Unsupervised classification of three specialty coffees from Java based on principal component analysis and UV-visible spectroscopy

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Unsupervised classification of three specialty coffees from Java based on principal component analysis and UV-visible spectroscopy

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Abstract. In this research, we investigated the feasibility of using UV-visible spectroscopy and chemometrics to classify three specialty coffees from Java Island: Java Preanger, Java Sindoro-Sumbing dan Java Ijen Raung. Total of 300 samples of Preanger, Sindoro-Sumbing and Ijen Raung ground roasted coffees were used as samples. Samples were extracted using hot distilled water and diluted. The spectral data was acquired using a UV-visible spectrometer in the range of 190-1100 nm. Unsupervised classification based on principal component analysis (PCA) was applied for original and modified spectral data. Using the original full spectrum of 190-1100 nm spectral data, the plot score of the first and second principal components (PC1xPC2) totally can explain 90% of data variance. It was difficult to separate the origin of Preanger, Sindoro-Sumbing and Ijen Raung using original full spectrum data. However, using modified spectral data in the range of 250-450 nm, the clear separation between Preanger, Sindoro-Sumbing and Ijen Raung was demonstrated. In conclusion, it was highly potential to use UV-visible spectroscopy and chemometrics to classify the specialty coffees from Java based on its origin.

1. Introduction

Recently, food authentication has become a great concern to food producers, customers and government in order to ensure food quality and food safety [1]. The term of food authentication is also associated with the process to avoid origin and quality fraud of food [2]. The quality of food is not only related to specific chemical composition but also related to specific origin. The information on food composition and food origin must be declared in the label of food [2]. In Indonesia, several coffees were traded based on its origins such as Gayo coffee from Aceh, Kalosi coffee from South Sulawesi, Java Preanger from Java and Kintamani coffee from Bali. Geographical Indications (GIs) is one of the label adopted by the Indonesian government 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.

In Java Island, there are three specialty coffees, which have been granted GIs. Java Preanger coffee (No. ID G 000000022) is origin from Priangan highland in west Java (at least 1000 meters above sea level). Java Sindoro-Sumbing coffee (ID G 000000030) is origin from the mountain of Sindoro-Sumbing in district Temanggung and Wonosobo in central Java and Java Ijen Raung coffee (ID G

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000000023) is origin from mountain Ijen-Raung (900-1500 meter above sea level) in east Java. Currently, there are several analytical method authentication based on spectral data analysis have been developed. For coffee authentication, near infrared spectroscopy (NIR), Fourier transform infrared (FT-IR) and Raman spectroscopy has been utilized as a useful analytical method for detection of coffee origin and quality with high-speed analysis, nondestructive and without laborious sample preparation [3–5]. Those methods are accurate and suitable for on-line measurement. However, the equipment of those three methods are still expensive. Several attempts have been done to develop a simpler and cheaper coffee authentication based on UV-visible spectroscopy [6–14]. To the best of our knowledge, there is no research related to Java specialty coffee authentication using UV-visible spectroscopy. The purpose of the current research is to evaluate the use of UV-visible spectroscopy along with principal component analysis to classify three specialty coffees from Java Island, Indonesia.

2. Materials and Methods

2.1. Specialty coffee samples

In total, 300 samples of ground roasted coffee specialty samples were used. The samples consist of three types of specialty coffee from Java island, Indonesia, which has been protected geographically (GIs): Java Sindoro-Sumbing (100 samples), Java Preanger (100 samples) and Java Ijen Raung (100 samples). The weight of each sample is 1.0 grams. To perform a uniform spectral acquisition, all samples were subjected to sieving using mesh 50 (particle size of 297 micrometers). The spectral acquisition was done using an aqueous coffee sample. For this purpose, an extraction of coffee samples was performedby using hot distilled water [6-14].

2.2. Spectral data measurement

The 2 mL of coffee aqueous samples were pipetted into a 10 mm of quartz sample cell holder. A commercial UV-vis spectrometer from Thermo Scientific (Genesys™ 10S UV-Vis, Thermo Scientific, USA) was used to acquire spectral data of aqueous coffee samples. The measurement was performed in the range of 190-1100 nm with 1 nm of spectral resolution and room temperature about 27-28°C. The original and modified spectra were used for chemometric analysis.

