classify various types of fruits using UV-Vis-NIR spectroscopy with wavelengths of 300-1041 nm and Principal Component Analysis (PCA). First derivative savitzky-golay with 9 smoothing points (dg1) and multiplicative scatter correction (MSC) were applied to correct the spectra. The results showed that the use of uv-vis-nir spectroscopy and PCA combined with spectra pre-treatment of the MSC method were able to classify various types of fruits with 100% success rate in all fruit samples including sapodilla, ridge gourd, mango, guava, apple and zucchini.*

Keywords: *dg1, Hotelling's* T^2*, MSC, NIPALS, PCA*

Citation
Kusumiyati, Hadiwijaya, Y & Putri, I. E. (2019). Non-destructive Classification of Fruits Based on UV-Vis-NIR Spectroscopy and Principal Component Analysis. *Jurnal Biodjati*, 4(1), 89-95

INTRODUCTION

Indonesia is a country that has fertile soils and tropical climate, various types of plants can grow well in Indonesia, especially horticulture plants. Therefore, the Indonesian agricultural sector, especially horticulture, has high potential to be able to compete with other countries. Horticulture products are generally divided into 4 major groups, namely fruit, vegetables, medicinal and ornamental plants. Fruits are the essential source of minerals and vitamins needed by humans. Generally, measurements of fruit quality such as vitamins, total soluble solids, and sugar content are made by extracting the fruit, then testing in the laboratory. This technique is conducted by destructing the fruits, hence the new technique is needed to measure the quality of fruit non-destructively.

Ultraviolet, visible and near-infrared (UV-Vis-NIR) spectroscopy is a non-destructive technique that has been studied by scientists for decades. The advantage of this technique is that it is possible to analyze a product non-destructively, environmentally friendly, no chemical materials needed, rapid analysis and high accuracy. UV-Vis-NIR spectroscopy is a technique where the sample is illuminated by light (photons) originating from the spectrometer. Then some photons are reflected back and spectrum data is obtained. The reflected photons carry information about internal composition of the sample.

In its application, UV-Vis-NIR spectroscopy requires chemometrics analysis to extract information of the spectra data. Chemometrics is an analytical technique that combines mathematics and statistics to interpret chemical data. The use of spectroscopy technique has been widely used to measure various fruit quality parameters including kiwifruit (Moghimi et al., 2010), banana (Zude-Sasse, 2003), passion fruit (Maniwara et al., 2014), apricot (Chen et al., 2006) and jujube (Wang et al., 2011). In addition, Kusumiyati et al. (2018) used wavelengths of 312-1050 nm to predict water content in sapodilla fruit.

Principal Component Analysis (PCA) is a technique to simplify data by transforming the data into new variables. PCA can also be used to classify or differentiate a product from other products. Yulia et al. (2017) performed the PCA to classify arabica and robusta coffee. This study aimed to classify various types of fruits based on UV-Vis-NIR spectroscopy and PCA analysis. Moreover, the spectra pre-treatment methods, such as first derivative savitzky-golay (dg1) and multiplicative scatter correction (MSC) were applied to the original absorbance spectra to improve the results of PCA analysis.

MATERIALS AND METHODS

Sample Preparation

Sapodilla samples (sukatali cultivar) were collected from plantation in the Situraja area, Sumedang, West Java, Indonesia. Samples of ridge gourd, mango (arumanis cultivar) and guava (crystal cultivar) were obtained from plantation in Tomo, Sumedang, West Java, Indonesia. Apple fruits (manalagi cultivar) were harvested from apple orchards in the city of Malang, East Java, Indonesia, while the zucchini samples were brought from the garden located in Lembang, West Bandung, West Java, Indonesia. All fruits were harvested at mature stage. Samples from each fruit commodity amounted to 20 samples, therefore the total samples amounted to 120 samples. Before analysis, all samples were numbered first. All observations and analysis were carried out at the Horticulture Laboratory, Department of Agronomy, Faculty of Agriculture, Universitas Padjadjaran.

Spectra Data Collection

The NirVana AG410 handheld spectrometer with wavelengths of 300-1041 nm and 3 nm interval was operated for spectra data collection. The wavelengths of 300-1041 nm are categorized as an area that includes ultraviolet, visible light, and near-infrared (UV-Vis-NIR). Before collecting the spectra data, the spectrometer was activated for at least 5 minutes for warming up. Each sample was scanned once in the middle part of fruit. The scan duration was around 5 seconds per sample. The spectra data obtained from the spectrometer were absorbance spectra, which is radiation absorbed by the sample. Thus, a total of 120 scans were collected to represent the spectra data of all fruit samples. The output data were processed using Integrated Software for Imagers and Spectrometers (ISIS). Furthermore, spectra data were analyzed using The Unscrambler version 10.4 for spectra pre-treatments and classification by the PCA.

