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Contributed Paper

Application of Artificial Neural Network for Tracing the Geographical Origins of Coffee Bean in Northern Areas of Thailand Using Near Infrared Spectroscopy

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ABSTRACT

The aim of this research study was to investigate the difference among coffee bean from different plantation areas in the northern of Thailand. Near infrared (NIR) spectra were recorded from Arabica coffee samples which were collected from Chiang Mai, Lampang and Mae Hong Son provinces in Thailand. In addition, color parameters and moisture content were analyzed. The data were exploratorily analyzed based on the uses of principal component analysis (PCA) and an artificial neural network (ANN) called self-organizing map (SOM). To identify the significant parameters of the spectroscopic data, a variable selection called self-organizing map discrimination index (SOMDI) was applied. As a result, SOM could overcome the PCA technique where the samples from the three different origins could be separated. Additionally, based on the SOMDI results, the coffee samples from Chiang Mai could be well discriminated using the NIR spectral regions of 880-1182, 1254-1326, 1896-2180 and 2260-2498 nm. This research demonstrated that using NIR spectroscopy coupled with the ANN algorithm allowed an efficient tracing method to differentiate the coffee bean samples in the northern of Thailand.

Keywords: coffee, geographical origin tracing, near infrared (NIR) spectroscopy, artificial neural network (ANN), self-organizing map (SOM)

1. INTRODUCTION

Coffee has been among the important agricultural products for many countries in Africa, Asia, Southern and Central America [1]. In general, coffee bean with good aroma quality, appropriate caffeine content and less bitter taste could have achieved high demand in the market [2, 3]. Due to the fact that environmental conditions such as soil composition, amount of rainfall, and height above the sea level can strongly affect the coffee quality, the coffee bean of various cultivation places could differently possess aroma and taste characteristics [4]. As a result, depending on the genuine trademarks, the price of the coffee bean from well-known origins can be relatively higher leading to an abusive price or the use of misleading package. Therefore, confirmation of the geographical origin of the coffee product is among the important matters not only to guarantee the quality of the coffee products but also to support the decision making process of customers in the market.

Since the environmental factors could have affected to the chemical composition in coffee bean, the coffee bean from various origins could be characterized using several analytical methods such as gas and liquid chromatography [5], nuclear magnetic resonance spectroscopy [6] and X-ray fluorescence spectrometry [7]. However, these chemical analysis methods have analytical limitations such as requirements of complicated sample preparation, long time analysis and high operating cost. Near infrared (NIR) spectrometry has been applied as an alternative technique. The prime advantage of NIR spectroscopy is that it can perform non-destructive measurement quickly without or less sample preparation [4]. With ease of chemometric computation, NIR spectroscopy has been successfully applied to analyze coffee samples, for example, coffee varietal discrimination [8], predictions of sensory properties [9] and coffee roasting degrees [10].

Artificial neural networks (ANNs) are mathematical tools that mimic the functioning of human brain to analyze multivariate data [11]. The ANN algorithm employs a model using a learning process based on previous known or training dataset. Therefore, they do not assume that the data should follow a multivariate normal distribution. In other words, the ANN models are nonlinear models where no mathematic equations are needed to describe the relationship between the studied samples. Proposed by Kohonen in 1991 [12], a self-organizing map (SOM) has been among the most popular of ANNs. This technique has been used for exploratory analysis of various samples such as water [13], food [14] and polymers [15]. Additionally, the SOM algorithm could be extended for variable selection purpose, called SOM discrimination index (SOMDI) [16-18]. For example, the predictive ability of the adulterated level was successfully improved when SOMDI was utilized to capture the significant NIR spectra of the adulterated Khao Dawk Mali 105 (KDML105) rice [19]. The aim of this research was to apply the chemometric ANN techniques to investigate the Arabica coffee beans of different original plantations from the three provinces in the northern Thailand. A SOM in supervised mode was used as a multivariate statistical tool for revealing the difference among the coffee samples. Some physicochemical parameters were also investigated in the relation to spectroscopic data. In addition, SOMDI was also used to indicate the significant parameters of the NIR spectra which could be used as the key parameters for identifying the sources of the coffee samples.

2. MATERIALS AND METHODS

2.1 Coffee Bean Samples and NIR Measurement

A total of 59 Arabica coffee bean samples were collected from three different areas located in the north parts of Thailand ranging from 736 to 1280 m above the sea level, mild temperatures between 23.8 and 28.6 °C and a yearly mean rainfall of 1274.3 mm. The coffee samples were categorized into three groups according to their plantation areas which were Chiang Mai (CM), Lampang (LP) and Mae Hong Son (MHS) provinces. The samples were measured using NIR spectrometer (NIR6500 system, Multi-Mode™ Analyzer, Foss, USA) with a NIR reflectance transportation module as an absorbance (log $(1/R)$) between 400 to 2498 nm at 2-nm intervals giving a total of 1050 data points for each spectrum. Each sample was scanned 32 times and the spectra were averaged to provide a mean spectrum. Prior to the

NIR analysis, the coffee samples were stored in a controlled room temperature at 25 °C for 6 hrs.

