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Authentication of Six Indonesian Ground Roasted Specialty Coffees According to Variety and Geographical Origin using NIR Spectroscopy with Integrating Sphere

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Abstract. Several factors such as type of bean (Arabica or Robusta), geographical origin (elevation, soil type, temperature, and solar radiation), and agronomic/postharvest practices (fertilization, bean processing, fermentation, and type of roasting) have a great influence on the quality of final taste of the coffee. In this research, an authentication of six Indonesian ground roasted specialty coffees according to different in variety and geographical origin using NIR spectroscopy with integrating sphere was evaluated. A total of 70 coffee samples of Arabica and Robusta coffee from different geographical origins were used as samples. NIR spectral data in the range of 1175.79 nm to 1651.222 nm were obtained using a portable NIR spectrometer equipped with an integrating sphere. The unsupervised classification was performed using PCA and supervised classification was conducted using the SIMCA method. The result of PCA shows that the samples were well clustered according to variety and geographical origin along the PC1 and PC2 axis both using original and preprocessed spectra. The SIMCA performed good results both for original and preprocessed spectral data, most of the testing sample set were properly classified to their corresponding classes.

Keywords: authentication, nir spectroscopy, pca, simca, specialty coffee

1. Introduction

In 2018, Indonesia can produce about 577 thousand tons of green bean coffee or about 5.5% of total production [1]. In Indonesia, two coffee species are commonly planted: *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta). Coffee beans harvested in Indonesia coming from a wide range of geographical areas from Aceh in the west region to Papua in the east area resulted in different chemical and organoleptic properties [2]. To protect the origin of each coffee origin, the Indonesian government issued an official label of geographical indications (GIs) as recognition of some specific food quality attributes, which have a specific geographical origin and characteristics or a reputation that are due to factors that are indigenous to that origin, such as nature and people [3]. The growing market of specialty coffee with GIs label and its high price has attracted farmers to provide a single-origin coffee. However, due to economic motivation to get as high as profit, it happens that intentionally mixing coffee from two

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or more different origins was the wrong label as a single one. For this reason, it is important to develop an analytical method to evaluate the authenticity of coffee from different geographical origins.

Several criteria have been proposed for differentiating coffee from different geographical origins, including physical dan chemical properties. In terms of chemical properties, several properties can be used to assess the quality of coffee from a different variety and geographical origin: the content of sucrose, lipids, amino acids, and trigonelline contents, chlorogenic acids, and caffeine content [3]. Different analytical methods have been used to perform coffee analysis to differentiate coffee from a different variety and geographical origin, including UV–Vis spectroscopy [4-7], chromatographic analysis [8-9], nuclear magnetic resonance (NMR) [10], and fluorescence spectroscopy [11]. Those methods are accurate in measurement but having several drawbacks such as time-consuming and generating chemical waste for sample preparation and expensive in a device.

NIR spectroscopy has been proposed for coffee quality evaluation with several advantages: minimum sample preparation, nondestructive analysis and allows to perform simultaneous analysis with the fast-spectral acquisition. Using benchtop NIR spectrometer, several types of research have been reported well for coffee geographical origins determination [12-13]. However, benchtop NIR spectrometer is an expensive device and it is a little bit difficult to be developed in developing countries, no exception Indonesia. For this reason, in this research, a low-cost analytical method for coffee differentiation of Arabica and Robusta coffee from several geographical origins in Indonesia was proposed using a handheld NIR spectrometer. Unsupervised and supervised classification was developed using principal component analysis (PCA) and soft independent modelling of class analogy (SIMCA).

2. Materials and methods

2.1 Coffee samples from five different geographical origins

A total of 70 coffee samples of Arabica and Robusta coffee from five different geographical origins were used as samples. The samples were including two Robusta coffee from Lampung (Codot and Lampung coffee) and four Arabica coffee from Gayo, Mandailing, Kintamani, and Wamena. All samples were collected from a trusted local coffee trader in Indonesia. Detailed information of samples was shown in Table 1. All samples were subjected to medium roasting at a temperature of 200°C for 10 minutes then ground and sieved using 50 mesh (297 micrometers of coffee particle size) [14].

Table 1. Detailed information of coffee samples used in this study.

