Identification of Gayo arabic coffee beans and powder using the FTIR-PCA combination method

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Abstract. The identification of Gayo Arabica coffee beans and coffee powder has been done to classify coffee plantation from several different regions using FTIR Spectroscopy and Principal Component Analysis (PCA). Samples were taken by purposive sampling from the Arabica coffee plantations in Pegasing, Jagong, and Celala areas, Aceh Tengah Regency, and also in Bandar, Permata, and Wih Pesam areas, Bener Meriah Regency. FTIR analyzed both the dry Gayo Arabica coffee beans and powder in the wavelength range of 4000 cm⁻¹-400 cm⁻¹. The spectra resulted were analyzed using PCA. FTIR spectra show the absorption of typical functional groups of caffeine, namely O-H (3400 cm⁻¹), C-H aromatic (2900 cm⁻¹), C-H aliphatic (2800 cm⁻¹), C=O (1743 cm⁻¹), C=C (1640 cm⁻¹), C=C aromatic (1550 cm⁻¹), C-H alkanes (1450 cm⁻¹) and C-N (1240 cm⁻¹). There was a loss of absorption of C=O and C-N groups in coffee powder samples from the Pegasing, Jagong, and Permata areas caused by high-temperature heating during the coffee powder making process. The PCA showed that coffee bean samples could be distinguished properly based on the coffee origin location, namely Aceh Tengah and Bener Meriah Regencies. Meanwhile, coffee powder samples showed poor separation of PCA plot patterns between coffee powder from the two regions. It can be concluded that the PCA method can be used for the classification of both Gayo Arabica coffee beans and powder, where the classification of beans is better than powder.

1. Introduction
Coffee is an agricultural product with high economic value and is quite popular with many people worldwide. Many types of coffee can be found on the market, one of which is Gayo Arabica coffee. There are two central areas of Gayo Arabica coffee plantations in Aceh Province, namely Aceh Tengah and Bener Meriah Regencies. Gayo Arabica coffee types are suitable to grow in areas with an altitude range of 900-1700 MASL [1].

In general, coffee contains various types of volatile compounds such as aldehydes, furfural, ketones, alcohols, esters, formic acid, and acetic acid. The caffeine compound (C₈H₁₀N₄O₂) is an alkaloid compound that is very important in coffee. Although similar in type of content, each coffee's detailed
chemical composition varies depending on the geographic factors, processing, and storage. This factor is also assumed to affect the taste of the coffee.

The identification of chemical composition in the organic sample can be made by several instrumental methods such as UV-Vis [2–4], Chromatography-Mass Spectrometry [5–8], FTIR [9,10], laser[11,12], and even image processing[13]. In identifying the chemical composition of coffee, the FTIR (Fourier Transform Infrared) spectroscopy method is the most commonly chosen, considered by the simple used and low cost. This method can identify the functional groups in coffee, enabling the chemical composition to be predicted [14].

However, FTIR spectra are so complex, complicating the differentiation between one coffee spectra and another. This makes it difficult for the coffee business to identify the possibility of knock-offs coffee. Therefore we need a statistical method that can identify complex data [15–18]. One of the popular statistical methods used to identify complex data is Principle Component Analysis (PCA)[19]. The combination of FTIR and PCA has been widely used in various fields, for example, to identify between Wheat Kernel and White Flour [20], falsification of Edible bird’s nests (EBNs) as a medicinal ingredient[21], differences in animal hair as raw material for making brushes[22] distinguishing of cattle bones [23] and also in the forensic analysis [24], as well as differentiating between Arabica and Robusta coffee [25].

In this study, FTIR analysis was carried out from coffee bean and powder samples taken from several BenerMeriah locations and Central Aceh. The resulting FTIR spectra were then analyzed by PCA to classify the coffee samples based on location and treatment.

2. Research methodology

Samples of Gayo Arabica coffee beans and powder were taken from the plantation areas of Aceh Tengah (Pegasing, Jagong, and Celala areas) and Bener Meriah (Bandar, Permata, and Wih Pesam Areas). Sampling was done by purposive sampling. The pretreatment of the obtained coffee beans was done by exfoliating, washing, and drying. Coffee powder samples were pretreated by roasting the dry coffee beans until they were evenly black and grounded until they became coffee powder.

2.1. Tools and materials

The equipment used was the maceration toolset, rotary evaporator, FTIR Spectroscopy (Shimadzu 50-IR Thermo Fischer), and statistical applications for FTIR data processing; The Unscrambler X 10.4.