2.2 Physicochemical Properties

In addition to the NIR absorbance, the color parameters and moisture content were measured from the coffee samples. To record the color parameters, each green coffee bean sample (100 g) was put in quartz cuvette cell (5×5×5 cm) and measured the color values in terms of lightness (L*), red–green component (a*) and yellow–blue component (b*) using a color meter (CR-400, Minolta, Japan) [20]. For the moisture content determination, the coffee bean of 100 g was contained into a chamber of a grain moisture tester (PM-450, Kett, Japan) to measure the moisture content.

2.3 Chemometrics

2.3.1 Artificial neuron network (ANN)

A self-organizing map (SOM) is an ANN technique which has been extensively used as a learning method for capturing the structure of multidimensional data [11]. After the iteration process, SOM can visualize the learning data into a two-dimensional map consisting of a certain number of units. Up to the present, a variation of the SOM learning processes has been proposed [14]. Generally, SOMs could be categorized into two different modes depending on how the models are trained: unsupervised and supervised SOMs. The unsupervised SOMs use only the information of the predictors (or measurements such as NIR spectra) during the training process. On the other hand, the supervised SOMs additionally utilize both of the predictors and responses (or the class membership). In this research study, the SOM was trained based on the algorithm presented by Lloyd et al. [15] with an initial map with the size of 8x10 map units. The other input parameters such as learning rate and neighborhood width were set following the literature [21].

2.3.2 SOMDI process

A SOM visualization method can be used to evaluate the parameters that strongly affect to the grouping of samples. For example, Figure 1 represents component planes of a supervised SOM map characterized by five variables and three class memberships. Each variable has different amount of variation reflecting the trend of the trained map. To evaluate the level of the variable contribution, the intensity of each variable should be visualized and considered in comparison to the organization in the respective class map. The distribution of the variables which most resembles to the class map component plane are basically indicated to be important variables for the respective class membership. For instance, Figure 2 shows the determination of the important variables which affect to trend of class map of A. In Figure 2(A), the dark shading of the map of variable 1 is analogous to the organization in the class map of the class membership A. Thus, this

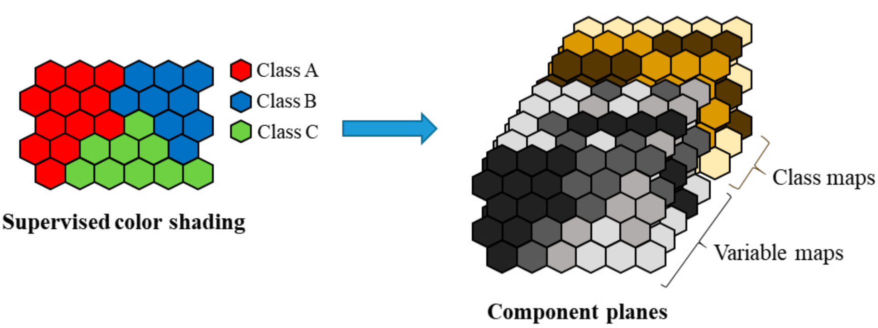


Figure 1. Supervised color shading of supervised SOM and its component planes.

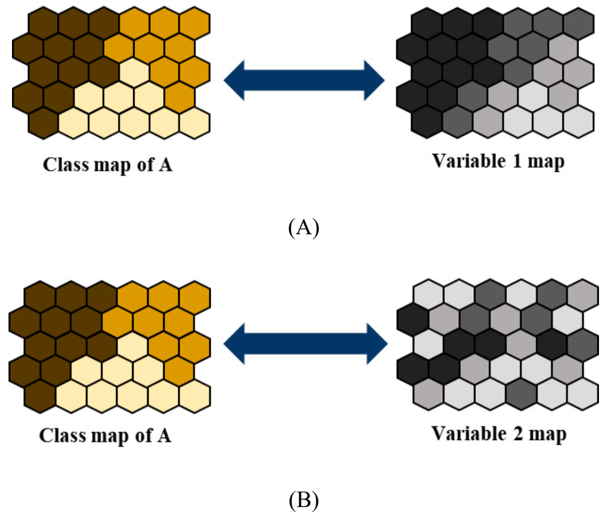


Figure 2. Determination of variable important to discrimination of class A.

variable could be important for the identification of the class A samples. On the other hand, the intensity in the component plane of variable 2, as is shown in Figure 2(B), is not quite associated to the class map implying that the variable 2 should not therefore be important in this case. This evaluation process could be simple; however, is impractical to investigate the complicated dataset having a large number of variables.

