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A novel application of artificial neural network for classifying agarwood essential oil quality

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ABSTRACT

This work studies the agarwood oil classification into high and low quality by using two different techniques. Initially, the Forest Research Institute Malaysia (FRIM) and Universiti Malaysia Pahang (UMP) are where the sample preparation and compound extraction of agarwood oil is collected. The data collections were done from the previous researcher consists of 96 samples from seven significant agarwood oil compounds. The artificial neural network (ANN) and the proposed stepwise regression technique were used in this study. The stepwise regression was done the feature selection and successfully reduced agarwood oil compounds from seven to four. Then, the ANN technique was used to classify agarwood oil into high and low using input from seven and four compounds separately. The performance of ANN with different inputs is compared (ANN with seven inputs compared with ANN with four inputs). All the experimental work was performed using the MATLAB R2017b using the “patternet” implemented Levenberg Marquardt algorithm and ten hidden neurons. It was found that the ANN technique using seven compounds obtained the best performance according to high accuracy and lower mean square error (MSE) value. Finally, 1 hidden neuron in ANN with seven inputs selected as the best neuron for grading the agarwood oil compounds.

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1. INTRODUCTION

Agarwood is dark resinous heartwood which comes from the main genus of Aquilaria Malaccensis, which grows in South Asia. The area is including Malaysia, Indonesia, Thailand and India [1], [2]. Agarwood has been given other names which are Aloeswood, Eaglewood, Kanankoh, Oudh, Jinkoh and others [1]–[5]. Generally, in the beginning, the agarwood plant has a light and pale color, but during the matured level, the plant turns into a dark color [6]. The productions of resin content from agarwood lead to the production of agarwood essential oil is due to infection either because of animal grazing, microbial invasions or attacks by insects [2], [6].

Agarwood essential oil is widely used in many countries [1], [3], [6]. It is well known because of its beneficial uses such as perfumes, medicines, incenses and ceremonies [1], [3]. In order to obtain high quality agarwood essential oil, it is important to undergo the best grading process. A previous study has been grade agarwood oil using the physical properties of the oil consists of the color intensity and infection level [2], [4].

Generally, the technique is done manually using human sensory panel but it has been proved not efficient for a long duration [2], [7]. In recent years, the grading process is using the chemical properties of agarwood oil and has been proven can provide accurate results [1], [3]. There are some modern techniques that have been introduced for grading agarwood oil such as by using artificial neural network (ANN), support vector machine (SVM), k-nearest neighbor (k-NN) and many others [2], [8]–[10]. Agarwood oil has successfully evaluated using SVM technique with different kernels which are radial basis function (RBF) and multilayer perceptron (MLP) [8].

Stepwise regression (SR) is a method of selecting the independent variables that can explain the dependent variable with step by step iterative construction very efficiently [11], [12]. The construction is through adding and removing of the independent variables from or into the model [12]. The two main procedures in SR are the forward selection method and backward elimination [12]–[17]. For the forward selection, the method starts with no independent variables in the model except the intercept. The process of adding the independent variables that give the most important factors that can improve the model is done one at a time until no more variables that significant to the model. Oppositely from forward selection, the backward elimination starts with the variables in the model and eliminates the variable that gives the least effect on dependent variables one at a time [12]–[14].

Some studies stated that, there are some selection criteria to be used to stop the process of stepwise regression of the model [14], [18]. They are F-test, Bayesian information criteria (BIC), Akaike information criterion (AIC), coefficient of determination R2, adjusted coefficient of determination R2adj, and P-value [13], [17], [19]. F-test and P-value are common to use in stepwise regression and they are tested using α value [13], [17]. Standard significance of α value in statistics is 0.05 [17], [20]. The advantages of stepwise regression can save time and cost due to only a significant parameter is selected, otherwise can reduce the error brought by the redundant variables [20].

