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# Optimizing nonlinear autoregressive with exogenous inputs network architecture for agarwood oil quality assessment

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**ABSTRACT**

Agarwood oil is highly valued in perfumes, incense, and traditional medicine. However, the lack of standardized grading methods poses challenges for consistent quality assessment. This study proposes a data-driven classification approach using the nonlinear autoregressive with exogenous inputs (NARX) model, implemented in MATLAB R2020a with the Levenberg-Marquardt (LM) algorithm. The dataset, sourced from the Universiti Malaysia Pahang Al-Sultan Abdullah under the Bio Aromatic Research Centre of Excellence (BARCE) and Forest Research Institute Malaysia (FRIM), comprises chemical compound data used for model training and validation. To optimize model performance, the number of hidden neurons is systematically adjusted. Model evaluation uses performance metrics such as mean squared error (MSE), root mean squared error (RMSE), mean absolute error (MAE), coefficient of determination ($R^2$), epochs, accuracy, and model validation. Results show that the NARX model effectively classifies agarwood oil into four quality grades which is high, medium-high, medium-low, and low. The best performance is achieved with three hidden neurons, offering a balance between accuracy and computational efficiency. This work demonstrates the potential of automated, standardized agarwood oil quality grading. Future research should explore alternative training algorithms and larger datasets to further enhance model robustness and generalizability.



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## 1. INTRODUCTION

Agarwood, scientifically known as *Aquilaria malaccensis* Lam, belongs to the Thymelaeaceae family and is renowned for its highly valuable, fragrant resin. This resinous wood, formed in the roots, stems, and branches of *Aquilaria* and *Gyrinops* trees, widely utilized in traditional medicine and religious practices across Southeast Asia and Northeast India. Over the years, these regions have become the primary producers of agarwood due to its increasing global demand [1]–[3]. Countries such as China, India, Vietnam, Indonesia, Malaysia, and Thailand recognize agarwood for its distinctive aroma, leading to its high market value. In the international trade, premium-grade agarwood is considered more valuable than gold. However, the immense demand has resulted in severe depletion of natural *Aquilaria* forests, as nearly all countries involved in agarwood harvesting have faced deforestation due to its high economic worth [2], [4], [5]. A unique characteristic of *Aquilaria* trees is that a healthy tree does not naturally produce agarwood. Only approximately 10% of these trees develop agarwood within the heartwood, primarily in response to external stressors such as lightning strikes, insect attacks, or bacterial and fungal infections. Traditional agarwood oil grading relies on sensory evaluation based on color, viscosity, odor intensity, and persistence [6]–[8]. However, this method is subjective, costly, and inconsistent, as it depends on the physical and emotional condition of evaluator, as well as external environmental factors. The limitations have demonstrated a high demand for an efficient and standardized method in grading agarwood oil. This study aims to address that gap by utilizing advancements in machine learning to develop a model for agarwood oil quality assessment [9]–[11].

Recent advancements in agarwood grading have shown that using chemical composition provides a more accurate and reliable solution for determining quality. Collaborations with industrial sectors have identified the key marker compounds that influence the scent of agarwood oil, including φ-eudesmol, α-agarofuran, β-agarofuran, and 10-epi-φ-eudesmol [12]–[14]. Regardless, there is no universally accepted classification system for grading agarwood oil yet to appear. Multiple countries still continue with their own grading method that are based on client preferences and perceptions. This indicates how demanding is the agarwood market for global standard in grading process, considering the established exploration of chemical profiling in agarwood [15]–[17]. The agarwood industry holds major economic value, with prices hitting the ranges from RM 19,999 to RM 29,999 per kilogram depends on the quality of the oil. From 2019 to 2025, agarwood oil has grown at a rate of 6.46% and is expected to reach US$201.03 million in global market. Malaysia ranks among the top exporters of agarwood for global distribution [18], [19]. In response to this, many collaborative efforts have emerged, including the partnership between Universiti Malaysia Pahang Al-Sultan Abdullah, Universiti Teknologi MARA (UiTM), and industry players, working to determine the quality of agarwood oil by identifying key chemical components [20]–[22].