2.2. FTIR Spectroscopic analysis

FTIR analysis was carried out at a wavelength of 400 – 4000 cm\(^{-1}\). Measurements were made in two repetitions to obtain a good spectrum. The spectrum data obtained were prepared for the chemometric purpose.

2.3. Preprocessing data and chemometric analysis

FTIR spectra were analyzed by The Unscrambler X 10.4 application to obtain the statistical information. Firstly, data preprocessing was needed to eliminate variations in data that were not related to analytical information [27]. The data preprocessing in this research was carried out by using The Unscrambler X 10.4 as the same as has been done by Van Horn et. Al. [28].

2.4. Principal component analysis (PCA)

FTIR spectra that have preprocessed were analyzed by The Unscrambler X 10.4 application to obtain the PCA plot. The plot was interpreted based on the grouping formed.
3. Results and discussion

3.1. FTIR spectrum

FTIR spectra of all samples can be seen in Figure 1 and Figure 2. In general, all the samples have similarities in functional groups that contained O-H (3400 cm\(^{-1}\)), C-H aromatic (2900 cm\(^{-1}\)), C-H aliphatic (2800 cm\(^{-1}\)), C=O (1743 cm\(^{-1}\)), C=C (1640 cm\(^{-1}\)), C=C aromatic (1550 cm\(^{-1}\)), C-H alkanes (1450 cm\(^{-1}\)) and C-N (1240 cm\(^{-1}\)). The differences are only in the intensity and a little bit on the spectral patterns. This functional group's presence indicated the existence of a well-known compound found in coffee, namely caffeine compounds, with one characteristic of it being present in a C-N functional group. The other functional group detected was C-O at 1010 cm\(^{-1}\) that indicated the presence of alcohol, ether, ester, and carboxylic acid [29].

![Figure 1. FTIR spectra of coffee powder from: (A) Aceh Tengah, and (B) Bener Meriah.](image)
Figure 2. FTIR Spectra of coffee beans from: (A) Aceh Tengah, (B) Bener Meriah.

There was a loss of absorption of C=O and C-N groups in coffee powder samples from the Pegasing, Jagong, and Permata. This may due to the heating process in the sample during the coffee sample treatment process[30], resulting in the breakdown of the C-N and C-O spectra. Despite that, the C-N and C-O functional groups may still be presented in the coffee powder samples, but the concentration has decreased, and the absorbance peak looks like invisible.

3.2. Pretreatment/preprocessing of the FTIR spectrum data
FTIR spectrum data requires a pretreatment to reduce noise caused by external influences, multiplication effects (scattering), particle size, and multi-collinearity changes that can cause large variations in the
spectrum. Thus, it is impertinent to apply the pretreatment method to avoid noise effects [31]. According to Savitzky and Golay [27], the FTIR spectrum is corrected by several data pretreatment methods, namely Smoothing, Baseline Correction, Derivative, and Standard Normal Variant (SNV).

3.3. Principal component analysis (PCA)

The principal component analysis aims to classify samples. In this study, the classification was based on the geographical origin of the coffee. Figure 3 showed that coffee beans and powder samples could be distinguished based on the coffee's location of origin, namely Aceh Tengah and Bener Meriah. However, the coffee powder samples overlap in two regions (blue and yellow circles), so the classification results were not as good as the coffee bean samples (red and black circles). Figure 3 shows that identifying the origin of coffee is better to use coffee beans as samples. The use of coffee bean samples as analysis material certainly has many advantages, like not having to do pretreatment to many samples, thus saving time and money.

![Figure 3. Classification of PCA plots by regencies.](image)

4. Conclusions

Identification of both Gayo Arabica coffee beans and powder by FTIR showed the presence of an identical functional group of caffeine and several other compounds of alcohol, ether, ester, and carboxylic acid. There was a loss of absorption of C=O and C-N groups in coffee powder samples from the Pegasing, Jagong, and Permata areas caused by high-temperature heating during the coffee powder making process. The PCA showed that coffee bean samples could be distinguished adequately based on the coffee origin location, namely Aceh Tengah and Bener Meriah Regencies. Meanwhile, coffee powder samples showed poor separation of PCA plot patterns between coffee powder from the two regions. It can be concluded that the PCA method can be used for the classification of both Gayo Arabica coffee beans and powder, where the classification of beans is better than powder.

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