ANN is first introduced by researcher McCulloch and Pitts in the year of 1940s. ANN is a favorite research tool among the researcher due to the ability to learn from example [21]. ANN is defined as a massively parallel distributed processor made up of simple processing units or known as “neurons” with large number and interconnections. The neurons are able to store any knowledge required by the network via synaptic weights [21], [22]. Generally, ANN mimics to biological neurons which applied human brain concept that able to learn [21], [23], [24]. The network of ANN can be grouped into two; feed-forward and recurrent networks. The first type is feed-forward networks which the connections are in feed-forward manners such as single layer perceptron, multilayer perceptron and radial basis function net. The second type is recurrent (has loop and feedback) or dynamic system contains many networks; competitive networks, Kohonen’s SOM, Hopfield network and adaptive resonance theory (ART) models [21]. According to the technique mentioned, in this study, the stepwise regression analysis technique and ANN technique were chosen to classify the agarwood oil into 1 and 0 which is high and low quality, respectively based on recommended by [9], [25], [26]. The paper is structured: section 1 is introduction, section 2 will be the project methodology followed by section 3 which is the results and discussion and conclusion is on section 4.

2. METHOD

Firstly, the data of agarwood oil compounds were obtained from the Forest Research Institute Malaysia (FRIM) and Bio Aromatic Research Centre Of Excellence (BARCE), Universiti Malaysia Pahang (UMP) that have been conducted by previous researcher based on GCMS analysis [27]. The compounds were consists of 96 samples (mixture of high and low quality oil) of seven significant compounds of agarwood oil and they were assigned as *C1=β-agarofuran, C2=α-agarofuran, C3=10-epi-ϒ-eudesmol, C4=ϒ-Eudesmol, C5=Longifolol, C6=Hexadecanol and C7=Eudesmol* [27]. From 96 samples, 78 samples were high quality and 18 samples were low quality. These data will be used in the ANN and proposed stepwise regression technique. Both of the ANN technique will be comparing towards the performance of ANN model. The entire experiment is carried out using MATLAB version R2017a for training and evaluates the performance of the network model.

The following step is to conduct the stepwise regression analysis and classify agarwood oil compounds using ANN. Stepwise regression is applied in this research study in order to identify the useful features for the next classification in the ANN. This technique is able to choose the variables that give the best fit statistic model by estimating the p-value wisely according to forward and backward technique [16]. The seven significant compounds are used as input features for the proposed method. In this experiment, the significance p-value is set into 0.05 or 5% as recommended by existing study [17]. In order to reject or accept the variables, the p-value need to be less than 0.05 for accept while reject when the p-value of 0.05 exceeds. The output from the stepwise regression is used as input feature for the neural network technique.

Next, the process continued by classifies agarwood oil compounds using ANN technique. The process is done separately for comparing purposes, where the first one is by using the seven compounds as input features and after that is repeated by using the four significant compounds from stepwise regression. The classification is using the special features in MATLAB which is pattern recognition neural network (patternnet) function. The data undergo data pre-processing stage which the data will be normalized, randomized and divide. The data is divided with the ratio of 70%:15%:15% respectively for training, validation and testing. The Levenberg Marquardt algorithm is used in ANN techniques as well as hidden neuron is set to 10 neurons. The model is test for the performance criteria which consists of confusion matrix, accuracy, sensitivity, precision, and mean square error (MSE) value. The results are appeared in the neural network training tool (nntraintool) that consists of plots and progress. The confusion matrix is used to describe the performance of the classification process as shown in the Table 1.

Table 1. The confusion matrix

Group	Low quality as positive	High quality as negative
Predicted as low quality	*kp*	*sn*
Predicted as high quality	*sp*	*kn*

For the *kp* is the number of accurately classified to low quality group, *kn* is the number of accurately classified to high quality group. While, *sp* is inaccurately classified to high quality group and *sn* is inaccurately classified to low quality group. The low quality of agarwood oil compounds will be appeared at *kp* section while the high quality of agarwood oil compounds will be appeared at *kn* section. The accuracy, precision, sensitivity and specificity are calculated to evaluate the performance of the ANN classification technique as shown in (1) to (4):

