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The development of classification model of peaberry and civet ground roasted coffee using UV-visible spectroscopy and two different compensation methods

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Abstract. In this research, an investigation on the influence of particle size variation in the authentication of peaberry and civet ground roasted coffee using UV-visible spectroscopy and two different compensation methods was conducted. A total of 398 samples of peaberry and civet coffee with two particle sizes of 1680 μm dan 297 μm (mesh 12 and mesh 50) were prepared. The all coffee samples were extracted using hot distilled water. The extracted aqueous coffee samples were pipetted into 10 mm of cuvette and the spectral data was acquired using a UV-Vis spectrometer in the range of 190-1100 nm. The result of PCA showed that the samples can be clustered based on types of coffee (peaberry and civet) and based on particle size (mesh 12 and mesh 50) using pre-processed spectral data in the range of 250-450 nm. Using the global calibration model of PLS1 and PLS2, the prediction results for prediction sample set at particle size of 1680 μm dan 297 μm (mesh 12 and mesh 50) were excellent with low RMSEP, low SEP and low bias. This result demonstrated the ability of global calibration model (both based on PLS1 and PLS2) to compensate the influence of particle size variation on the authentication of peaberry and civet ground roasted coffee.

1. Introduction

The application of UV-visible spectroscopy along with several different chemometrics for authentication of several ground roasted coffee has been reported [1-9]. The authentication involved the process of grinding and sieving ground roasted coffee into samples having homogeneous particle size (mesh 40) and then it was followed by an extraction process with hot distilled water. This sample preparation is time consuming and a laborious task. It was demonstrated in previous work that the performance of calibration model for authentication of coffee using UV-visible spectroscopy was highly influenced by the variation in particle size of the coffee sample [10].

Several methods have been investigated for developing calibration models that can compensate for sample physical properties variations such as temperature variations and particle size variations. One of the most common approach is to include physical properties variation in the calibration model both

explicitly and implicitly. In implicit approach, a global calibration model is developed using PLS1 regression in combination with calibration samples from a broad range of physical properties variation [11-12]. By doing so, it is possible to include all possible wavelengths for optimal determination of the target. However, this method requires a large data set [13].

Another way to compensate the influence of physical properties variations is using partial least squares 2 (PLS2) regression method. In this method, we add directly the particle size information as predicted variable results in an X block containing only the UV-visible spectra and a Y block containing the information of particle size and the information of types of coffee. This method was called as an explicit method [14-15]. The explicit inclusion of the particle size information into the calibration model is expected to improve the accuracy of peaberry and civet authentication.

In term of ground roasted coffee, several previous reports have been published for particle size compensation. For example, Suhandy and co-worker used NIR spectroscopy with implicit and explicit method to compensate the influence of particle size variations and established a more robust calibration model for coffee authentication [16]. However, there is a few report on the use of global calibration model (both implicit and explicit) to compensate the influence of particle size variations in coffee authentication using UV-visible spectroscopy. Therefore, in this study, we evaluate the performance of global PLS-DA (partial least squares discriminant analysis) model using PLS1 (implicit) and PLS2 (explicit) for compensation of particle size variations in the authentication of peaberry and civet ground roasted coffee using UV-visible spectroscopy. It is expected to develop a more robust PLS-DA model with minimal sample preparation (without sieving the samples).

2. Material and Methods

2.1. Samples
A total of 398 samples of peaberry and civet ground roasted coffee were prepared. To evaluate the influence of particle sizes in coffee powder to spectral analysis, two particle sizes of 1680 μm dan 297 μm were used by sieving through a nest of U. S. standard sieves (mesh number of 12 and 50) on a Meinzer II sieve shaker (CSC Scientific Company, Inc. USA) for 10 minutes. The experiments were performed at room temperature (around 27-29°C).

2.2. Sample preparation and spectral measurement
The all coffee samples were extracted using hot distilled water using extraction procedure of the coffee samples as described by Suhandy and co-workers [1-9]. Before the spectral measurements step, the reference spectra was measured by putting 3 mL of distilled water. It was followed by sample measurement by putting 3 mL of coffee aqueous samples. UV-Visible spectra of the aqueous extracts were measured using a UV-Vis spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, USA) in the range of 190-1100 nm with spectral resolution of 1 nm at a room temperature.

