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Application of spectra pre-treatments on firmness assessment of intact sapodilla using vis-nir spectroscopy

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Abstract. This study aimed to obtain the best calibration model from various spectra pretreatment methods to assess sapodilla fruit firmness using vis-nir spectroscopy. Before the spectra data measurement, samples were treated with storage of 0, 5 and 10 days at room temperature. Spectra data measurement was carried out using the NirVana AG410 visible and near infrared spectrometer from 312 to 1050 nm with interval of 3 nm. RAW spectra were pretreated using the multiplicative scatter correction (MSC), standard normal variate (SNV), and Savitzky-Golay first derivative (dg1) with 9 points of smoothing. The calibration model was developed using PLS (partial least squares) method. Validation was done by K fold cross validation method. The results showed the MSC and SNV spectra were able to eliminate noises of RAW spectra, whereas in the dg1 spectra, noises were still visible. The best model was acquired by SNV spectra with R^2 (coefficient of determination) of calibration and validation of 0.882 and 0.870, root mean square error of calibration (RMSEC) and root mean square error of cross validation (RMSECV) values of 2.92 and 3.08, and the ratio of performance to deviation (RPD) of 2.76. The result indicated the spectra pre-treatments were able to improve the accuracy of calibration model on assessment of sapodilla fruit firmness.

1. Introduction

Sapodilla (Achras zapota L.) is one of the commodities that grows in the tropics. Climate and environmental conditions in Indonesia cause this commodity to be widely cultivated as a plantation commodity. One of parameters that is generally used as an indicator of the quality of sapodilla fruit is firmness. Fruit firmness is one of the main factors of fruit quality because it is related to maturity and shelf life [1]. Storing sapodilla fruit for a long period will result in softer fruit. Sapodilla fruit, which harvested before the ripening phase experiences an increase in respiration rate, hence sapodilla is classified into climacteric fruit. After harvesting, the fruit continues the life process by carrying out respiration and metabolic activity [2].

Conventional determination of fruit firmness is done by destructive method. This method causes the measured fruit to be damaged. So it's needed a measurement method without damaging the fruit. The most used non destructive technology is near infrared (NIR) spectroscopy. Determining the fruit firmness using NIR has some advantages, such as environmentally friendly, fast measurement, and without damaging the fruit. This method has been widely used to measure the firmness of fruit, including kiwi [3], apple [4], tomato [5], peach [6], mango [7] and melon [8]. The firmness of sweet cherries was detected in reflectance NIR with wavelengths of 800-1700 nm [9]. Kiwi fruit firmness can be predicted at wavelengths of 800 to 1100 nm [10].

Fruit quality measurements using NIR could produce noises in the original spectra. The obtained spectra require pre-treatment in order to reduce noises, because it affects the accuracy of the resulting model [11]. There are several spectra pre-treatment methods that are commonly practiced, for example, multiplicative scatter correction (MSC), standard normal variate (SNV) and Savitzky-Golay first derivative (dg1). Spectra pre-treatments minimize the effects of various factors that reduce the accuracy of the model, for instance, noise, light scattering, and baseline drift. Various pre-treatment methods of the spectra were used for analyzing coffee bean [12], grape [13], persimmon [14] and mango [15]. The

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purpose of this study was to obtain the best calibration model to assess sapodilla fruit firmness from several spectra pre-treatment methods, such as MSC, SNV and dg1.

2. Materials and methods

2.1. Samples collection

Sapodilla fruit samples were harvested from sapodilla plantation located in Situraja, Sumedang. Thereafter sapodillas were brought to the Horticulture Laboratory, Faculty of Agriculture, Padjadjaran University. Sapodilla fruits were numbered first, then stored for 0, 5 and 10 days at room temperature. The numbers of sapodilla samples used in this study were 265 samples.

2.2. Spectra data collections

Spectra data were collected from intact sapodilla fruits using NirVana AG410 visible and near infrared spectrometer with wavelengths of 312 nm - 1050 nm. Light source from the spectrometer illuminated sapodilla fruit samples, the light could be absorbed, reflected, transmitted, or even scattered by the sample. The reflected light from the fruit was captured by a sensor (detector) in the spectrometer. Afterwards, the reflected light was digitized and translated into numbers, the data were later stored within the spectrometer internal storage. Once spectra data collections were completed, the data were transferred to a computer using ISIS (Integrated Software for Imagers and Spectrometers).