- The accuracy (ACRY) [28] is defined the overall effectiveness of a classifier to classify agarwood oil compounds:

$$\mathrm{ACRY} = (\mathrm{kp} + \mathrm{kn})/(\mathrm{kp} + \mathrm{kn} + \mathrm{sn} + \mathrm{sp}) \quad (1)$$

- The sensitivity (STVY) of a classifier is its ability to classify low-quality groups:

$$\mathrm{STVY} = \mathrm{kp}/(\mathrm{kp} + \mathrm{sn}) \quad (2)$$

- The practicable of the partitioned detects negative tag is known as specificity (SPCT):

$$\mathrm{SPCT} = \mathrm{kn}/(\mathrm{sp} + \mathrm{kn}) \quad (3)$$

- The precision, PRCS is the degree to which the data labels agree with the classifier's positive labels:

$$\mathrm{PRCS} = \mathrm{kp}/(\mathrm{kp} + \mathrm{sp}) \quad (4)$$

3. RESULTS AND DISCUSSION

This section explains the results obtained from the ANN technique using seven compounds and using the four compounds from proposed stepwise regression technique. The results included the comparison between the architecture of ANN, accuracy, MSE value and comparison of confusion matrix. Finally, ANN with the best performance is chosen as the best model for classified agarwood oil.

3.1. Artificial neural network using seven agarwood oil compounds

Figure 1 shows the architecture of neural network by using the patternnet function in MATLAB. According to the Figure 1, the input is seven refer to seven significant compounds, six hidden neurons and one output neuron. The target output is between value 0 and 1 based on MSE value as the default performance in MATLAB.

Table 2 tabulated the accuracy results for training, validation and testing for Levenberg Marquardt (LM) algorithms using seven agarwood oil compounds with the MSE value. From the table, the minimum accuracy from three dataset obtained by testing dataset which is 85.7% while the maximum accuracy is 100% and the validation dataset obtained the good performance. By referring the MSE value, hidden neuron 6 obtained the lowest value, which is 1.39x10-9 while the maximum obtained by hidden neuron 7 which is 1.55x10-2. Overall, the 1 hidden neuron is chosen as the best hidden neuron in classifying the seven agarwood oil compounds as it achieved accurately 100% for training, validation and testing accuracy at early stage of network training.

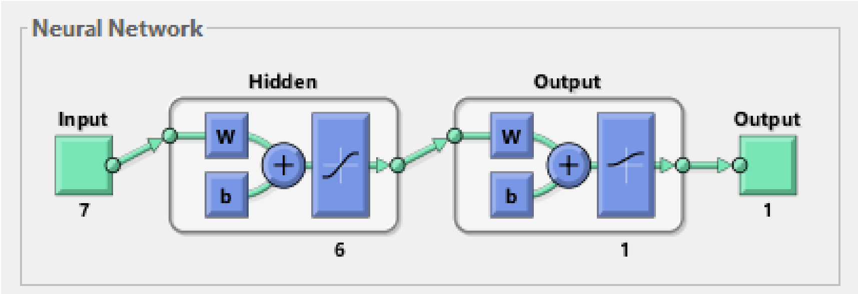

Figure 1. Architecture of neural network using seven significant compounds

Table 2. Training dataset using seven significant compounds

Hidden Neuron	Accuracy			MSE value
	Training	Validation	Testing	
***1**	**100**	**100**	**100**	**$6.98x10^{-9}$**
2	100	100	100	$3.36x10^{-9}$
3	100	100	100	$8.77x10^{-9}$
4	94.1	100	85.7	$2.20x10^{-2}$
5	100	100	100	$1.61x10^{-8}$
6	100	100	100	$1.39x10^{-9}$
7	92.6	100	92.9	$1.55x10^{-2}$
8	94.1	100	85.7	$1.87x10^{-2}$
9	100	100	100	$2.36x10^{-9}$
10	92.9	100	92.9	$3.42x10^{-2}$