In this research study, SOM discriminant index (SOMDI) was employed to solve this problem by scoring the component planes according to how strong they could be related to the class membership data. The calculation of the SOMDI values was based on the literatures [16, 17]. After that, the ΔSOMDI can be calculated using the following steps as illustrated in Figure 3:

Step 1: Matrices of variable maps and class maps were generated from the three-dimensional trained map.

Step 2: To consider the influence variables of each class, the classes must be identified as "in-group" and "out-group". For example, in the case of identifying important variables in relation to the class A sample, the samples in this class will be defined as an in-group vector (gray color vector). On the other hand, the other classes are defined as an out-group matrix (green color matrix). A SOMDI score of each variable can be then calculated for the in-group and out-group vectors. It is noted that the values of the out-group matrix for each sample were combined to be an out-group vector before the calculation of the SOMDI scores [17].

Step 3: The difference between the "in-group" and "out-group" SOMDI values (ΔSOMDI) was calculated as follows:

$$\Delta \text{SOMDI} = \text{SOMDI}_{\text{in-group}} - \text{SOMDI}_{\text{out-group}}$$

If the ΔSOMDI of a variable is greater than 0, this implies that the SOMDI value from "in-group" is higher than SOMDI value from "out-group". Consequently, this variable will be defined as an important parameter for the respective class.

3. Results and Discussion

3.1 Details of the Studied Coffee Bean Samples

Table 1 presents the characteristic information,

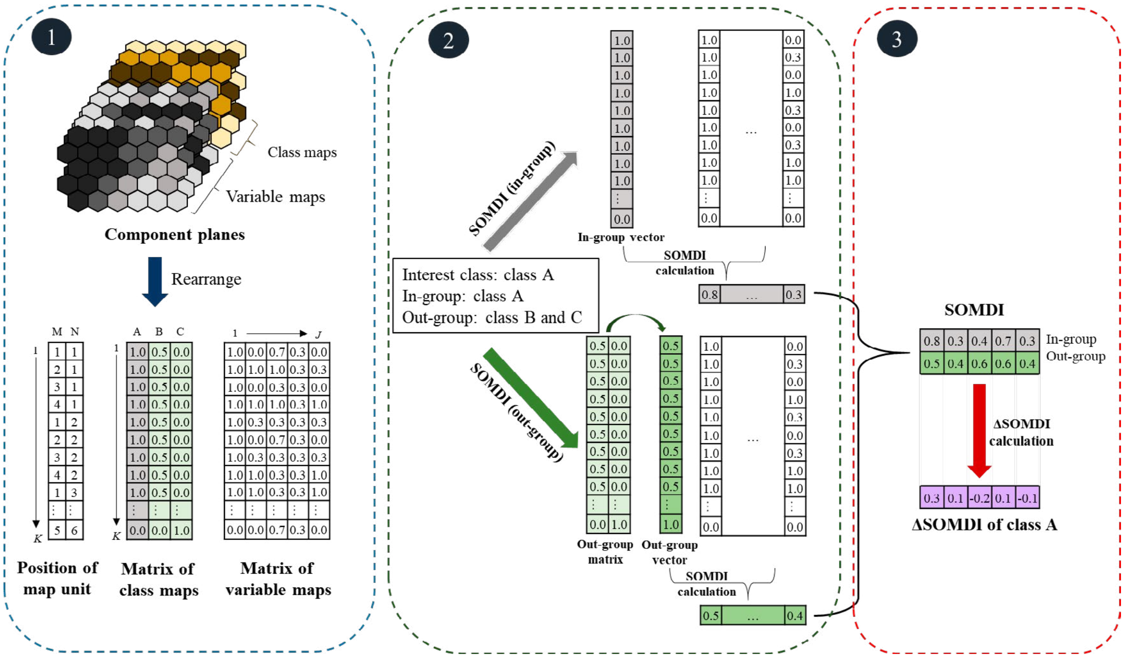


Figure 3. Diagram of a ΔSOMDI calculation.

Table 1. Details of the coffee bean used in this study. The values represent mean ± standard deviation.

Plantation area	Altitude (m)	Density (g/dm^3)	Moisture content (%)	Color values		
				L*	a*	b*
Chiang Mai (n=32)	979.9 ± 166.6a	667.14 ± 12.10a	8.53 ± 1.57a	47.23 ± 1.40a	1.22 ± 0.34a	15.43 ± 0.86a
Lampang (n=17)	947.9 ± 169.2a	672.09 ± 10.00a	8.33 ± 1.29a	47.91 ± 1.09a	1.45 ± 0.20b	15.84 ± 0.78a
Mae Hong Son (n=10)	1128±3.4b	673.58 ± 27.24a	6.87 ± 0.89b	49.21 ± 1.44b	1.52 ± 0.25b	16.15 ± 0.82a