2.3. Firmness measurement

Measurement of fruit firmness was carried out using the AD-4932A-50N force gauge. The value of fruit firmness was measured based on the level of fruit resistance to the probe. The greater the force required, the greater the firmness value of the fruit. After all samples were measured, firmness reference data along with spectra data (RAW) were transferred to Microsoft Excel 2016 and The Unscrambler 10.5 for further data processing.

2.4. Chemometrics

In the analysis of spectra data, chemometrics is useful for extracting information obtained from the measurement of spectra data. Chemometrics is a branch of chemistry that combines statistics and chemical analysis. There are several chemometric stages, for example, performing spectra pre-treatment, building calibration and validation model, then transferring model into NIR device [16]. Data acquired from the NIR measurement was RAW spectra. The spectra pre-treatment stage was performed using several pre-treatment methods including SNV, MSC and dg1. The next step was calibration and validation analysis.

The calibration model was developed using the PLS (partial least squares) method. Calibration aims to produce the estimated value of sapodilla fruit firmness based on spectra data. PLS is a multivariate calibration technique, which is used to interpret large amounts of data, has many X variables (predictor) and some Y variables (response) [17]. This method reduces the dimension of data without eliminating the characteristics of the data, PLS reduces predictor variables that are not relevant to data variation.

Validation was done by the K fold cross validation method, which was computed by dividing the entire samples into 20 segments with each segment containing as many as 13-14 samples. The 20 segments were splitted into training sets and test sets. A total of 19 segments were taken as train sets and 1 segment as a test set, cross validation was completed until the entire segments have been validated (test set). In addition to verifying the calibration model, cross validation was also run to avoid the overfitting.

Resulting from calibration and validation analysis, coefficient of determination (R^2), root mean square error of calibration (RMSEC) and root mean square error of cross validation (RMSECV) were obtained. Moreover, the ratio of performance to deviation (RPD) was also calculated. These values describe how well the calibration and validation model.

3. Results and discussion

3.1. Sapodilla fruit firmness during storage

Table 1 shows the average value of sapodilla fruit firmness at 0, 5 and 10 days storage. At 5 days storage, the mean value of firmness significantly decreased. Before harvesting, the fruit gets supply of nutrients

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from the plant to perform the ripening process. But after harvesting, the fruit doesn't get it anymore. The fruit is like other living things, which still carry out respiration activity. During respiration activity, fruit undergoes a process of breaking down the carbohydrates, which results in fruit becoming soft [18]. Storage at room temperature encourages fruit enzymes to run more actively than storage in cold temperatures. Pectinase and cellulase enzymes used to operate the protopectin decomposition to move more actively at room temperature [19]. Therefore, the longer storage period resulted in decreasing the firmness of sapodilla fruit. By doing 0, 5 and 10 days storage, it was expected that the firmness values of sapodilla fruits would be varied, so that bigger range of value would be obtained in the calibration model.

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Storage duration	Mean	Min	Max	Standard deviation				
0	22.52							
5	12.77	0.5	27.81	8.53				
10	12.42							

Table 1. Effects of storage durations on sapodilla fruit firmness

3.2. Spectra pre-treatments

Images of the RAW and pre-treated spectra are shown in Figure 1. The RAW spectra (Figure 1-a) evinces the presence of noises at wavelengths of 650 nm to 800 nm, which could be caused by the external interference while spectra data measurement. The lowest RAW spectrum value was 623, while the highest was 57,989. MSC spectra (Figure 1-b) removed noises at wavelengths of 650 nm to 800 nm. The lowest MSC spectrum value was -495, while the highest value was 58,232. The range of MSC spectra values was wider than the RAW spectra. The MSC spectra pre-treatment aims to reduce the amplification and offsets of the RAW spectra [20]. By performing pre-treatment of spectra using the MSC method before calibration analysis, the use of PLS factor was supposed to be reduced, so that a more stable and precise model could be acquired. Likewise, SNV spectra (Figure 1-c) pre-treatment successfully eliminated noises at wavelengths of 650 to 800 nm. But it was inversely proportional to the MSC spectra, the range of SNV spectra was narrower than the RAW spectra. The lowest SNV spectrum value was equal to -0.82, while the highest value was 2.35. Basically, the objectives of the SNV and MSC spectra pre-treatment methods were to reduce multiplicative interference in RAW spectra. SNV spectra pre-treatment individually processes each spectrum without relying on other spectrum, whereas the MSC spectra pre-treatment doesn't process every spectrum individually, but each spectrum needs other spectrum as reference. RAW spectra were transformed into dg1 spectra (Figure 1-d) without removing important information of the spectra. The smoothing was carried out by 4 points on left and right sides, respectively, with a total of 9 smoothing points. The lowest spectrum value of dg1 was -1.308, while the highest value was 4.241. Pre-treatment of spectra using the dg1 method is able to clarify the peaks and valleys of the spectra [16]. In addition, the dg1 method is also used to reduce overlapping spectra. Pre-treatments of spectra using the MSC and SNV methods were able to eliminate noises in RAW spectra, whereas the noises were still visible in spectra pre-treatment using dg1 method. After the spectra pre-treatments completed, the next stage was calibration and validation analysis.