Spectra Pre-treatments

The spectra obtained from the spectrometer require spectra pre-treatment to improve the analysis results. Spectra pre-treatment can reduce various influences such as pericarp thickness and skin disorder. It is also able to improve the spectra classification. According to Rinnan et al. (2009) spectra pre-treatment can reduce spectrum diversity due to light emission and nonlinearity, it is

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also effective in improving accuracy of model to be obtained. The spectra pre-treatment methods applied in this study were dg1 with 9 smoothing points and MSC. Both are common methods used to correct the spectra data. The MSC correction method can decrease the effects of light emission and minimize diversity in the spectrum. The working principle of the MSC is to examine each spectrum and correct it based on the reference spectrum by utilizing the results of simple linear regression estimation. The dg1 method is able to separate the overlapping spectrum in order to acquire the hidden information in the spectrum.

Classification Using PCA

Once the spectra pre-treatment was finished, PCA analysis was performed using the Non-linear Iterative Partial Least Squares (NIPALS) algorithm. PCA is a multivariate analysis method that works by reducing correlated variables and then converting them into new variables that are not correlated with each other. NIPALS was used due to large numbers of samples and variables. PCA modifies the large numbers of variables into the principal component (PC), which are few in number but still can explain diversity in the original data. In addition, PCA transforms the original absorbance data into scores and loading vectors. Hotteling's T^2 was used to detect the outliers in diversity of PCA analysis data.

RESULTS AND DISCUSSION

The absorbance data were obtained from the measurement of spectra with wavelengths of 300-1041 nm, which includes ultraviolet (UV), visible (Vis) and near-infrared (NIR) radiation. When light with various wavelengths is radiated to organic matter, a portion of light at certain wavelengths will be absorbed. The amount of absorbed light depends on composition of the irradiated organic material. Each species of fruits has different composition from other fruits such as chlorophyll, carotenoids, vitamins, sugar content, etc. This causes different absorption responses in each species. Information obtained from UV-Vis-NIR radiation uptake in organic materials includes optical, physical and chemical properties. Absorbance spectra in various fruit

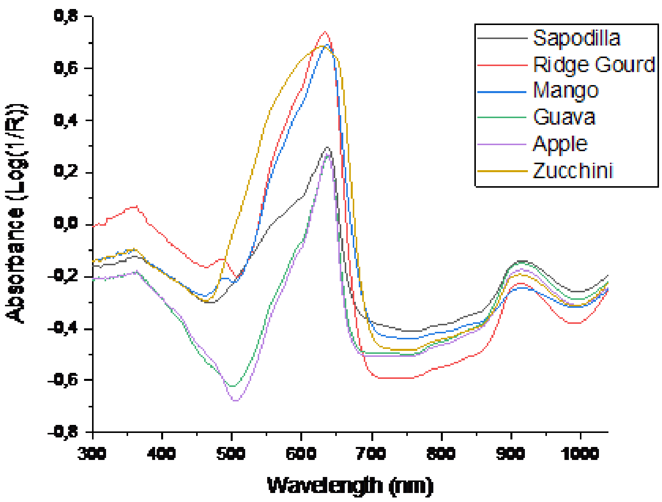

Figure 1. Absorbance spectrum in each fruit

commodities (Figure 1).

Various parameters of fruit quality can be predicted with wavelengths in the UV-Vis-NIR region, peaks at wavelengths of 470 and 500 nm correlated with absorption bands of lycopene content (Bunghez et al., 2011), while Bhumsaidon & Montip (2016) used wavelengths of 453, 505, 645 and 663 nm to measure lycopene and beta carotene. Another study stated that absorption at wavelength of 660 nm was detected as chlorophyll content (Solovchenko et al., 2001). Kusumiyati et al. (2018) predicted total soluble solids, firmness, skin color (L*, a*, b*, hue and chroma) of sapodilla fruit with wavelengths of 312-1050 nm and obtained high accuracy rate.

Pre-treatment of spectra is an important stage in interpretation of spectra data. When collecting spectra data, the data often noises, scattering spectra and various other disturbances are also detected. Therefore, spectra pre-treatment is needed to minimize the effect of the disturbances, with the intention of interpreting spectra data can be enhanced. The most widely used methods include dg1 and MSC.