In each column, the values with different superscript letters are significantly different according to the Tukey test ($p < 0.05$).

including height above the sea level (altitude), density, moisture content and color parameters of the coffee bean samples from Chiang Mai (CM), Lampang (LP) and Mae Hong Son (MHS). It can be seen that the samples from the three provincial areas were grown at the different heights from the sea level. The average altitudes of coffee samples from CM and LP were significantly lower than those of the samples from MHS. This fluctuation difference could result in the variations in air temperature, the shading and water levels of the cultivation areas influencing the characteristic quality of the coffee bean [22]. The average density values of three coffee origins were approximately 667.14 to 673.58 g/dm^3. In this case, no significant difference of the density values among all of the samples from different locations could be observed. However, the samples from MHS have lower moisture content (MC = 6.87) in comparison with those from CM and LP (8.33-8.53). The average color values of coffee including lightness, red–green component and yellow–blue component represented ranged from 47.23-49.21, 1.22-1.52 and 15.43-16.15 in terms of L*, a* and b* values, respectively.

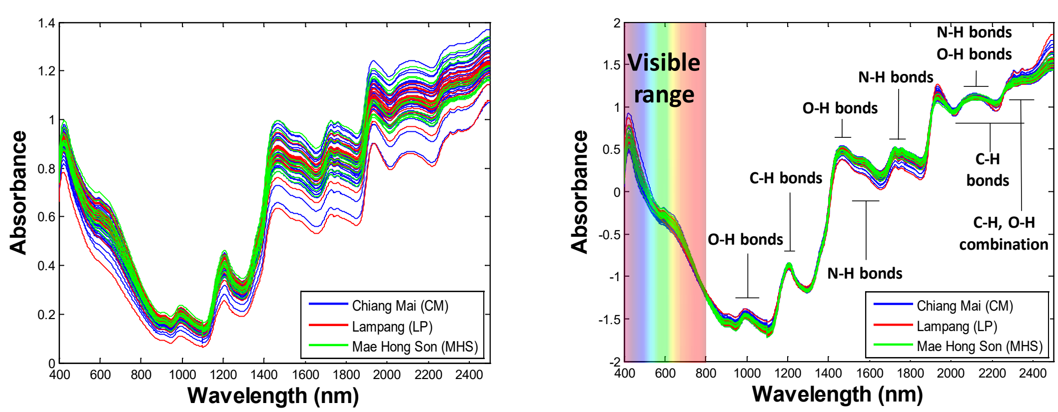
3.2 Spectra Feature

The NIR spectra of all coffee bean samples are shown in Figure 4 where the samples collected in Chiang Mai (CM), Lampang (LP) and Mae Hong Son (MHS) are labelled using blue, red, and green lines, respectively. The deviation from baseline shifts could be observed from the raw NIR spectra in Figure 4(A). This deviation of the NIR spectra could be obtained from the samples with inhomogeneity in size causing by scattering of light during the NIR measurement. To eliminate this error, standard normal variate (SNV) was applied to transform the spectra into a uniform of variation [23]. The NIR spectra after the SNV pretreatment are presented in Figure 4(B). The deviation on the spectra in the range of 400-800 nm could be related to the variation of the sample colors. In addition, the dominant absorbances which could be associated to the organic chemical compounds in coffee beans were also observed. In Figure 4(B), the labeled bands corresponding to the functional groups in caffeine, lipids, water, protein and amino acid, carbohydrate, sugars and trigonelline were labelled in agreement with the main components found in coffee [4, 9].

3.3 Data Exploratory Based on PCA

3.3.1 Determination of NIR data

To exploratorily analyze the pattern in the coffee samples, PCA was applied after the data was pretreated by SNV. Figure 5 demonstrates a PCA score plots where the samples were labelled according to their origins. When the whole spectral data were used as shown in Figure 5(A), no clear separation among sample groups was observed. The coffee samples were organized into a single region. However, it was possible to observe that the samples from the same location were located nearby each other. For example, most of the coffee samples from the LP and MHS provinces were located on the lower side of the PCA space. On the other hand, the samples from the CM province had higher of the PC2 scores, so tended to locate on the upper part of the score plot. Remarkably, when the PCA was modelled exclusively using the NIR absorbance from the short-wave NIR region ranging from 950 to 1050 nm (Figure 5(B)), the difference among the three groups were noticeably



(A) (B)

Figure 4. NIR spectra of 59 coffee samples with no data preprocessing (A) and SNV (B).