**Best hidden neuron*

3.2. ANN using compounds from proposed stepwise regression

The seven significant compounds are firstly being the input features to the stepwise regression technique. They are assigned into variables X1 to X7 according to compounds C1 to C7. By the analysis of p-value by stepwise regression, there are four compounds have been listed to have p-value less than 0.05 and they fit to the model as well. The compounds are *X1(compound 1)=β-agarofuran, X4(compound 4)=ϒ-Eudesmol, X5(compound 5)=Longifolol and X7(compound 7)=Eudesmol*. These four compounds are fed into neural network as the input features. Figure 2 shows the architecture of neural network with the input feature from stepwise regression by using the patternnet function. The input neuron is four according to four compounds selected from stepwise regression, one hidden neuron and one output neuron.

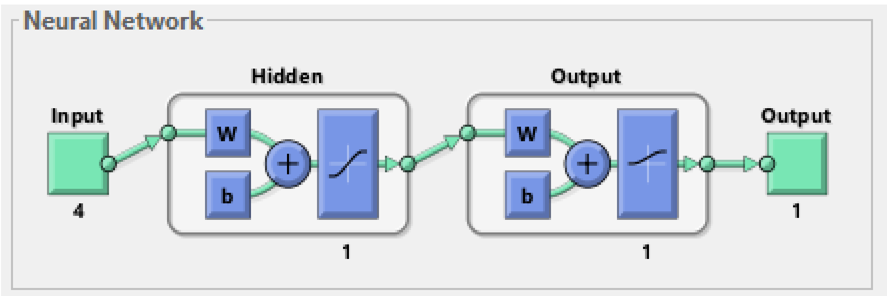

Figure 2. Architecture of neural network using four significant compounds

Table 3 tabulated the accuracy results for training, validation and testing of LM algorithm using four agarwood oil compounds chosen by stepwise regression with the MSE value. From the table, the minimum accuracy is obtained by training dataset which is 92.6% while the maximum accuracy is 100%. By referring the MSE value, 3 hidden neurons obtained the lowest value, which is 0.0134 while the maximum obtained by 1 hidden neuron which is 0.0384. Overall, the 1 hidden neuron is chosen as the best hidden neuron in classifying the agarwood oil compounds from proposed stepwise regression.

Table 3. Training dataset using four compounds

Hidden Neuron	Accuracy			MSE value
	Training	Validation	Testing	
***1**	**92.6**	**100**	**100**	**0.0384**
2	95.6	92.9	92.9	0.0271
3	98.5	100	100	0.0134
4	98.5	100	100	0.0149
5	97.1	100	100	0.0145
6	94.1	92.9	92.9	0.0316
7	94.1	92.9	92.9	0.0276
8	92.6	100	100	0.0318
9	95.6	100	100	0.0341
10	94.1	100	100	0.0314

**Best hidden neuron*

3.3. Comparison of ANN with seven compounds and ANN with compounds from the proposed stepwise regression

The Figures 3 and 4 show the overall confusion matrix for ANN technique using input of seven and four compounds respectively. Figure 3 shows that from 96 numbers of samples, the predicted group has successfully predicted 18 samples to low quality (group 1) and 78 samples to high quality (group 2). Besides, in Figure 4 shows that, from 96 numbers of samples, the predicted group has successfully predicted 17 samples and 4 samples to group 1, and 74 samples and 1 sample to group 2.

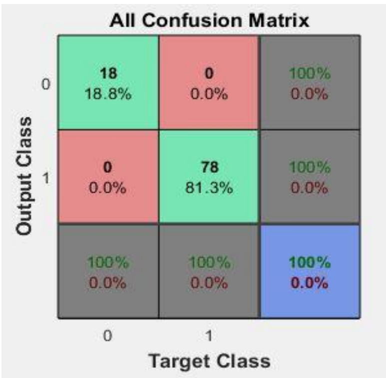

Figure 3. Overall confusion matrix for ANN technique using seven compounds

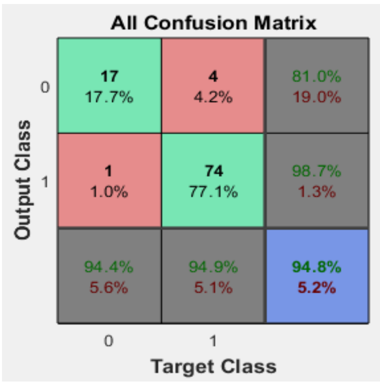

Figure 4. Overall confusion matrix for ANN using four compounds from stepwise regression

