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Agarwood oil quality identification using artificial neural network modelling for five grades

Siti Mariatul Hazwa Mohd Huzir[1], Saiful Nizam Tajuddin[2], Zakiah Mohd Yusoff[1], Nurlaila Ismail[3], Ali Abd Almisreb[4], Mohd Nasir Taib[3]

[1]Electrical Engineering Studies, College of Engineering, Universiti Teknologi MARA, Johor Branch, Pasir Gudang Campus, Johor, Malaysia
[2]Bioaromatic Research Centre of Excellence, Universiti Malaysia Pahang, Pahang, Malaysia
[3]School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Selangor, Malaysia
[4]Faculty of Computer Science and Engineering, International University of Sarajevo, Sarajevo, Bosnia and Herzegovina

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ABSTRACT

Agarwood (*Aquilaria Malaccensis*) oil stands out as one of the most valuable and highly sought-after oils with a hefty price tag due to its widespread use of fragrances, incense, perfumes, ceremonial practices, medicinal applications and as a symbol of luxury. However, nowadays the conventional method that rely on color alone has its limitations as it yields varying results depending on individual panelists' experiences. Hence, the quality identification system of Agarwood oil using its chemical compounds had been proposed in this study to enhance the precision of the Agarwood oil grades thus addressing the shortcomings of traditional methods. This study indicates that the primary chemical compounds of Agarwood oil encompass γ-Eudesmol, *ar*-curcumene, β-dihydroagarofuran, Υ-cadinene, α-agarofuran, *allo*-aromadendrene epoxide, valerianol, α-guaiene, 10-epi-γ-eudesmol, β-agarofuran and dihydrocollumellarin. This study employed artificial neural network analysis with the implementation of Levenberg-Marquardt algorithm to identify the Agarwood oil grades. The study's findings revealed that this modeling system of five grades got 100% accuracies with mean square error of 0.14338×10^{-08}. Notably, this lowest mean square error (MSE) value falls within the best hidden neuron 3. These study outcomes play a pivotal role in highlighting the Levenberg Marquardt-artificial neural network (LM-ANN) modeling that contribute to the successful of Agarwood oil quality identification using its chemical compounds.

Corresponding Author:

Nurlaila Ismail
School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA
40450, Shah Alam, Selangor, Malaysia
Email: nurlaila0583@uitm.edu.my

1. INTRODUCTION

The Aquilaria trees are renowned as a wood infused with resin and known for its fragrant qualities, commonly alluded to as Agarwood [1]. Globally, Agarwood goes by diverse names, often associated with specific religions or countries. It is commonly referred to as "Gaharu" in Malaysia and "Chexiang" in China. Other names include "Jinkoh", "Kalambak", "Agalloch", "Kanankoh", "Aloeswood" and "Eaglewood" [2], [3]. Agarwood, in particular, is extremely valuable as a non-timber forest resource due to its substantial demand. It plays a pivotal role in traditional medicine, contributes to the production of fragrant products and is used in religious and cultural ceremonies and festivals across many nations and faiths [1], [4]–[6].

Agarwood oil has gained universal and Malaysian acclaim for its diverse and valuable applications, particularly in the realms of fragrances, incense, perfumes, ceremonial practices, medicinal uses and as symbols of premium goods [7]–[10]. The unique essence of Agarwood is rooted in a complex blend of chemical compounds, proving the quality of the essential oil [10]. In the 20th century, an abrupt evaluation occurred in the grading of Agarwood oil, moving towards an emphasis on its chemical compounds. This approach stands as a key strategy for assessing oil quality, with the potential to enhance the identification precision and address issues posed by traditional techniques [11], [12]. Collaborative efforts involving academia and industry partners have sought to identify crucial marker compounds responsible for Agarwood's unique aroma. Research findings advocate for the quality classification of Agarwood or *Aquilaria* based on their chemical compounds abundance with a primary focus on *φ*-eudesmol, *α*-agarofuran, *β*-agarofuran and 10-epi-φ-eudesmol known as the key contributors to its robust woody aroma [13], [14]. Consequently, an imperative arises to distinguish the critical chemical compounds that underlie the diverse qualities of Agarwood oils.