2.3. Compensation using PLS1-DA and PLS2-DA method
For each particle size of 1680 μm dan 297 μm (mesh 12 and mesh 50), the samples were randomly divided into two groups, calibration and cross-validation sample set and prediction sample set. A calibration and cross-validation sample set was used for developing the calibration model and performing the full cross-validation test. The calibration will be developed for two types: local model and global model. Local calibration model was developed using samples having same particle size (mesh 12 or mesh 50). Global calibration model was developed using samples having different particle size (combination of mesh 12 and mesh 50). Local model was developed using PLS1 regression with an X block containing only the spectra and a Y block containing the types of coffee (peaberry and civet). This PLS algorithm works with a dummy response variables: Y=1 is belong to peaberry class and Y=0 is belong to civet class. Global calibration was developed using explicit and implicit method. First, global calibration models will implicitly compensate the influence of particle size variation by developing calibration model using PLS1 regression and samples having combination of mesh 12 and mesh 50

(global model PLS1-DA). Second, we add the particle size (mesh 12 and mesh 50) as predicted variable results in an X block containing only the spectra and a Y block containing the types of coffee (peaberry and civet) and particle size (mesh 12 and mesh 50) (global model PLS2-DA). The simultaneous prediction of the Y variable (types of coffee and particle size) is seen as a way to enable the model to identify the spectral regions which are particle size dependent. The performance of local and global calibration model will be evaluated based on the following parameters: RMSEP (root mean squared error of prediction), SEP (standard error of prediction) and bias.

3. Results and Discussions

3.1. Spectra of peaberry and civet ground roasted coffee samples with two different particle sizes
Figure 1 showed pre-processed spectra of peaberry and civet coffee samples in the range of 250-450 nm with two different particle size of 1680 μm dan 297 μm (mesh 12 and mesh 50). Three pre-processing spectra were used namely Savitzky-Golay smoothing with 9 segments, mean normalization and standard normal variate (SNV). The all spectra are similar in shape and intensity and in line with previous reported studies [1-9]. Based on this figure, it is difficult to find the spectral difference due to particle size variation. The high intensity of absorbance was detected at wavelength of 255 nm, 277 nm and 320 nm. Those wavelengths re related with the absorbance of caffeine in ground roasted coffee [2-3]. In order to evaluate the influence of particle size variation, further analysis including PCA and PLS-DA was performed.
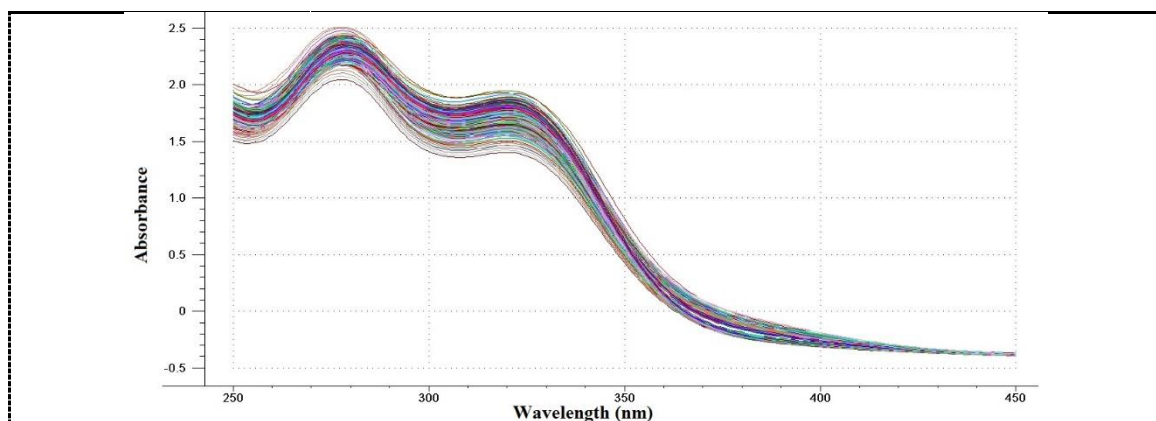

Figure 1. Spectra of peaberry and civet coffee samples for pre-processed spectra in the range of 250-450 nm with two different particle sizes.

3.2. Results of PCA
Figure 2 showed the result of PCA. In general, it can be seen that using the PC1 and PC2 (represent 88% of the total spectral variation), the samples can be clustered into 4 groups based on type of coffee (peaberry and civet) and based on particle size (mesh 12 and mesh 50). Peaberry coffee mostly are located in the left side of PC1 and civet coffee sample are clustered in the right side of PC1. Based on this result we can easily understand that the particle size has great influence on the authentication of peaberry and civet coffee.