2.3. Chemometric analysis

Principal component analysis or PCA (unsupervised chemometric analysis) method was used to classify Java specialty coffee samples according to its origin (Java Preanger, Java Sindoro-Sumbing, and Java Ijen Raung). PCA was performed using all samples (300 samples) using original spectral data in the range of 190-1100 nm and modified spectral data in the range of 250-450 nm. In order to improve the quality of spectral data, original spectral data were preprocessed into modified spectral data using two algorithms: standard normal variate (SNV) and moving average smoothing with 11 segments. PCA is a popular unsupervised method and widely used to reduce the dimension of multivariate data sets. The principle and application of PCA can be found in several previous reported works [15-16]. Mathematically, PCA represents the eigenvectors for the covariance or correlation matrix of a data matrix. The eigenvector associated with the greatest eigenvalue is known as the first principal component (PC1). The second principal component (PC2) is the eigenvector that is associated with the next greatest eigenvalue and so on [16]. The acceptance of the PCA result was evaluated using a value of cumulative percentage of variance (CPV) of the calculated PC. The CPV of more than 70%-85% is desirable to accept the PCA result [17]. The calculation of PCA was done using the multivariate software of the Unscrambler 9.7 (CAMO Software AS, Oslo, Norway).

3. Results and Discussion

3.1. Spectral analysis of coffee samples with different origin

Figure 1 showed the original spectra of 300 samples of Java specialty coffee from Sindoro-Sumbing, Preanger and Ijen Raung in the range of 190-1100 nm (UV, visible region and near infrared region). In general, it can be seen that it was not easy to discriminate the origin of coffee based on direct

investigation of original spectra. The effective wavelength range region is located at 250-450 nm. In this selected range, several peaks were identified at a wavelength of 250 nm, 285 nm, 305 nm, and 322 nm. These wavelengths have been previously reported to be present in the spectra data of ground roasted arabica and robusta coffee samples. For example, the wavelength at 250 nm is close to the wavelength of 275 nm which is related to the C=O chromophore absorption of caffeine [18]. The wavelengths at 285 nm and 322 nm are closely related to the absorbance of chlorogenic acids and trigonelline, respectively [18]. To improve the quality of spectral data, two preprocessings (SNV and moving average smoothing) were applied and the result was depicted in Figure 2.

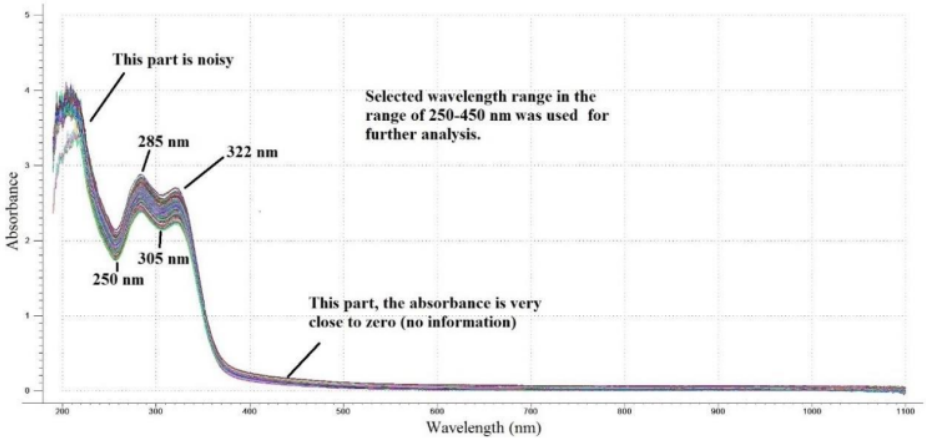

Figure 1. The original spectra of 300 samples of Java specialty coffee from Sindoro-Sumbing, Preanger and Ijen Raung in the range of 190-1100 nm.

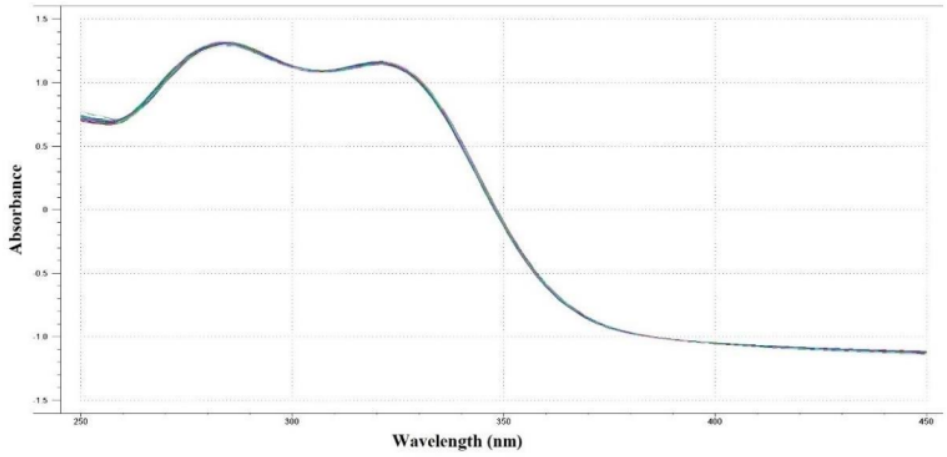

Figure 2. The modified spectra of 300 samples of Java specialty coffee from Sindoro-Sumbing, Preanger and Ijen Raung in the range of 250-450 nm.