The results of PCA analysis of absorbance spectra without spectra pre-treatment attained PC1 values of 80% and PC2 by 8%. PC1 is a component that explains the greatest variability in the analyzed data set, while PC2, PC3, and so on explain the remaining variability. The scores plot illustrates that only sapodilla samples were able to be classified properly without being mixed with other fruit samples (Figure 2). Additionally, when Hotelling's T^2 was projected onto the data set, there was one outlier in sapodilla sample. The outlier is a different sample from most other samples. The existence of this outlier is not beneficial for the PCA model because it can cause bias. The usual handling for outliers includes eliminating outliers or applying spectra pre-treatment.

The values of PC1 and PC2 acquired from the PCA analysis and spectra pre-treatment of the dg1 method were 58% and 28%, respectively (Figure 3). Moreover, once Hotelling's T^2 was applied to scores plot, there was still one outlier in the ridge gourd fruit sample. Pre-treatment of spectra using the dg1 method was carried out in order to disperse the overlapping spectrum with the aim of clearer spectrum of peaks and valleys would be obtained (Cen & He, 2007). The dg1 method was an effective method for improving the calibration model of estimating starch content in arumanis mango (Agustina et al., 2015). But on the results of PCA analysis, this method was not able to classify various types of fruits properly. Similar to absorbance spectra without spectra pre-treatment, which only sapodilla fruit samples can be classified properly, while other fruit samples were still mixed together.

The use of the PCA classification method combined with the pre-treated spectra of the MSC method was able to classify fruits with accuracy rate of 100%. This can be witnessed from the distribution of scores plot data (Figure 4), each group of fruits can be separated without being mixed with different fruits. Guava and apple were grouped in positive X-axis, while ridge gourd, zucchini and mango were categorized in negative X-axis. This denoted that guava and apple fruits have composition that is inversely proportional (opposite) to ridge gourd, zucchini and mango. On the other hand, sapodilla was in the middle between the two groups. Apple and guava samples displayed very close data distribution, this indicates that guava and apples have proximity in terms of fruit composition, this comprises physical or chemical composition. The values of PC1 and PC2 were 78% and 9% respectively, with a total of 87% variance can be explained on PC1 and PC2. Hotelling's T^2 projected on the results of the PCA analysis of the MSC method found no outliers in the entire population. Therefore, the MSC method achieved the best results in classifying fruits. This is in line with research conducted by Munawar et al. (2017) that the use of near-infrared at wavelengths of 1000-2500 nm and the pre-treatment method of MSC was able to classify biodiesel based on different KOH concentrations with 100% success rate. In other study, Ramadhan et al. (2016) reported that the use of PCA and spectra pre-treatment of the MSC method were able to classify Aceh and Bali coffee beans well. The MSC method works by circling each spectrum and then correcting the spectrum to obtain similarities to the standard spectrum.

The use of UV-Vis-NIR spectroscopy with wavelengths of 300-1041 nm and PCA combined with spectra pre-treatment of the MSC method were able to classify fruits non-destructively with a success rate of 100% in all fruit samples including sapodilla, ridge gourd, mango, guava, apple and zucchini.