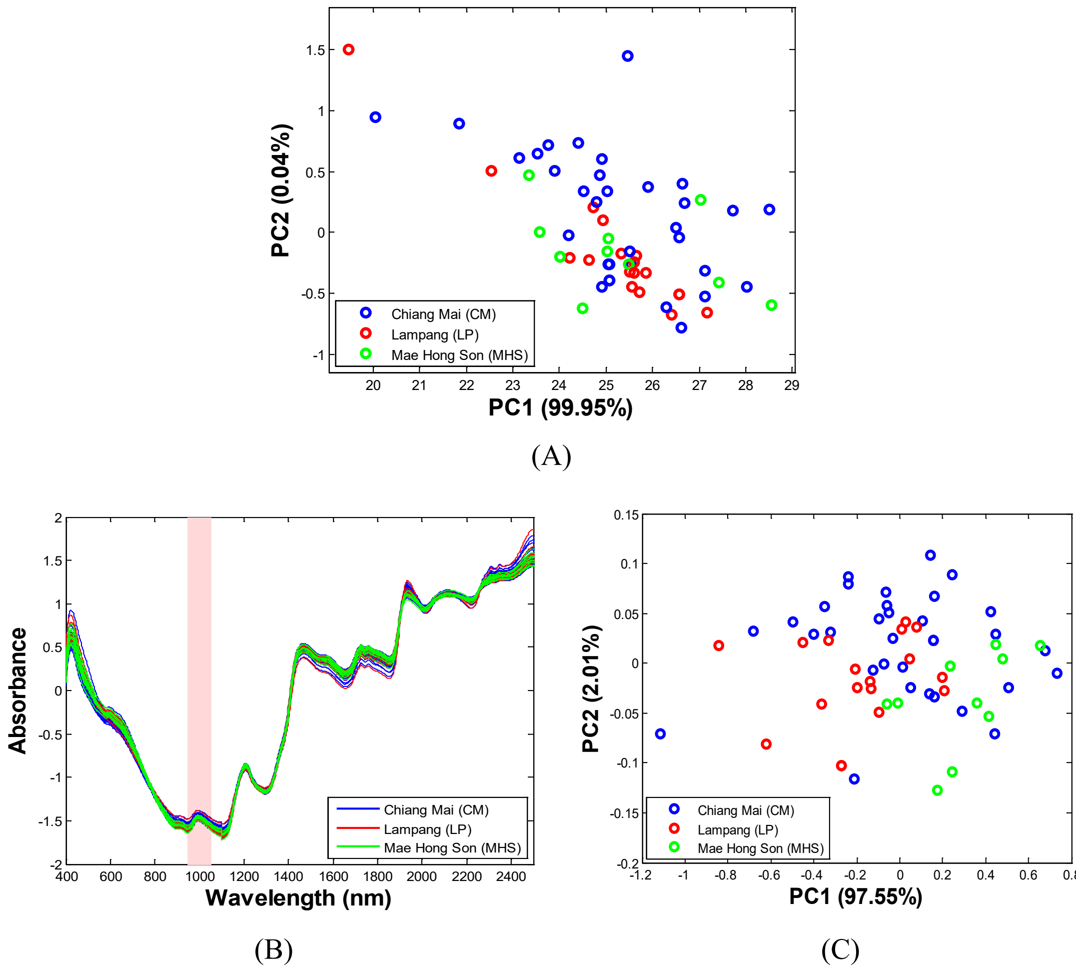


Figure 5. PCA scores plot of 59 coffee samples using the whole NIR spectra (A); selected NIR wavelengths (B), and the PCA scores plot of the selected wavelengths (C).

clear. From Figure 5(C) which is the PCA scores plot of the selected wavelength from Figure 5(B), the difference of samples from different locations were clearer than using the whole spectra as seen in Figure 5(A). This indicated that PCA could reveal the difference in the production sources of coffee beans if a set of appropriate wavelengths can be chosen for the exploratory analysis task. This could pose the possibility of the effective use of the short-wave NIR detection leading to a relatively low-cost reduction in development of the detection instrument.

3.3.2 Relationship between the physicochemical properties and the NIR spectra

The color parameters (L*, a*, b*) are among the important features that can be used to determine the quality of the green coffee beans [20]. In addition, moisture content (MC) can be used as an indicator for estimating the drying process of the coffee bean. If green coffee has the MC greater than 12.5%, it demonstrates that it is not properly dried and stored. The high MC in coffee bean, leading fungal growth and mycotoxin productions which are harmful to human, is therefore not allowed for commercial trading [24].

Figure 6(A), 6(B), 6(C), and 6(D) illustrate the changes of the MC, L*, a* and b* values, respectively, in relation to the PCA scores. The changes of the parameters of MC and L* could be obviously observed. In Figure 6(A), the MC values appeared to increase with the decrease of the PC1 score. While the coffee samples on the left side of the cluster possessed the higher MC. On the other hand, the trend of the lightness parameter (L*) in Figure 6(B) increased with the increment of the PC1 score but dropped along with the PC2 score. In case of the a* and b* parameters shown in Figure 6(C) and 6(D), the parameters indicated a slight inverse trend from the MC and L* values. The higher value appeared in the upper part of PC2 score with high PC1 score.