Neural networks have been used in classification tasks and are known for their ability to handle complex datasets. In particular, the nonlinear autoregressive with exogenous (NARX) model effectively captures dynamic relationships in sequential data, making it useful for agarwood oil grading [23]–[25]. Quality evaluation based on chromatographic techniques, chemical composition analysis, and aromatic assessment such as gas chromatography-flame ionization detection (GC-FID) and gas chromatography-mass spectrometry (GC-MS) known for high precision. However, these methods require high costs, specialized expertise to operate the equipment, and still involve subjective sensory evaluation [26], [27]. Machine learning offers scalable and automated classification methods. Therefore, this study leverages the capabilities of machine learning by applying the NARX model using the Levenberg-Marquardt (LM) algorithm to assign four distinct grades of agarwood oil: high, medium-high, medium-low, and low. Although various studies have explored machine learning for oil classification, research on the application of NARX for agarwood oil grading is still limited. Moreover, none of them emphasize the impact of varying the number of hidden neurons on classification accuracy. By systematically modifying the hidden neurons and evaluating performance, this study offers a deeper understanding of optimizing NARX for classification tasks [28], [29]. Deep learning models such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs) have improved oil classification accuracy, particularly in feature extraction [30], [31]. Hence, this study aligns with the ongoing development of machine learning by adopting NARX-based classification techniques and focusing on hidden neuron optimization. MATLAB R2020a software is used in this grading process to support the implementation, simulation, and validation of the agarwood oil model. By incorporating all this information, this study contributes to the development of a standardized intelligent grading system for high-value oils like agarwood oil.

## 2. METHOD

This section is divided into three main parts: subsection 2.1 is NARX model development with LM algorithm, subsection 2.2 is experimental set-up, and subsection 2.3 is performance evaluation. The first part walkthrough the development of the NARX model, highlight on how the LM algorithm is applied with an open-loop structure and selected network configurations. The second part discusses the experimental set-up, covering dataset preprocessing, feature selection, and data partitioning. The final part covers performance evaluation, explaining the statistical and validation approaches used to measure model accuracy and robustness.

### 2.1. NARX model development with LM algorithm

The agarwood oil samples used in this study were obtained through a collaboration between the Universiti Malaysia Pahang Al-Sultan Abdullah under the Bio Aromatic Research Centre of Excellence

(BARCE) and Forest Research Institute Malaysia (FRIM). The samples from the datasets used in this study had been analyzed by previous researchers through statistical and pattern analysis methods [32]–[34]. In this study, a NARX model implemented the LM algorithm in an open-loop structure. In this arrangement, predictions are driven by real outputs and input variables, with no feedback from the previous predictions. Figure 1 shows a three-layer network architecture consists of input, hidden, and output layers to allow complex relationships within the data to be captured [35].

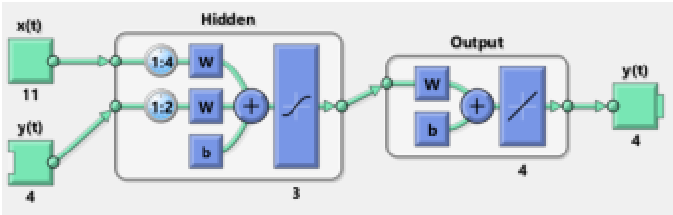


Figure 1. Feedforward LM-NARX network configuration

The NARX model development follows a structured workflow starting with sample collection and data preparation; the dataset consists of 660 samples containing eleven key chemical compounds identified via statistical and pattern analysis. Feature selection and preprocessing; key chemical compounds were selected based on their relevance to agarwood oil quality. Preprocessing steps includes normalization, randomization, and dataset partitioning (70:15:15) were applied to enhance model generalization [36]. Next on the network structure selection; a three-layer feedforward architecture was chosen, comprising input, a hidden (1-10), and output. The NARX in (1) defines the dependency on previous inputs and outputs, with input delay (Dx) and output delay (Dy) capturing temporal dependencies [37]:

$$y(t) = f(x(t-1), x(t-2), \dots, x(t-D_x), y(t-1), y(t-2), \dots, y(t-D_y)) \quad (1)$$

Training phase; the model was trained using the LM algorithm, selected for its fast convergence and stability in handling nonlinear regression problems. After that, the validation and performance evaluation where the model was validated using multiple performance metrics (mean squared error (MSE), root mean squared error (RMSE), mean absolute error (MAE), coefficient of determination ($R^2$), epochs, and accuracy). The model was also assessed through performance plots, and regression plots.

Optimization and model tuning; if performance thresholds were not met, iterative adjustments such as modifying the number of hidden neurons or tuning training parameters were implemented to improve predictive accuracy. To improve the ability of model to learn complex patterns within the dataset, the input delay is adjusted from 1:2 to 1:4. This enhancement allows the NARX model to capture longer temporal dependencies, providing a more comprehensive understanding of past inputs [38], [39]. By incorporating a broader historical context, the model achieves better generalization, reduces the risk of overfitting, and ultimately enhances predictive accuracy.