3.3. Calibration and validation

Table 2 displays the results of the calibration and validation analysis before and after the spectra pretreatments. The results showed calibration and validation analysis using RAW, dg1, and MSC produced values that are similar to each other. PLS factor used in dg1 and MSC spectra were 6 and 7, respectively. Noises removal carried out by MSC spectra pre-treatment method was able to reduce the PLS factor by 1. dg1 method with 9 smoothing points was able to minimize 2 PLS factors. The estimation of soluble solids content and tannin of persimmon using MSC and PLS methods were able to reduce the PLS factor by 1 [14]. Determination of factor in PLS is very important. The factors that are too high cause a weakening of the ability of a calibration model to predict new (different) samples due to disturbances in the spectra. The PRESS (predictive residual error sum of square) value determines the optimum factor in PLS analysis. The optimum PLS factor for a model is obtained at a minimum PRESS value [21]. The highest value was resulted by SNV spectra with R² of calibration and cross validation were equal to 0.882 and 0.870, respectively. Besides, the RMSEC and RMSECV values of SNV spectra were found to be the lowest compared to the other three spectra, which were 2.92 and 3.08. A good model is characterized by a high R² value, which means the predictor variables are able to explain variations in

the response variables well. In addition, R² value of calibration and validation is expected to have values that are close to each other, as well as for RMSEC and RMSECV. Although the PLS factor in SNV spectra was as high as the RAW spectra, but SNV spectra showed highest model accuracy with the RPD value of 2.76. Calculation of RPD is yielded from the standard deviation of the response variable divided by the error value in cross validation. The RPD value above 2.5 indicates the model is categorized as good [22]. RAW, dg1, MSC and SNV spectra had RPD values above 2.5, so the four models above were categorized as good models.



Figure 1. Original and pre-treated spectra (a) RAW, (b) MSC, (c) SNV, and (d) dg1.

Factor	Calibration	Validation	RMSEC	RMSECV	RPD				
	(\mathbf{R}^2)	(R^{2})							
8	0.873	0.860	3.02	3.20	2.65				
6	0.873	0.862	3.03	3.16	2.69				
7	0.875	0.861	3.00	3.17	2.68				
8	0.882	0.870	2.92	3.08	2.76				
	Factor 8 6 7 8	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$				

Table 2. Effects of spectra pre-treatments on calibration and validation.

3.4. Regression coefficients

Figure 2 shows some wavelengths that significantly contributed to the value formation of response variables by SNV spectra. It is characterized by several wavelengths that have high and low values of regression coefficients. The peak means the wavelength contributes to the increase in value of response variables, whereas the valley means the wavelength contributes to the decline in value of response variables. The greater the peak or valley, the higher contribution of the wavelength to the increase or decrease in value of response variables. Peaks and valleys of SNV spectra presenced at 507 nm, 591

nm, 615 nm, 672 nm, 726 nm, 735 nm, 768 nm, 864 nm, 909 nm, and 975 nm. Wavelengths of 651 nm, 672 nm, 768 nm, 864 nm, and 909 nm are sensitive to the detection of firmness values [23]. The wavelength of 864 nm correlates with absorption of carbohydrates [24]. The wavelength of 975 nm relates to absorption of carbohydrates and water contents [25]. This indicated that carbohydrates and water contents played an important role in the value of sapodilla fruit firmness, as the breakdown of carbohydrates into more liquid compounds caused the fruit to become soft so that the value of fruit firmness was decreased.