However, an internationally recognized standard for Agarwood oil has yet to be established [15], [16]. Agarwood oil is graded differently in different countries [2], [3], with the existing grading system heavily reliant on consumer perception and preferences. Therefore, it encourages adulteration in the Agarwood trade [15], [16]. Agarwood oil's market value is determined by its inherent quality with higher-quality variants commanding premium prices [17], [18]. As previously stated, human sensory panels are used to evaluate the quality of Agarwood oil, a practice fraught with inefficiencies, fatigue and time consumption [13], [14], [19]. Consequently, doubts may arise and the grading process varies between exporting countries [7], [20]. The lack of a standardized identification method perpetuates the possibility for manipulations and fraudulent practices in which subpar oil is sold at exorbitant prices.

A comprehensive study on the United Arab Emirates, UAE's Agarwood market conducted by the Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES) team (2010) identified critical quality assessment criteria including factors such as country of origin, fragrance longevity, oil aroma and color, density and thickness [21]. Identifying pivotal marker compounds shaping Agarwood's distinctive aroma has been the focus of a collaborative effort between Universiti Malaysia Pahang (UMP), Universiti Teknologi MARA (UiTM) and industrial partners [22], [23]. In light of these endeavors, it is proposed that Agarwood identification align with its chemical compounds with φ-eudesmol, α-agarofuran, β-agarofuran and 10-epi-*φ*-eudesmol emerging as primary contributors to the high grade [22]. Extensive research supports the importance of these compound groups in providing Agarwood with a robust woody aroma [22].

In recent years, the prevailing approach adopted by most researchers involves the utilization of intelligent techniques based on the chemical compounds of Agarwood oil [4], [20], [24], [25]. This study proposes the utilization of an artificial neural network (ANN) with the Levenberg Marquardt (LM) algorithm as an intelligent grading method for categorizing Agarwood oil. The focus is on five grades of Agarwood oil including high, medium high, upper low, medium low and low qualities. The assessment of the ANN's performance entails the examination of parameters such as the mean square error (MSE), the number of epochs and the utilization of a confusion matrix.

2. MATERIALS AND METHODOLOGY

Figure 1 depicts the flowchart illustrating the process of classifying Agarwood oil quality utilizing the LM-ANN approach. The process of Agarwood oil quality classification started with data collection and pre-processed using boxplot analysis and stepwise regression which already explained in paper [26]. Data pre-processing method is important as it is to study the dataset before handling the dataset using intelligent model. The significant chemical compounds were found during this process as a marker to grade the oil based on their quality. Hence, development of ANN method to model the Agarwood oil grades were discussed in detail in this manuscript. The focus of this paper was implementing LM algorithm into ANN and also the ration of training, validation and testing dataset into 70:15:15. The output of accuracy and MSE were observed to conclude the effectiveness of LM-ANN technique in classified the Agarwood oil quality.

2.1. Data collection and pre-processing

A total of twenty-two raw Agarwood essential oil samples underwent gas chromatography-mass spectrometry (GC-MS) extraction analysis to extract the 103 identified chemical compounds. Subsequently, these 103 identified chemical compounds underwent a pre-processing technique to determine their significance, employing methods such as principal component analysis (PCA) and Pearson's correlation. Then, eleven significant chemical compounds from PCA analysis were used as inputs for boxplot and stepwise regression to identify the remarkable compounds that contribute into high grades. A detailed analysis of experimental procedures for boxplot and stepwise regression can refer to previous published papers as cited in [26], [27]. In

the initial stage, the input and output data are loaded. The input data comprises the significant chemical compounds of Agarwood oil identified through the pre-processing technique while the output data represents the grades of Agarwood oil: high, medium high, upper low, medium low and low. The dataset consists of 660 samples each of which contains eleven significant compounds.