### 2.2. Experimental set-up

As illustrated in Figure 2, the dataset consists of 660 samples, each containing eleven key chemical compounds: γ-eudesmol, β-dihydroagarofuran, allo-aromadendrene epoxide, α-agarofuran, ar-curcumene, valerianol, α-guaiene, 10-epi-γ-eudesmol, dihydrocollumellarin, γ-cadinene, β-agarofuran. All chemical compounds exhibit varying abundance (%) across samples, providing variability for analyzing the relationship between chemical composition and agarwood oil quality. Prior to training, the dataset undergoes preprocessing, including normalization, randomization, and partitioning into training, validation, and testing subsets. These steps help to regulate the range of input, improve data quality, and reduce noises within the dataset.

The dataset is divided using divider and function of MATLAB as follows: 70% of training (462 samples), 15% of validation (99 samples), and 15% of testing (99 samples). This split helps to balance training process and ensure model to perform well on unseen data. In assessing the performance, different number of neurons utilized in hidden layer configurations (1 to 10 neurons). MATLAB R2020a is selected for implementation due to its specialized neural network toolbox, which provides built-in capabilities for dynamic system modeling and time-series forecasting, making it a suitable choice over alternatives such as TensorFlow and PyTorch [40].

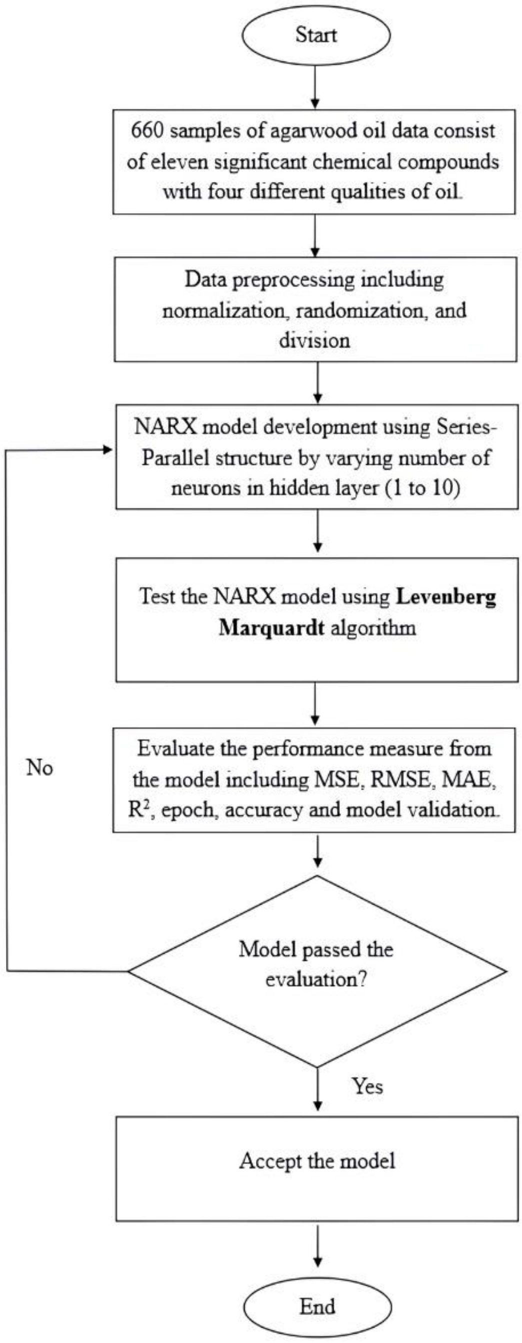


Figure 2. Detailed experimental setup for the LM-NARX model, illustrating dataset preprocessing, development, testing, and evaluating workflow

## 2.3. Performance evaluation

The effectiveness of the NARX model was assessed using multiple performance metrics, including MSE, RMSE, MAE, $R^2$, and accuracy. These performance metrics were chosen for their significance in evaluating both regression and classification tasks. MSE measures the average squared error but is sensitive to large deviations. RMSE, expressed in the same unit as the target variable, improves interpretability but does not distinguish over- and under-predictions. MSE and RMSE quantify prediction errors, with RMSE placing greater emphasis on larger discrepancies. MAE, which calculates absolute errors, is less sensitive to outliers but does not heavily penalize large deviations. $R^2$ assesses model fit, with values near 1 indicating strong correlation, though high $R^2$ does not guarantee generalization. Accuracy measures correct classifications but may overlook class imbalances. Another key factor is the number of epochs, which represents the total iterations the model undergoes during training. Selecting an optimal epoch count is critical whereas insufficient epochs may lead to underfitting, whereas excessive training can cause overfitting [41].