Overall, the patterns of the coffee samples in relation to the investigating parameters could be revealed using the plots of PCA scores. In fact, the differences in these parameters could be generally associated to several factors such

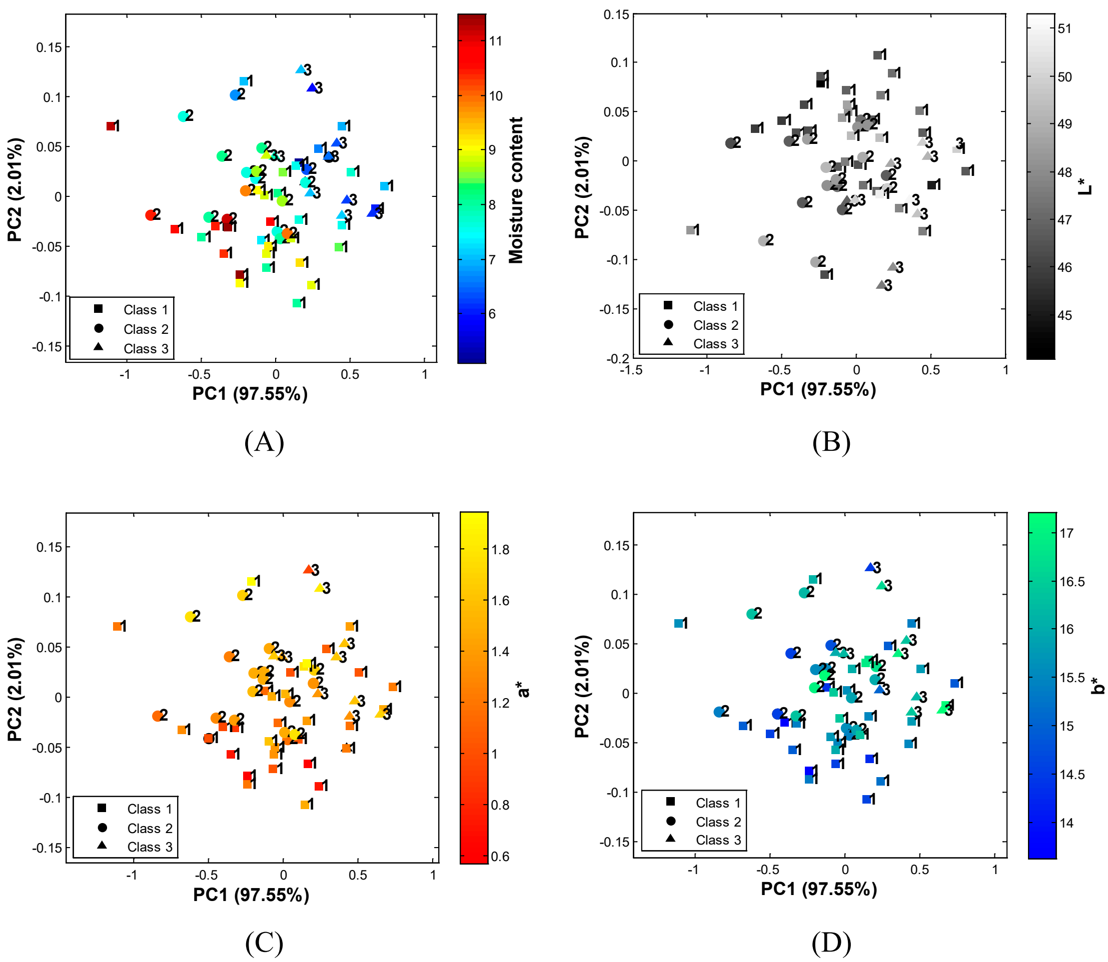


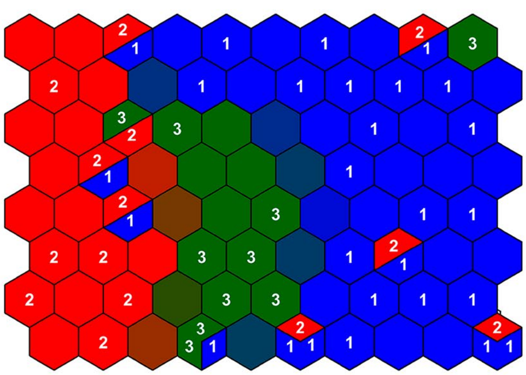
Figure 6. Comparison of the PCA scores plots labelled according to the moisture content (A), L* (B), a* (C) and b* values (D). The numbers 1, 2 and 3 indicated the class memberships of CM, LP and MHS, respectively.

as coffee been processing, variety and especially the age of coffee [20, 25]. However, based on the simple linear modelling of PCA, these parameters could not be used as parameters for determining the coffee origins in this research study.