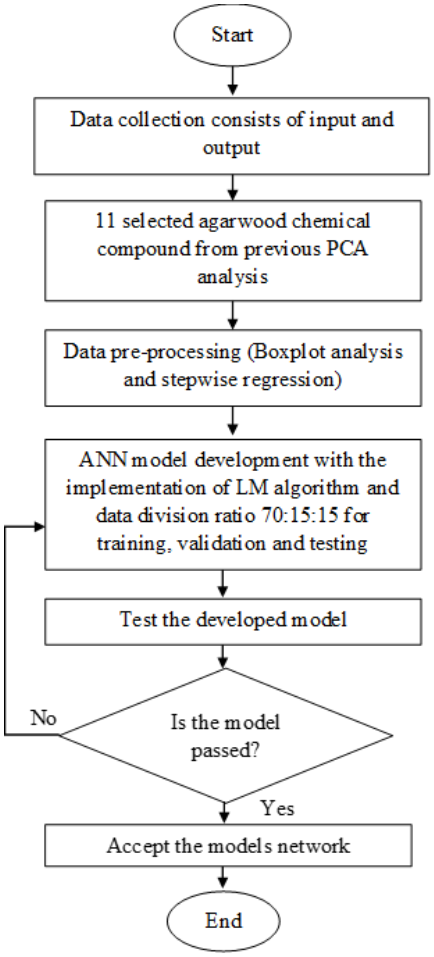


Figure 1. Flowchart of LM-ANN modelling

2.2. Data division for ANN modelling

Subsequently, the data undergoes sequential pre-processing, involving data normalization, randomization, and division. This step holds significant importance as it serves to mitigate the adverse effects of varying input ranges and to render the data suitable for network inputs and targets [28]. Following this, the data is divided into three distinct datasets, namely training, validation, and testing using the "dividerand" function in MATLAB. The distribution ratio among these datasets is 70% for training (462 samples), 15% for validation (99 samples) and 15% for testing (99 samples), respectively.

2.3. ANN model using LM algorithm

Moving on to the development of the ANN, this study employed a three-layer network configuration, encompassing input layers, hidden layers and output layers as shown in Figure 2. Regarding the hidden layers, the number of hidden neurons was subject to variation, ranging from just one to a maximum of ten neurons in this study. The model was trained utilizing the LM algorithm.

2.5. The measurement of performance

The evaluation of the ANN performance of classification model is conducted through the assessment of MSE, the number of epochs and a confusion matrix comprising accuracy, sensitivity, precision and specificity. The structure and table content of confusion matrix are illustrated as table of 5×5 which

indicate five grades (high, medium high, upper low, medium low and low) of Agarwood oil. The formula for accuracy, sensitivity, specificity and precision is expressed in (1) to (4) [29]:

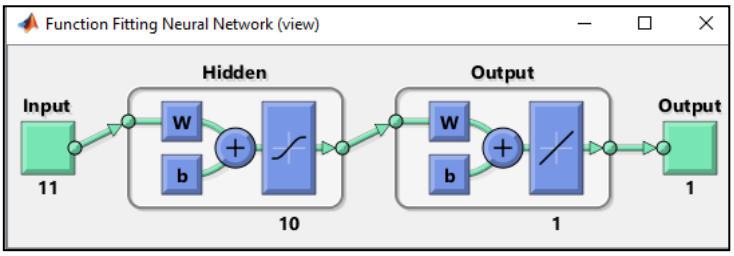


Figure 2. The layers of feed forward multi-layer perceptron LM-ANN configuration

$$Accuracy = \frac{tp+tn_t}{tp+tn_t+fp_t+fn_t} \times 100 \quad (1)$$

$$Sensitivity = \frac{tp}{tp+fn_t} \times 100 \quad (2)$$

$$Specificity = \frac{tn_t}{tn_t+fp_t} \times 100 \quad (3)$$

$$Precision = \frac{tp}{tp+fp_t} \times 100 \quad (4)$$

Note that tp is the number of correctly classified to low group. tn_t is the number of correctly classified to the not group examples. Symbol fp_t is the example wrongly classified to the low group. Symbol fn is the example wrongly classified to the not group examples.