To assess the reliability of NARX model, validation techniques such as performance and regression plots were utilized. The performance plot illustrates training, validation, and test errors across epochs, provide information on the learning behavior of model and generalization capabilities. Ideally, a well-trained model displays steadily decreasing errors that later stabilize. In contrast, a growing gap between training and validation errors may indicate overfitting [42]. The regression plot highlights the predictions of model with actual values; when y=x, whereas data points lie close to the line indicating strong accuracy of the model. While presences of deviations and outliers may signal that the patterns of the model have not fully captured.

## 3. RESULTS AND DISCUSSION

This section discusses the outcomes from the study with figures and tables. The section is divided into two subsections. Section 3.1 focuses on NARX model performance using evaluation metrics such as MSE, RMSE, MAE, $R^2$, epochs, and accuracy. Section 3.2 addresses the model validation, interpreting the plots from the performance and regression plots. This ensures the reliability, helps detect potential issues such as overfitting or underfitting, and provides information for generalization ability.

### 3.1. MSE, RMSE, MAE, $R^2$, epochs and accuracy

For the evaluation of the LM-based NARX model, the number of neurons in hidden layer was varied from 1 until 10 as shown in Table 1 that summarizes the results. The MSE values ranged from $10^{-2}$ to $10^{-3}$, indicating precise predictions and consistent data quality. Most configurations achieved classification accuracy above 80%, while $R^2$ values remained at 0.99, reflecting a strong correlation between predicted outputs and actual grades. The most optimal configuration across the performance measure is three neurons, achieving an MSE of $2.158\times10^{-3}$, RMSE of 0.046, MAE of 0.019, $R^2$ of 0.99, 7 epochs and 99.54% accuracy. This approach effectively classifies agarwood oil into four grades while maintaining model simplicity. Beyond three neurons, additional complexity provided minimal improvement. These results confirm the LM-NARX efficiency and robustness of model across all configurations.

Table 1. Performance metrics of LM-NARX model with varying hidden neurons (1-10)

| Hidden neurons | MSE | RMSE | MAE | $R^2$ | Epochs | Accuracy (%) |
|---|---|---|---|---|---|---|
| 1 | $5.882\times10^{-2}$ | 0.243 | 0.151 | 0.69 | 17 | 81.71 |
| 2 | $1.543\times10^{-2}$ | 0.124 | 0.048 | 0.92 | 12 | 95.27 |
| *3 | $2.158\times10^{-3}$ | 0.046 | 0.019 | 0.99 | 7 | 99.54 |
| 4 | $1.991\times10^{-3}$ | 0.045 | 0.015 | 0.99 | 9 | 99.54 |
| 5 | $1.971\times10^{-3}$ | 0.044 | 0.016 | 0.99 | 8 | 99.54 |
| 6 | $1.595\times10^{-3}$ | 0.040 | 0.013 | 0.99 | 8 | 99.54 |
| 7 | $1.528\times10^{-3}$ | 0.039 | 0.012 | 0.99 | 7 | 99.85 |
| 8 | $1.656\times10^{-3}$ | 0.040 | 0.013 | 0.99 | 10 | 99.70 |
| 9 | $1.522\times10^{-3}$ | 0.039 | 0.016 | 0.99 | 9 | 99.70 |
| 10 | $1.875\times10^{-3}$ | 0.043 | 0.010 | 0.99 | 13 | 99.70 |

*Best hidden neuron in LM-NARX model

### 3.2. NARX model validation

Subsection 3.1 established that three hidden neurons yielded the best performance, but this section evaluates the NARX model with three hidden neurons to further analyze its behavior. The performance plot in Figure 3 illustrates the learning process, tracking training, validation, and test errors of model over epochs. Initially, all errors decline together, reflecting effective pattern learning. They eventually stabilize, indicating optimal training with no further significant improvement. A small gap between training and validation/test errors suggests good generalization, while a large gap would indicate overfitting. The parallel trend between validation and test errors confirms model consistency. Since all curves converge smoothly without divergence, the model demonstrates effective regularization and avoids overfitting.

The regression plot in Figure 4 evaluates the correlation between predicted and actual outputs. The regression lines for training, validation, and test sets closely align with the ideal y=x line, confirming a strong predictive relationship. Low residual values in the plots indicate high accuracy of the model, thus by having these fourteen data points of outliers most likely result from the variability within the dataset and did not significantly affect the overall model performance. The findings assures that the proposed NARX model is capable in producing accurate and consistent classification results with only minor variances.