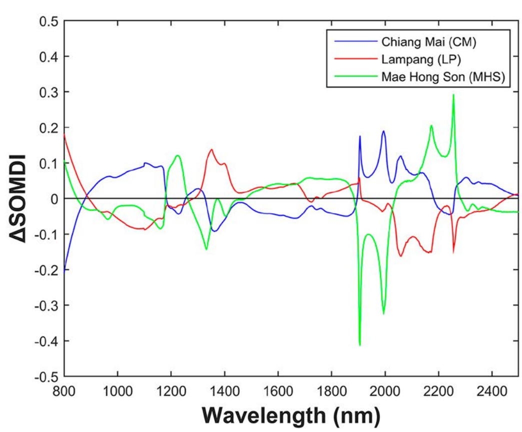
3.3.3 Supervised SOM and variable selection using SOMDI

Supervised self-organizing map (SOM) was applied to reveal the feature of the 59 coffee samples. The supervised color shading diagram in Figure 7(A) indicates that the supervised SOM could clearly discriminate the coffee samples into the three different clusters according to their origins. The coffee from CM (class 1) was mostly projected on half-right side of the map where the others from LP (class 2) and MHS (class 3) were located on the left side of the map. To investigate the important parameters in relation to the coffee discrimination result in Figure 7(A), the ΔSOMDI values of each sample class were calculated using the whole NIR spectra (800-2498 nm) and presented in Figure 7(B). The blue, red and green lines represented, respectively, the sample groups from CM, LP and MHS. The high values of this variable screening index indicated that the variables could be significant and play an important role in the SOM organization. The grater ΔSOMDI values in the regions could be related to the absorbance of several important chemical components in the coffee bean. For instance, the NIR region of 1180-1262 nm could be related to the amount of cellulose and caffeine [2, 4]. The absorption in the regions of 1480-1882 nm and 1896-2180 nm corresponded to the presence of caffeine, chlorogenic acid, proteins, lipids, and carbohydrates [4, 26]. In addition, the detected absorbance during 2260-2498 nm represented to carbohydrate, protein and caffeine contents [4]. To inspect the significant NIR absorbance of each coffee groups, the SOM maps were regenerated using the variables indicated as significance for each of the coffee origins. In this research, the ΔSOMDI values greater than zero were identified as significance and, after that, the variables with the significant ΔSOMDI were used for the reconstruction of the SOM maps.

Figure 8 displays the selected wavelengths and the regenerated SOM maps. Clear separation among the coffee samples could be obtained from all of the SOM maps. Figure 8(A) is the investigation of the coffee from CM (class 1) where



(A)



(B)

Figure 7. Supervised color shading of the NIR spectra (800-2498 nm) (A) and ΔSOMDI of the three sample classes (B).