3. RESULTS AND DISCUSSION

This section explained the findings of the research while also providing a comprehensive discussion. The results presented in figures, tables and also confusion matrix visualization for the reader to easily understand. The discussion was made in several sub-sections where sub section 3.1. explain on the confusion matrix and sub section 3.2. about MSE findings and number of epochs.

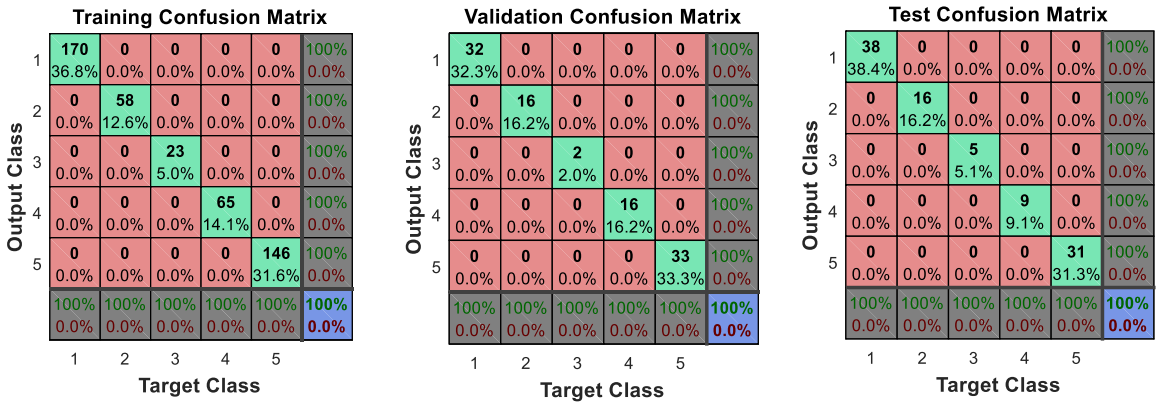
3.1. Confusion matrix

Table 1 displays the sensitivity, precision, specificity and accuracy performance during the training, validation and testing phases of the network, utilizing the LM algorithm. The training accuracy exhibits perfect 100% with one hidden neuron to ten hidden neurons. For the validation dataset, all hidden neurons achieved 100% accuracy without any exceptions. Subsequently, the testing accuracy also varies with values of 100%. Considering the overall accuracy results across training, validation and testing, it shows that evaluation for five grades of Agarwood oil achieve perfect performance in term of its confusion matrix. Theoretically in neural networks, minimizing the number of hidden neurons used for training can mitigate prolonged computational training times and the risk of overfitting [30], [31].

Table 1. Training, validation and testing accuracy of LM algorithm

Number of hidden neurons	Accuracy (%)			Sensitivity (%)	Precision (%)	Specificity (%)
	Training	Validation	Testing			
1	100.00	100.00	100.00	100.00	100.00	100.00
2	100.00	100.00	100.00	100.00	100.00	100.00
3	100.00	100.00	100.00	100.00	100.00	100.00
4	100.00	100.00	100.00	100.00	100.00	100.00
5	100.00	100.00	100.00	100.00	100.00	100.00
6	100.00	100.00	100.00	100.00	100.00	100.00
7	100.00	100.00	100.00	100.00	100.00	100.00
8	100.00	100.00	100.00	100.00	100.00	100.00
9	100.00	100.00	100.00	100.00	100.00	100.00
10	100.00	100.00	100.00	100.00	100.00	100.00

Figure 3(a) to (c) shows the best accuracy of training, validation and testing, respectively from the ten hidden neurons. The training, validation and testing accuracies achieved accurate classification of 100.00%. Based on the x-axis and y-axis of confusion matrix table, numbering label of 1, 2, 3, 4, 5 indicate high, medium high, upper low, medium low and low grade.



(a) (b) (c)

Figure 3. LM-ANN confusion matrix for (a) training, (b) validation, and (c) testing

3.2. MSE and epochs

Since the accuracy for all training, validation and testing dataset achieved 100%, the MSE values were evaluated to determine the best hidden neuron. Table 2 summarize the MSE values and the number of Epoch for the training of a neural network with ten hidden neurons employing the LM algorithm. It is worth noting that all MSE values for the ten hidden neurons fall within the category of small values as they are all less than 1.0. However, the table highlights that among the ten hidden neurons, three hidden neurons emerge as the optimal choice for classifying Agarwood oil with MSE value of 0.14338×10^{-08}, given their consistently strong performance at epoch 21. This is because hidden neuron 3 has the lowest MSE value compared to other neurons.