Figure 2. Regression coefficients of SNV spectra.

4. Conclusion

This study showed spectra pre-treatments using the MSC and SNV method eliminated noises from RAW spectra at wavelengths of 650 nm - 800 nm. The use of MSC and dg1 spectra were able to diminish PLS factor values in the calibration and validation analysis. But the best model to assess sapodilla fruit firmness was shown by SNV spectra due to the highest calibration, validation, and RPD values, besides, the lowest RMSEC and RMSECV compared to the other three spectra.

References

- J. Xue, S. Zhang, H. Sun, and J. Zhou, "Study of Malus Asiatica Nakai's firmness during different shelf lives based on visible/near-infrared spectroscopy," *Math. Comput. Model.*, vol. 58, no. 11–12, pp. 1829–1836, 2013, doi: 10.1016/j.mcm.2012.12.021.
- [2] I. K. Arah, H. Amaglo, E. K. Kumah, and H. Ofori, "Preharvest and postharvest factors affecting the quality and shelf life of harvested tomatoes: A mini review," *Int. J. Agron.*, vol. 6, pp. 1–6, 2015, doi: 10.1155/2015/478041.
- [3] H. Li, D. Billing, P. Pidakala, and J. Burdon, "Textural changes in 'Hayward' kiwifruit during and after storage in controlled atmospheres," *Sci. Hortic. (Amsterdam).*, vol. 222, pp. 40–45, 2017, doi: 10.1016/j.scienta.2017.05.013.
- [4] B. Shi, L. Zhao, H. Wang, and D. Zhu, "Signal optimization approaches on the prediction of apples firmness by near infrared spectroscopy," *Sens. Lett.*, vol. 9, no. 3, pp. 1062–1068, 2011, doi: 10.1166/sl.2011.1381.
- [5] Kusumiyati, T. Akinaga, M. Tanaka, and S. Kawasaki, "On-tree and after-harvesting evaluation of firmness, color and lycopene content of tomato fruit using portable NIR spectroscopy," *J.*

Food, Agric. Environ., vol. 6, no. 2, pp. 132–137, 2008.