Figure 5 shows the graph comparison of performance evaluation between ANN using seven compounds and four compounds by ANN-Levenberg Marquardt, respectively. From the graph, it is obviously shown that the ANN using seven compounds performed better percentage of performance evaluation with 100% for the accuracy, sensitivity, specificity and precision. However, for ANN using four input compounds obtained 94.8%, 81%, 98.7% and 94.4% for accuracy, sensitivity, specificity and precision, respectively.

Based on the MSE value of the chosen best hidden neuron, the ANN with seven compounds obtained MSE value with 6.98x10-9 (1 hidden neuron) while ANN with compounds from the proposed stepwise regression is 0.0384 (1 hidden neuron). Both of the value is considered minimum as the value are less than 0 significant with the targeted output. For the comparison, both ANN obtained great performance at 1 hidden neuron. Nevertheless, by looking at the accuracy performance, ANN with input of seven compounds performed better as it achieved overall 100% for three dataset and classified accurately 96 compounds into its group classes. 1 hidden neuron is sufficient in this research study as it can avoid long computational time and overfitting problems [29], [30].

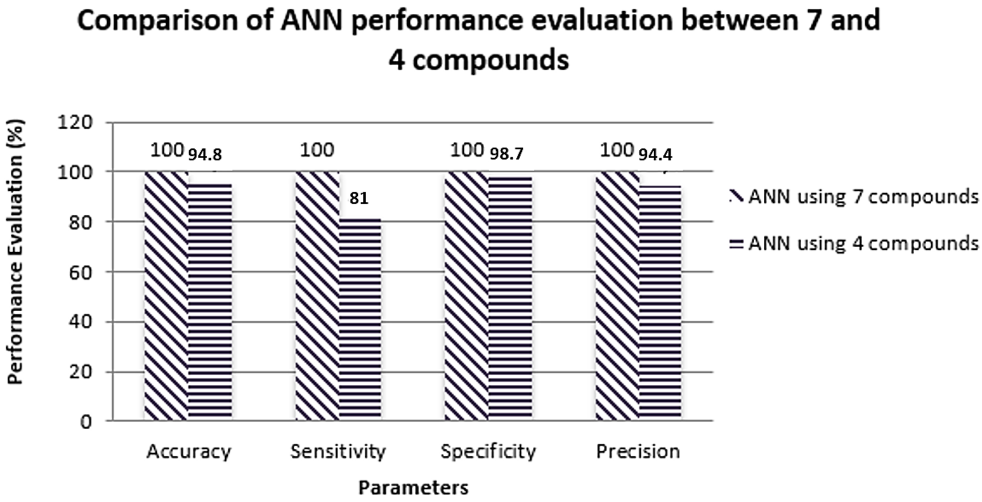

Figure 5. The performance evaluation between ANN using seven and four compounds

4. CONCLUSION

The study in this research has successfully differentiated the agarwood oil compounds to low and high quality using different amount of agarwood oil compounds by using ANN. The seven significant compounds are used as input features for ANN and stepwise regression. For the stepwise regression, the feature is reduced from seven to four compounds by feature selection. According to the results based on the MSE value and confusion matrix percentage evaluation between ANN with seven and four compounds, the ANN with seven compounds performed a better performance where the accuracy, specificity, precision and sensitivity obtained accurately 100% classification as well as lower MSE value. The ANN using compounds from proposed stepwise regression also performed good performance but the training accuracy makes it differentiated with the ANN with seven compounds due to not accurately classified. Therefore, this technique will benefit the agarwood oil industry in the future, particularly to its grading system.

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