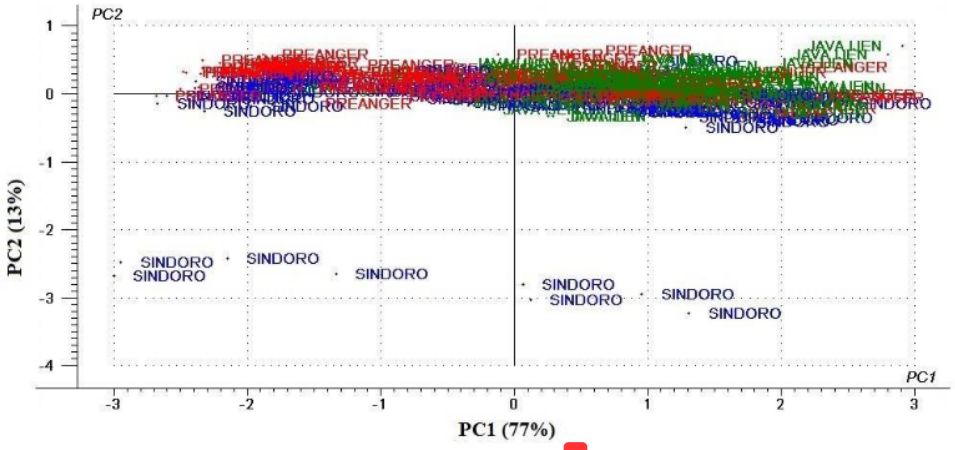

Figure 3. The result of the PCA analysis of all samples using original spectra in the range of 190-1100 nm.

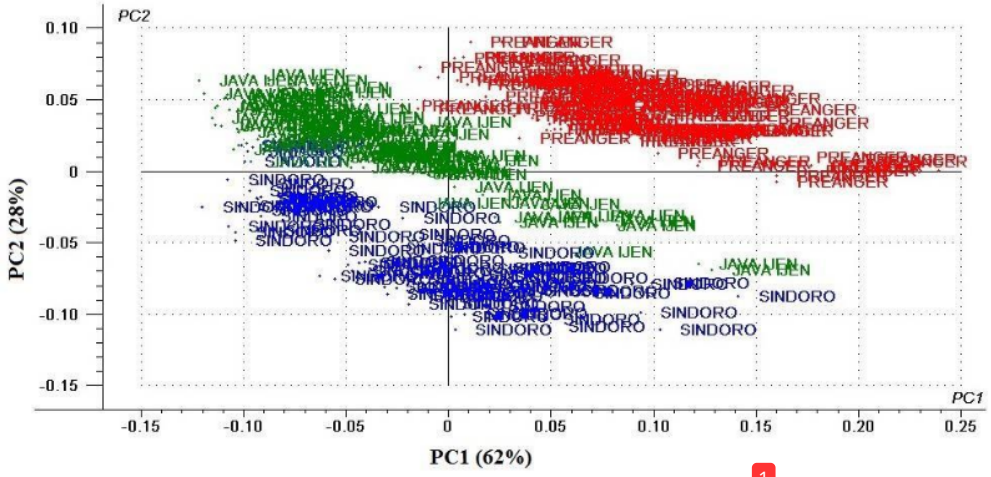

Figure 4. The result of PCA analysis of all samples using modified spectra in the range of 250-450 nm.

3.2. Unsupervised method using PCA analysis for original spectra

The result of the PCA analysis of all samples (300 samples) using original spectra in the range of 190-1100 nm was depicted in Figure 3. Using two PCs (PC1 and PC2), a cumulative percentage of variance (CPV) of 90% was obtained. However, it was difficult to see a clear separation of coffee samples based on their origin.

3.3. Unsupervised method using PCA analysis for modified spectra

To improve the PCA result, PCA was also applied to all samples (300 samples) using modified spectra in the range of 250-450 nm. The result was demonstrated in Figure 4. The cumulative percentages of variance (CPV) of 90% was obtained. A clear separation was achieved. The coffee samples were well

separated according to their origin. This result showed the importance of proper wavelength region selection and effective spectral preprocessing before applying PCA analysis.

4. Conclusion

This present research demonstrated the potential application of UV-visible spectroscopy and PCA to classify Java specialty coffees. A clear separation was obtained using modified spectra in the wavelength range of 250-450 nm. It is confirmed that the proper selection of wavelength region and preprocessing spectral data is quite important to improve the result of PCA. It is concluded that an authentication system of Indonesian specialty coffees based on UV-visible spectroscopy can be realized in the near future.

Acknowledgment

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