Sample Name	Variety	Number of samples		Origin	Geographical Indication Certificate
		Training set	Testing set		
Wamena	Arabica	9	6	Wamena, Papua	ID G 000 000 0083
Gayo	Arabica	9	6	Gayo, Aceh	ID G 000 000 005
Kintamani	Arabica	6	4	Kintamani, Bali	ID G 000 000 001
Codot	Robusta	6	4	Lampung	ID G 000 000 026
Lampung	Robusta	6	4	Lampung	ID G 000 000 026
Mandailing	Arabica	6	4	Mandailing, North Sumatera	ID G 000 000 048

2.2 NIR spectral data acquisition

NIR spectral acquisition of each sample was performed in interactance mode by directly placing the sample holder about 1.33 grams in weight of ground roasted coffee samples on a flat surface. A NIR handheld spectrometer from Ocean Optics (USA), NIRQuest512 operated in the range of 900–1650 nm, was used for spectral acquisition. This spectrometer was equipped with a fiber optic and an integrating sphere with a built-in tungsten-halogen light source was located at the bottom of the integrating sphere.

2.3 PCA and SIMCA

Multivariate analysis of PCA and SIMCA was applied for both original and preprocessed spectral data. Preprocessed spectral data were obtained by applying three algorithms simultaneously: moving average smoothing with 11 segments (MAS 11), standard normal variate (SNV), and Savitzky-Golay first derivative with 7 segments and second polynomial order (SG 1d). In PCA, the result of PC scores of PC1 and PC2 was plotted. In SIMCA, each class's classification model was developed on a training sample set using NIPALS (nonlinear iterative partial least squares) algorithm with full cross-validation. The result of testing was visualized using a confusion matrix based on Cheah and Fang [15]. The calculation of PCA and SIMCA was done using the multivariate software of the Unscrambler 9.7 (CAMO Software AS, Oslo, Norway).

3. Results and discussion

3.1 NIR spectral data of coffee samples with different variety and geographical origin

Averaged original NIR spectral data of Arabica and Robusta coffee samples from five different geographical origins is shown in Figure 1. In general, Arabica samples (Gayo, Mandailing, Kintamani, and Wamena) had higher absorbance intensity than Robusta samples (Codot and Lampung). A critical peak was observed in a wavelength of 1450 nm related to the O-H bonding of water molecules (first overtone of O-H stretching) in coffee [16]. Figure 2 shows the averaged preprocessed spectra showing several peaks and shoulders. The selected peaks were closely related to the C-H aliphatic second overtone (1195-1225 nm) and the O-H first overtone of aliphatic (1410 nm) and aromatic alcohol (1420 nm) [17].

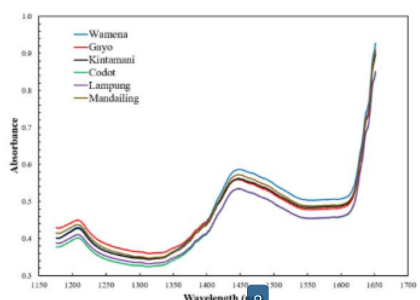

Figure 1. The averaged original spectra of 70 samples of Indonesian specialty coffee from different in variety and geographical origins in the range of 1175.79 -1651.222 nm.

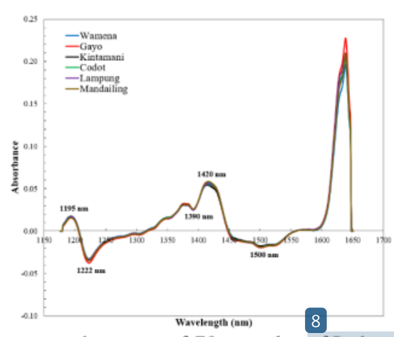

Figure 2. The averaged preprocessed spectra of 70 samples of Indonesian specialty coffee from different in variety and geographical origins in the range of 1175.79 -1651.222 nm.

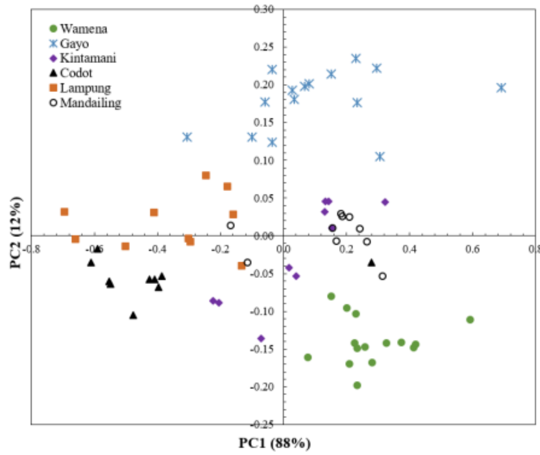

Figure 3. The plot of PCA (PC1xPC2) for original spectral data in the spectral window of 1175.79 nm to 1651.222 nm.