Figure 2. Score plot of PC1 and PC2 of peaberry and civet ground roasted coffee samples using pre-processed spectra in the range of 250-450 nm with two different particle sizes.
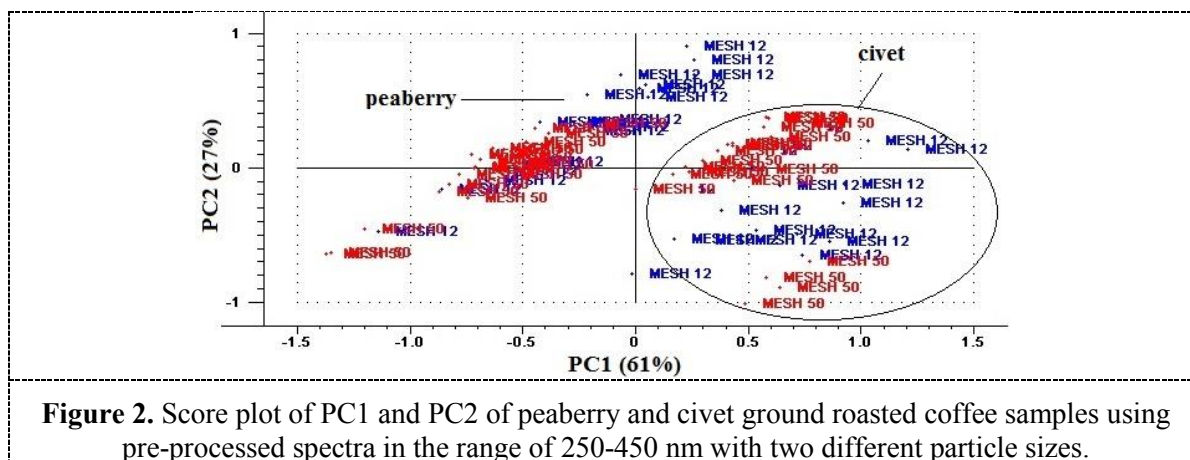
3.3. Compensation of particle size variation using PLS1 method
Using PLS1 regression method, local and global PLS-DA model was developed using pre-processed spectra in the range of 250-450 nm and the result was presented in Table 1. Local PLS-DA model was developed using samples having same particle size. For this purpose, two local PLS-DA models of mesh 12 and mesh 50 were established. A global PLS-DA model was developed using samples having particle size of combination of mesh 12 and mesh 50. As seen in Table 1, all developed models have high quality with coefficient of determination 0.98-0.99 for both calibration and validation.

Table 1. The result of PLS-DA model development for local and global model using pre-processed spectra in the range of 250-450 nm using PLS1 method.

Models	Samples	Latent variables	R^2_{cal}	R^2_{val}	RMSEC	RMSECV	bias
Local 12	158	4	0.99	0.99	0.056517	0.059232	-0.000137
Local 50	160	2	0.98	0.98	0.068911	0.070666	0.000172
Global 12 and 50	318	4	0.98	0.98	0.065042	0.066946	-0.000389

To evaluate the model performance of the local and global calibration models, a prediction using external sample set was conducted. A number of 80 samples of peaberry and civet coffee was used. The results were presented in Figure 3. Using the local calibration model at mesh 50, the prediction results were poor with high RMSEP, SEP and bias. Using the global calibration model, the prediction results were excellent with low RMSEP, SEP and bias.
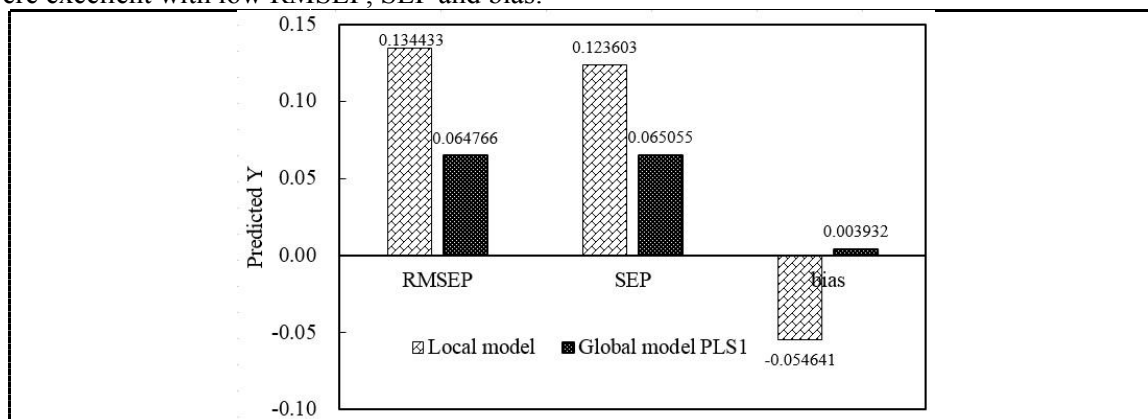