Table 2. Summarization of MSE values and number of epochs

Hidden Neurons	Percentage value	Epoch
1	0.01896	80
2	0.0018786	27
*3	0.14338×10^{-08}	21
4	3.0915×10^{-08}	11
5	0.49862×10^{-08}	12
6	2.6147×10^{-08}	12
7	0.42095×10^{-08}	11
8	0.25284×10^{-08}	13
9	1.07×10^{-08}	12
10	0.18084×10^{-08}	11

*Best hidden neuron in LM-ANN model

4. CONCLUSION

This research study effectively showcases the performance of the ANN. The LM-ANN algorithm has proven its ability to classify eleven chemical compounds, differentiating between high, medium high, upper low, medium low and low qualities based on default performance metrics including MSE, epochs and the confusion matrix using feed forward multi-layer perceptron technique. Among the configurations tested, the setup with three hidden neurons emerged as the top performer, demonstrating the highest accuracy during training, validation, and testing while achieving lower MSE values and fewer epochs. The percentage of precision, sensitivity and specificity for the whole LM-ANN model of five grades also develop 100% classification. The presence of intelligent modelling based on the abundance of chemical compounds contributes to the grading identification system for industry, ultimately influencing the Agarwood oil's market value and remarkable as reference in future study.

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BIOGRAPHIES OF AUTHORS

Siti Mariatul Hazwa Mohd Huzir was born in Malaysia who is currently pursue her studies as a postgraduate student majoring in electrical engineering at UiTM Johor Branch, Pasir Gudang Campus. She received her B. Eng (Hons) of Electronics Engineering from Universiti Teknologi MARA (UiTM) Shah Alam Malaysia. She can be contacted at email: mariatulhazwa97@gmail.com.

Saiful Nizam Tajuddin received his PhD from Universiti Malaysia Pahang (UMP). He is a professor and director of Bioaromatic Research Center of Excellence (BARCE) at Universiti Malaysia Pahang. He is a director and researcher at Synbion Sdn Bhd, Kuantan, Pahang, Malaysia. He has been a very active researcher and over the years had author and/or co-author many papers published in refereed journals and conferences. He can be contacted at email: saifulnizam@ump.edu.my.

Zakiah Mohd Yusoff is a senior lecturer who is currently working at UiTM Pasir Gudang. She received the B.Eng. in electrical engineering and PhD in electrical engineering from UiTM Shah Alam, in 2009 and 2014, respectively. In May 2014, she joined UiTM Pasir Gudang as a teaching staff. Her major interests include process control, system identification, and essential oil extraction system. She can be contacted at email: zakiah9018@uitm.edu.my.

Nurlaila Ismail received her PhD in electrical engineering from Universiti Teknologi MARA, Malaysia. She is currently a senior lecturer at School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Malaysia. Her research interests include advanced signal processing and artificial intelligence. She can be contacted at email: nurlaila0583@uitm.edu.my.

Ali Abd Almisreb is currently an associate professor at the Faculty of Computer Sciences and Engineering, Director of Graduate Council and editor in chief at International University of Sarajevo. He received a master's degree in computer science and doctorate doctor's degree in electrical engineering/computer engineering from Universiti Teknologi MARA, Malaysia. His major interests include deep learning, machine learning, computer vision voice recognition and quantum computing. He can be contacted at email: alimes96@yahoo.com.

Mohd Nasir Taib received his PhD from UMIST, UK. He is a senior professor at Universiti Teknologi MARA (UiTM). He heads the Advanced Signal Processing Research Group at the School of Electrical Engineering, College of Engineering, UiTM. He has been a very active researcher and over the years had author and/or co-author many papers published in refereed journals and conferences. He can be contacted at email: dr.nasir@uitm.edu.my.