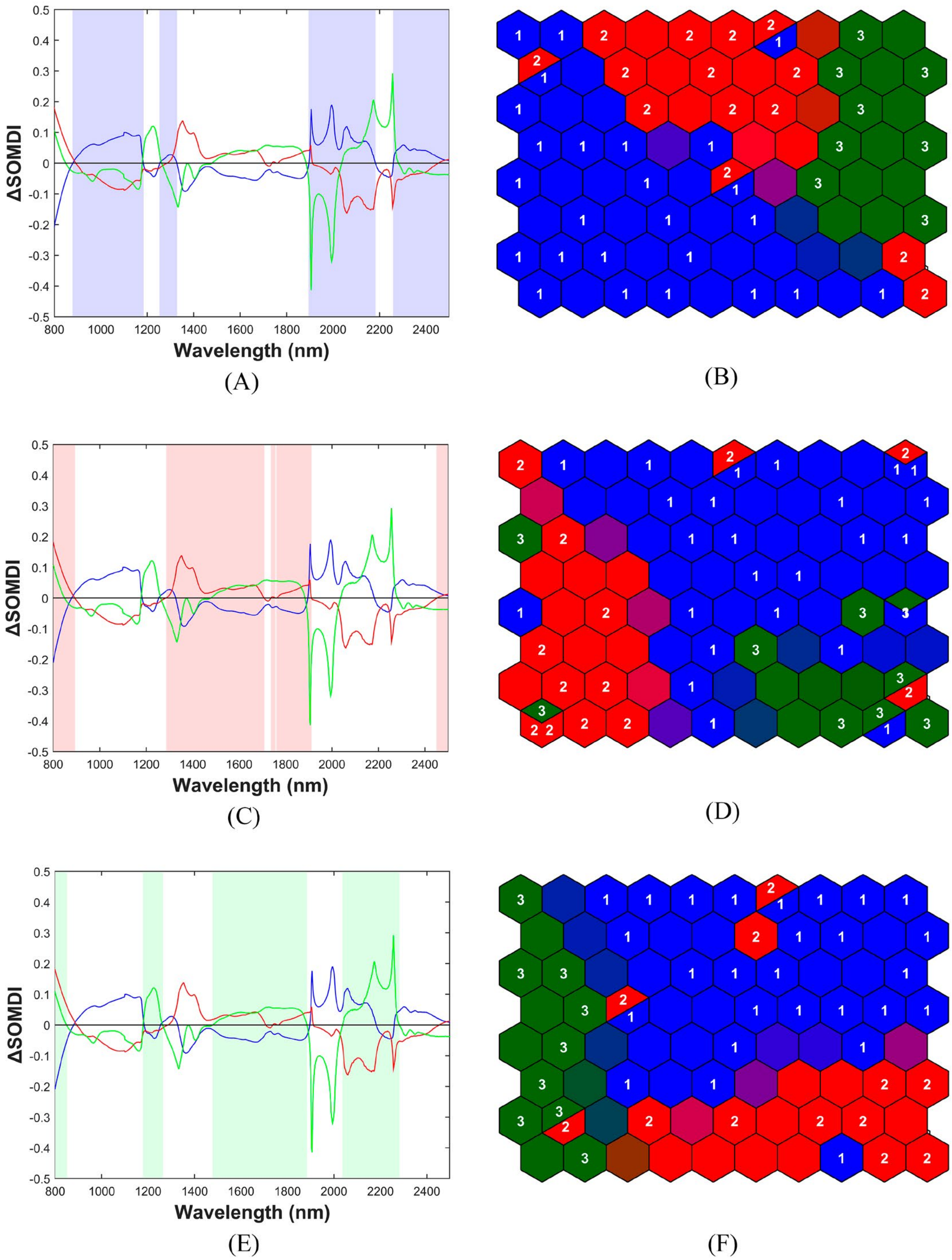


Figure 8. The highlighted significant ΔSOMDI values of class 1 (A) class 2 (C) and class 3 (E). The highlighted wavelength regions were used to generated the SOM maps for class 1 (B) class 2 (D) and class 3 (F), respectively, presented using the supervised color shadings; where 1 = Chiang Mai, 2 = Lampang and 3 = Mae Hong son.

the highlighted NIR spectral regions (880-1182, 1254-1326, 1896-2180 and 2260-2498 nm) were selected by the ΔSOMDI and used to construct the respective supervised color shading map shown in Figure 8(B). In this case, the use of the selective NIR wavelengths based on class 1 resulted in a more united cluster of samples from the CM region. After the screening, only one sample of class 1 was located out of the main group and only the samples from LP (class 2) was wrongly superimposed onto the CM region.

In case of the supervised color shading maps in Figure 8(D) and Figure 8(F), the use of NIR regions, which were prominently corresponded to the samples of LP (class 2) and MHS (class 3), also well revealed the clustering of the samples according to their geographical origins. Nevertheless, the selection of significant regions based on LP and MHS still provided poor separation in the other classes. For example, using the NIR ranges based on the significant ΔSOMDI of class 2 (Figure 8(C)), the majority of poor clustering appeared with the samples of class 3. Likewise, the clustering of class 2 was low effective when the important NIR ranges based on class 3 (Figure 8(E)) were used to generate the SOM map in Figure 8(F).

It could be noticed that using the selected wavelength based on class 1 showed a superior distinguishing model for tracing the geographical coffee origins of the samples. Remarkably, the significant wavelengths for the LP and MHS samples appeared not to be the same as those for the CM samples. The ΔSOMDI of class 1 showed that the main wavelength, which was not picked for the SOM process, was the NIR range approximately around 1300-1900 nm. The absorbance within this region generally correspond to protein, cellulose [9] and strongly relate to the first overtone of water [27]. This could possibly relate to the PCA score plot of MC in Figure 6(A). The MC, the water determination in coffee beans, were quite not much different according to their origins. This implied that, in this case, the amount of water in coffee might not be a good discriminator for differentiating the class of each sample. The NIR region with associating of water could be less correlated to the difference of the coffee beans from the different origins. Therefore, they could be discarded from the ANN analysis.

Finally, the NIR parameters selected based on the significant ΔSOMDI of class 1 successfully provided the best discrimination. Although the variable selection based on the individual class could lead to the overfitting problem, this process enlighten that the specific variables could be exclusively used for identifying whether the coffee bean has been from the expected origin or not. The developed model could be further used for evaluating the coffee bean samples if they were mislabeled or adulterated by the coffee from the other sources.

4. Conclusions

NIR measurement coupled with SOM could be successfully used to identify the difference among coffee samples collected from different geographical origins in the northern areas of Thailand. The exploratory results showed that SOM offered more the separation ability than PCA. This could be that using SOM, the topology of the data could be better maintained, and the samples were distributed across the established map. Whereas, using PCA, the samples were rather scattered around the center of the PCA space. To enhance the identification results, the potential NIR wavelengths which could be important were identified using the ΔSOMDI parameter.

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