- [6] X. P. Fu, Y. Bin Ying, Y. Zhou, L. J. Xie, and H. R. Xu, "Application of NIR spectroscopy for firmness evaluation of peaches," *J. Zhejiang Univ. Sci. B*, vol. 9, no. 7, pp. 552–557, 2008, doi: 10.1631/jzus.B0720018.
- [7] C. Watanawan, T. Wasusri, V. Srilaong, C. Wongs-Aree, and S. Kanlayanarat, "Near infrared spectroscopic evaluation of fruit maturity and quality of export Thai mango (Mangifera indica L. var. Namdokmai)," *Int. Food Res. J.*, vol. 21, no. 3, pp. 1109–1114, 2014.
- [8] SuhSang-Ryong, LeeKyeong-Hwan, YuSeung-Hwa, ShinHwa-Sun, ChoiYoung-Soo, and YooSoo-Nam, "A melon fruit grading machine using a miniature VIS/NIR Spectrometer: 1. calibration models for the prediction of soluble solids content and firmness," *J. Biosyst. Eng.*, vol. 37, no. 3, pp. 166–176, 2012.
- [9] R. Lu, "Predicting firmness and sugar content of sweet cherries using near-infrared diffuse reflectance spectroscopy," *Trans. Am. Soc. Agric. Eng.*, vol. 44, no. 5, p. 1265-1271, 2001, doi: 10.13031/2013.6421.
- [10] V. A. McGlone and S. Kawano, "Firmness, dry-matter and soluble-solids assessment of postharvest kiwifruit by NIR spectroscopy," *Postharvest Biol. Technol.*, vol. 13, no. 2, p. 131– 141, 1998, doi: 10.1016/S0925-5214(98)00007-6.
- [11] Å. Rinnan, F. van den Berg, and S. B. Engelsen, "Review of the most common pre-processing techniques for near-infrared spectra," *Trends Anal. Chem.*, vol. 28, no. 10, pp. 1201–1222, Nov. 2009, doi: 10.1016/J.TRAC.2009.07.007.
- [12] S. Citra Yuliana Madi, I. W. Budiastra, Y. Aris Purwanto, and S. Widyotomo, "Analysis of the Effect of Variation of Bean Layers on Prediction Accuracy of Minor Compound in Green Arabica Coffee Beans of Bondowoso by NIR Spectroscopy," *J. Ilmu Pertan. Indones.*, vol. 23, no. 2, pp. 81–87, 2018, doi: 10.18343/jipi.23.2.81.
- [13] R. Ferrer-Gallego, J. M. Hernández-Hierro, J. C. Rivas-Gonzalo, and M. T. Escribano-Bailón, "Evaluation of sensory parameters of grapes using near infrared spectroscopy," *J. Food Eng.*, vol. 118, no. 3, pp. 333–339, 2013, doi: 10.1016/j.jfoodeng.2013.04.019.
- [14] I. Kurniasari, Y. Aris Purwanto, I. W. Budiastra, and S. Ridwani, "Prediction of Tannin and NonSoluble Solid Content of Persimmon (Diospyros kaki L.) Using NIR Spectroscopy," J. *Keteknikan Pertan.*, vol. 5, no. 3, pp. 245–252, 2017, doi: 10.19028/jtep.05.3.245-252.
- [15] Y. A. Purwanto, H. P. Sari, and I. W. Budiastra, "Effects of preprocessing techniques in developing a calibration model for soluble solid and acidity in 'Gedong Gincu' mango using NIR spectroscopy," *Int. J. Eng. Technol.*, vol. 7, no. 5, pp. 1921–1927, 2015.
- [16] Y. Cen, H. & He, "Theory and application of near infrared reflectance spectroscopy in determination of food quality," *Trends Food Sci. Technol.*, vol. 18, no. 2, pp. 72–83, 2007, doi: 10.1016/j.tifs.2006.09.003.
- [17] A. Kuno and M. Matsuo, "Nondestructive speciation of solid mixtures by multivariate calibration of X-ray absorption near-edge structure using artificial neural networks and partial leastsquares," *Anal. Sci.*, vol. 16, no. 6, pp. 597–602, 2000, doi: 10.2116/analsci.16.597.
- [18] M. I. Syafutri, F. Pratama, and D. Saputra, "Physical and chemical characteristics of mangos (Mangifera indica L.) during storage with various methods of packaging," J. Teknol. dan Ind. Pangan, vol. 17, no. 1, pp. 1–11, 2006.
- [19] N. K. Ilmi, R. Poerwanto, and Sutrisno, "Hot water treatment and storage temperature control to maintain the quality mango fruit (Mangifera indica L.) cv. Gedong," J. Hortik., vol. 25, no. 1, pp. 78–87, 2015.
- [20] S. Ramadhan, A. A. Munawar, and D. Nurba, "NIRS and principal component analysis (PCA) application for rapid clasification of arabica coffee beans (Coffea arabica)," J. Ilm. Mhs. Pertan. Unsyiah, vol. 1, no. 1, pp. 954–960, 2016.
- [21] R. Jankovská and K. Šustová, "Analysis of cow milk by near-infrared spectroscopy," Czech J. Food Sci., vol. 21, no. 4, pp. 123–128, 2003, doi: 10.17221/3488-cjfs.
- [22] B. M. Nicolaï *et al.*, "Nondestructive measurement of fruit and vegetable quality by means of NIR spectroscopy: A review," *Postharvest Biol. Technol.*, vol. 46, no. 2, pp. 99–118, 2007, doi: 10.1016/j.postharvbio.2007.06.024.
- [23] Z. Qing, B. Ji, and M. Zude, "Wavelength selection for predicting physicochemical properties of apple fruit based on near-infrared spectroscopy," *J. Food Qual.*, vol. 30, no. 4, pp. 511–526,

2007, doi: 10.1111/j.1745-4557.2007.00139.x.

- [24] D. Suhandy, "Soluble solids content prediction in sapodilla fruit using NIR spectroscopy," J. *Bionatura*, vol. 11, no. 1, pp. 1–12, 2009.
- [25] M. Zude, B. Herold, J. M. Roger, V. Bellon-Maurel, and S. Landahl, "Non-destructive tests on the prediction of apple fruit flesh firmness and soluble solids content on tree and in shelf life," J. Food Eng., vol. 77, no. 2, pp. 254–260, 2006, doi: 10.1016/j.jfoodeng.2005.06.027.