Figure 3. Prediction result using local and global PLS-DA model using PLS1 algorithm for pre-processed spectra in the range of 250-450 nm.

3.4. Compensation using PLS2 method

A global PLS-DA model was developed using pre-processed spectra in the range of 250-450 nm using PLS2 algorithm. In this model, predictor variables are spectral data in wavelengths of 250-450 nm. In PLS2 algorithm we add directly two target variables: types of coffee (civet and peaberry) and particle sizes (mesh 12 and 50). The result was summarized in Table 2. The quality of the model is quite good with low RMSEC and RMSECV. To assess the performance of this model, a prediction using external sample set was conducted and the result was presented in Figure 4. It is clearly seen that global calibration model has better performance in prediction with low RMSEP, SEP and bias comparing to local calibration model.

Table 2. The result of PLS-DA model development for global model using pre-processed spectra in the range of 250-450 nm using PLS2 method.

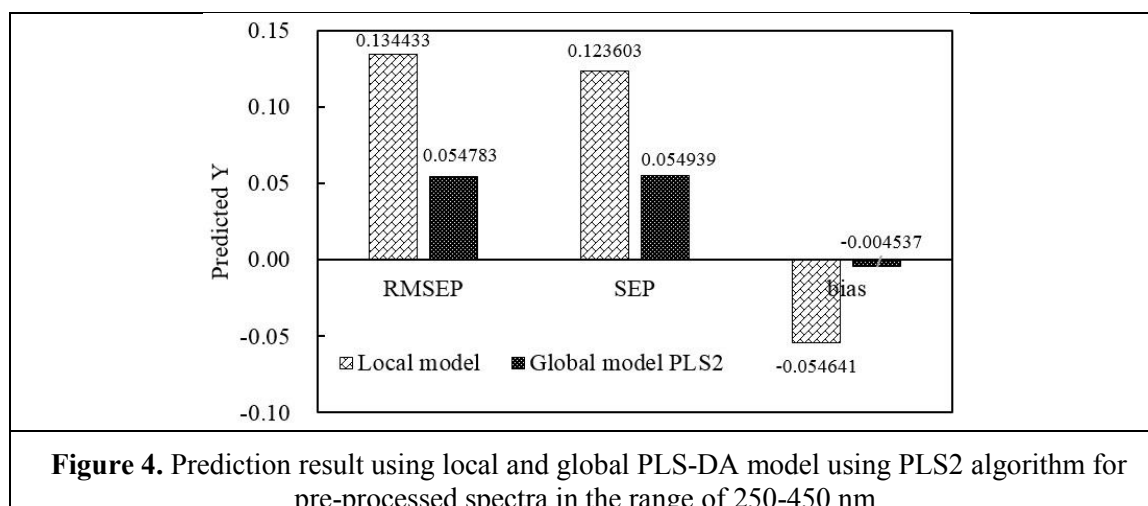| Models	Samples	Latent variables	R^2_{cal}	R^2_{val}	RMSEC	RMSECV	bias
Global 12 and 50	318	9	0.99	0.99	0.053658	0.059444	-0.001361

Figure 4. Prediction result using local and global PLS-DA model using PLS2 algorithm for pre-processed spectra in the range of 250-450 nm.

4. Conclusion

The result of PCA showed that the coffee samples can be clustered based on types of coffee (peaberry and civet) and based on particle size (mesh 12 and mesh 50) using pre-processed spectral data in the range of 250-450 nm. Using the two compensation methods of global calibration model of PLS1 and PLS2, the prediction results for prediction sample set at particle size of 1680 μm dan 297 μm (mesh 12 and mesh 50) were excellent with low RMSEP, low SEP and low bias. This result opens a possibility to develop a robust PLS-DA model for faster authentication of civet and peaberry coffee with minimal sample preparation.

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