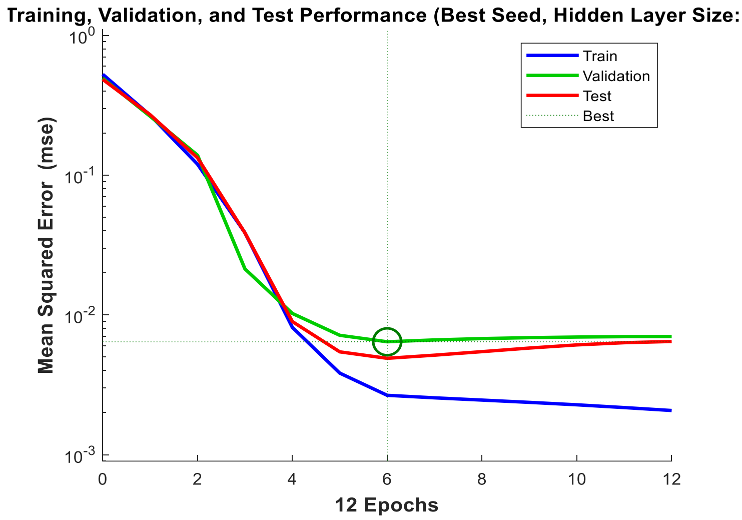


Figure 3. Training, validation, and test performance of the NARX model with three hidden layers, showing error convergence and stability across epochs

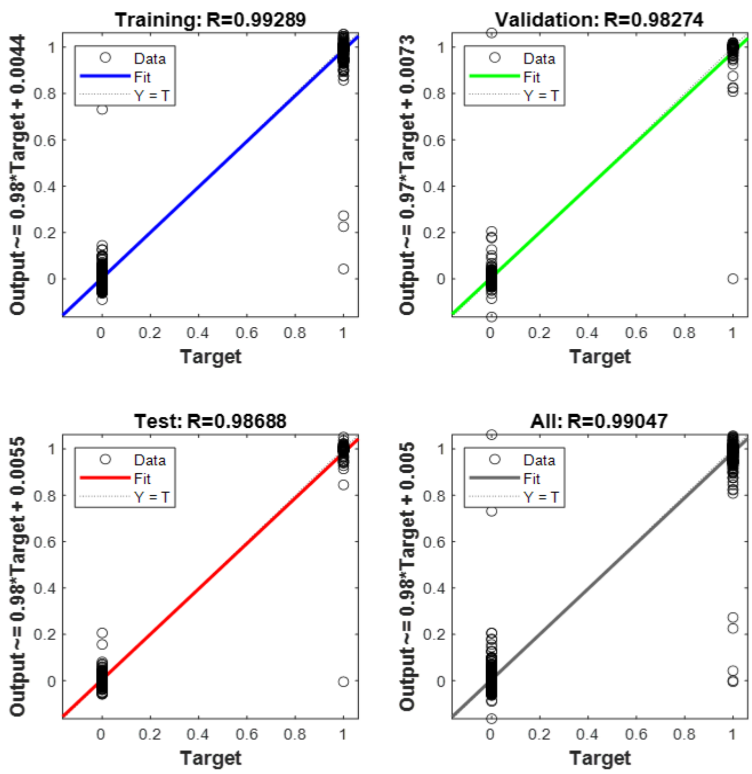


Figure 4. Regression plot of NARX model on three hidden neurons with small residuals and outliers

## 4. CONCLUSION

This study optimizes the application of the NARX neural network in classifying agarwood oil quality using the LM algorithm. By modifying the hidden neuron, model performance was measured using metrics, including MSE, RMSE, MAE, $R^2$, number of epochs, and accuracy. The configuration with three hidden neurons come out as the most effective, strikes a balance between accuracy and efficiency. The results showed minimal prediction error, and strong convergence behavior. The regression analysis proved good balance of predicted and actual values with distributed residuals. These findings suggest that the LM-NARX model is suitable for classifying agarwood oil. However, there is limitations to highlight in this study.

While the dataset of 660 samples provides a robust result, expanding the datasets could improve generalizability. Further improvements could also be made by fine-tuning hyperparameters, such as the learning rate. Exploring other models like LSTM may offer advantages in handling complex data structures. For real-world use, the model would need to be validated against standardized industry datasets to confirm its scalability and resilience. Future work may involve experimenting with alternative training techniques to further enhance the adaptability. Overall, this study underscores the value of machine learning in product quality evaluation and its potential to improve grading consistency and commercial value.

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## AUTHOR CONTRIBUTIONS STATEMENT

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C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

## CONFLICT OF INTEREST STATEMENT

Authors state no conflict of interest.

## DATA AVAILABILITY

Data availability is not applicable to this paper as no new data were created or analyzed in this study.

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