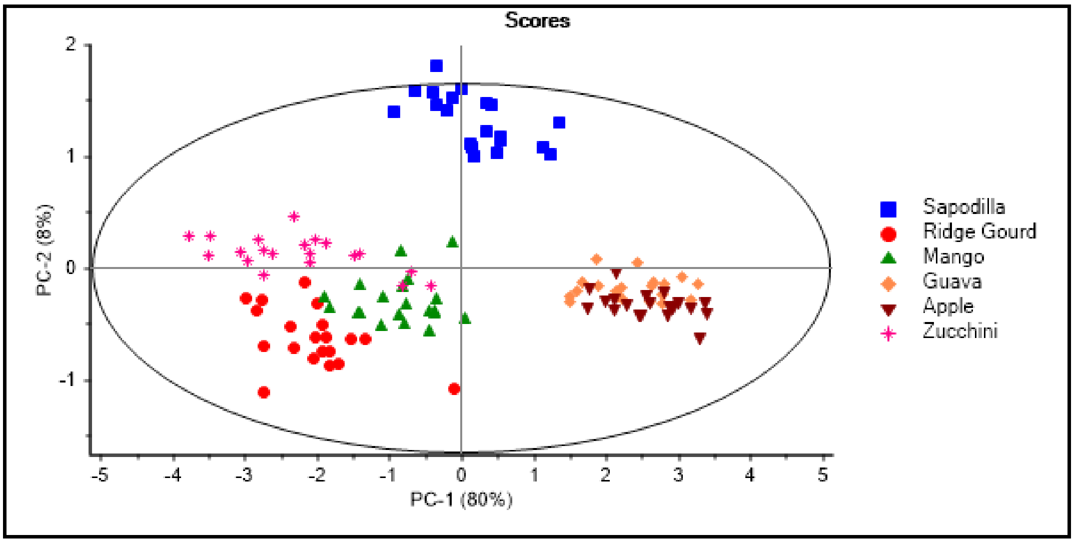

Figure 2. PCA scores plot of absorbance without spectra pre-treatment

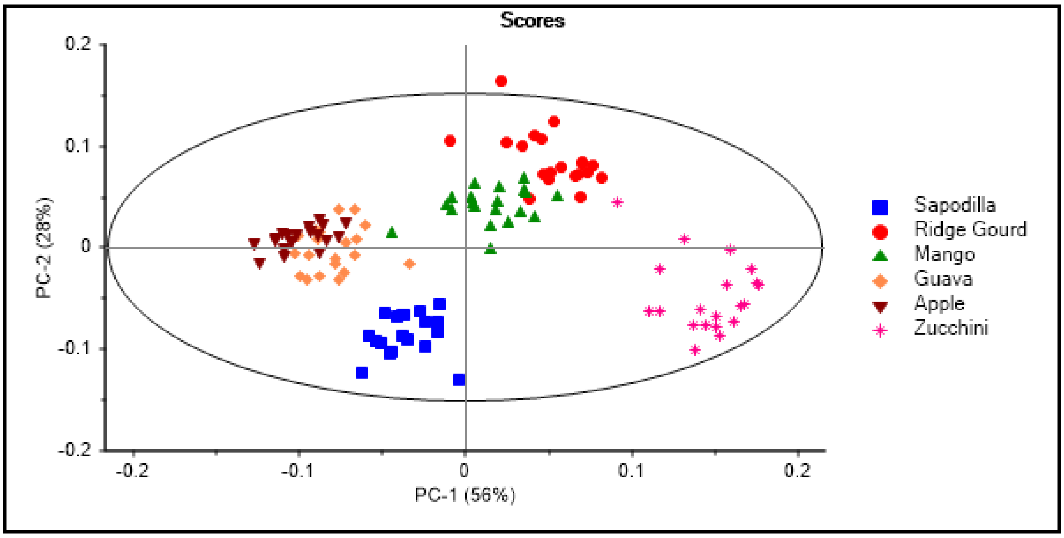

Figure 3. PCA scores plot with dg1 pre-treated spectra

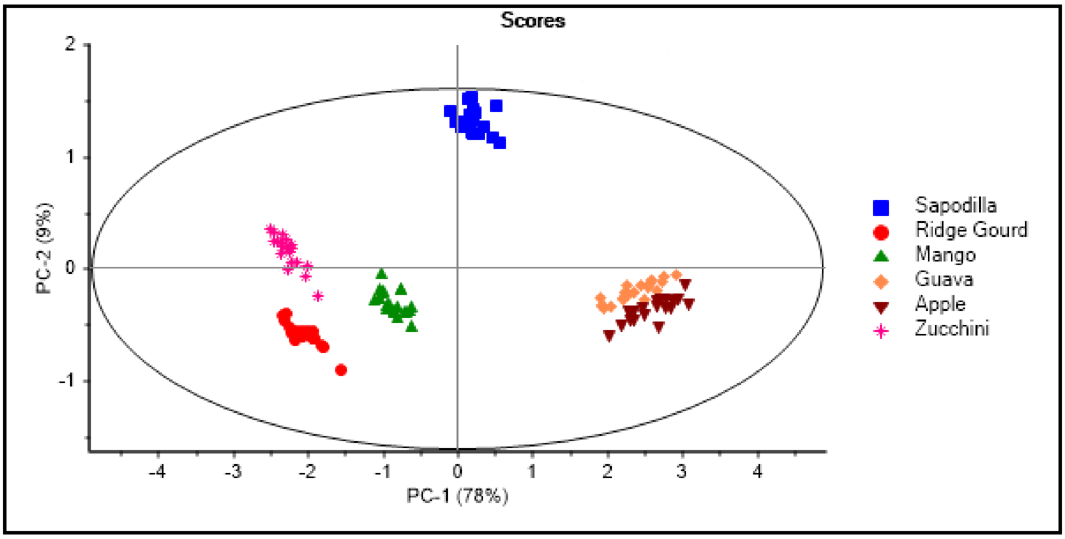

Figure 4. PCA scores plot with MSC pre-treated spectra

ACKNOWLEDGMENTS

This study was supported by DRPMI of Universitas Padjadjaran.

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