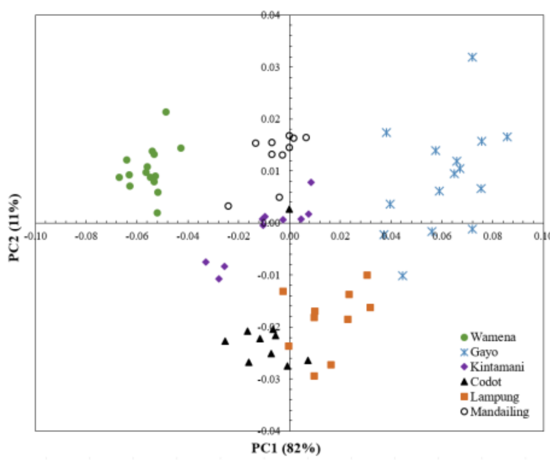

Figure 4. The plot of PCA (PC1xPC2) for preprocessed spectral data in the spectral window of 1175.79 nm to 1651.222 nm.

3.2 Result PCA analysis for original and preprocessed spectra

Figures 3 and 4 show the result of the PCA analysis of all samples (70 samples) using original and preprocessed spectral data in the range of 1175.79 nm - 1651.222 nm. Using two PCs (PC1 and PC2), a cumulative percentage of variance (CPV) of 100% and 93% was obtained for original and preprocessed spectral data, respectively. In general, separation of coffee samples according to variety and geographical origins was achieved. However, a clearer clusterization was obtained using preprocessed spectral data. Lampung clusters are laid very close to Codot one. Lampung and Codot coffee samples are the same in variety (Robusta) and from the same geographical origin (Lampung).

3.3 SIMCA results

Using a training set, the SIMCA model was developed for each class. A testing sample set was used to evaluate the performance of the SIMCA model in classification coffee samples. Figure 5 shows the result of testing sample set classification in the form of a confusion matrix for original (left) and preprocessed spectra (right). Using original spectra, of 4 Kintamani samples (true class 3), 1 sample was misclassified as Lampung coffee. Of 4 Codot samples (true class 4), none samples correctly classified as Codot, and 3 samples were misclassified as Lampung coffee. For true class 5 and 6 (Lampung and Mandailing coffee), 1 sample was misclassified as Kintamani coffee. A better confusion matrix was obtained using preprocessed spectral data. Only 1 sample of Codot coffee was misclassified as Lampung coffee. The reason for this misclassification may be coming from the similar characteristic of Codot and Lampung coffee. The two coffee of Codot and Lampung coffee coming from the same variety (Robusta) and same geographical origin (Lampung).

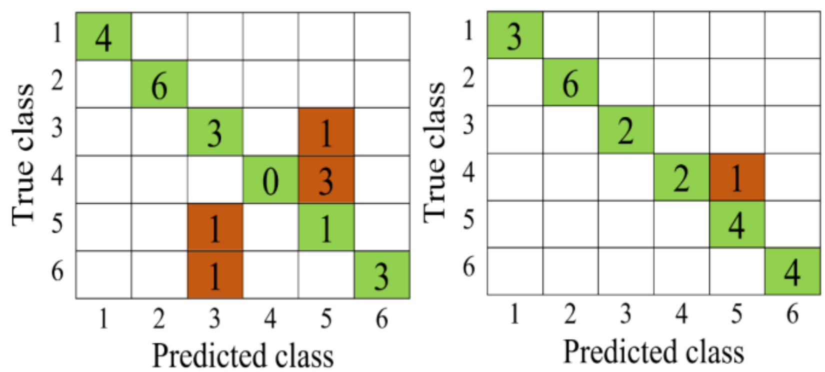

Figure 5. Confusion matrix for testing result for original (left) and preprocessed spectra (right) (class 1= Wamena coffee; class 2= Gayo coffee; class 3= Kintamani coffee; class 4= Codot coffee; class 5= Lampung coffee; class 6= Mandailing coffee).

4. Conclusion

This paper demonstrated a classification of Arabica and Robusta coffee from five different geographical origins in Indonesia using a low-cost NIR spectrometer. A clear separation was obtained using original and preprocessed spectra in the wavelength range of 1175.79 nm to 1651.222 nm. Using SIMCA, a classification of testing sample set was performed using original and preprocessed spectra. The preprocessed model was better than that of the original one in the low number of misclassified samples. It can be concluded that the developed low-cost NIR spectrometer equipped with an integrating sphere was highly applicable for the differentiation of Indonesian specialty coffee according to different in variety and geographical origins.

5. Acknowledgements

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