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A Novel Quality Grading Determination using Boxplot Analysis and Stepwise Regression for Agarwood Oil Significant Compounds

Siti Mariatul Hazwa Mohd Huzir¹, Aqib Fawwaz Mohd Amidon², Zakiah Mohd Yusoff³, Nurlaila Ismail² and Mohd Nasir Taib³

¹School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Cawangan Johor, Kampus Pasir Gudang, 81750 Masai Johor Malaysia, ²School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Shah Alam, Selangor, Malaysia, ³Malaysia Institute of Transport (MITRANS), Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

zakiah9018@uitm.edu.my

Abstract— This product presents the intelligent technique on the oil chemical properties to get accurate results. Agarwood essential oil is frequently connected with wealth that has been great demand all over the global market due to its aroma and various usages. Unfortunately, there is still no standard method for classifying the quality of Agarwood oil since mostly graded by using the human sensory panel. Therefore, the performance of Boxplot analysis and Stepwise Regression model is trained using MATLAB version R2015a. This research project involved the proposed statistical analysis which is Boxplot analysis and Stepwise Regression. In this work, there are eleven significant compounds of Agarwood Oil that consists of 660 samples from low, medium low, medium high and high. The experiment involved all the independent variables have been selected by observing the p-value of each variable where all of them have p-value less than 5% significance level. The parameter concerned is on the value of correlation coefficient, R and the mean squared error (MSE). Based on the results of the research project, successfully show that 4 out of 11 compounds show the best performance towards regression value and MSE which are γ -Eudesmol, 10-epi- γ -eudesmol, β -agarofuran and dihydrocollumellarin. The finding in this proposal will be significant and can contribute to the agarwood oil industry as well as its quality grading classification system.

Keywords— *boxplot analysis, stepwise regression, Agarwood oil, quality grading*

I. INTRODUCTION

Based on the Medical News Today, Essential Oil therapy is also one of the alternative medicine for psychological treatment. It is commonly used in the practice of aromatherapy [1]. Recently, Agarwood oil valued in many cultures where it is being used to treat various illnesses, perfumery and incense for religious and spiritual ceremonies purposes [2]. Currently, the quality of Agarwood oil had been measured and graded manually by using sensory evaluation based on its physical properties. Based on human perception and experience, Agarwood oil with the greatest grade has a lot of resin, dark oil colour, strong odour and long-lasting aroma [2], [3]. However, the sensory evaluation method is somehow inaccurate since different people may come with different perceptions and decisions about the technique. There is no guarantee that grading using human sensory evaluation can secure the purity or quality of the Agarwood oil. Human trained grader technique has a significant disadvantage in terms of objectivity and repeatability due to the continuous process when deal with a bulk of samples at once, contribute to the high labor-intensive process and time-consuming [4], [5]. Thus, several methods have been proposed and applied to determine the Agarwood oil quality grading by using intelligent techniques [4]–[9]. Chemical profiles can be used to classify essential oils into their respective classes (high, medium high, medium low or low grade). This paper presented the Boxplot analysis and Stepwise Regression technique in analyse the Agarwood oil chemical profiles based on its abundance from four different qualities. The parameter concerned is the value of correlation coefficient, R and the mean squared error (MSE). The best fit line from the chemical compounds that are significant to the model will be a good marker to be used as future classifier for Agarwood essential oil to be grading into high, medium high, medium low and low quality.

II. THEORETICAL WORK

A. Boxplot Analysis

Several researchers mentioned that Boxplot Analysis is the most common technique for early step of data pre-processing and summarizing data based on the minimum and maximum range values, the upper quartile (Q3), the lower quartile (Q1) and the median (Q2) [10]–[12]. Here, Boxplot method is one of a technique that can be implemented for this study to compare the chemical compound abundance (%) for different qualities. The box plot has become the industry standard for displaying the minimum and maximum range values, upper and lower quartiles and the median [13]. By summarising the distribution with a minimal set of parameters, the median and quartiles are used to extract the important characteristics of a dataset. Tables, charts, and graphical plots can be used to show data summaries from multiple datasets [14]. According to several academics, the boxplot is the most efficient and effective visualisation method [11], [15], [16]. The interior of this box between upper and lower quartiles where indicates the inner quartile range, consists 50% of the distribution.

In addition, the round bullet (0') in the box plot reveals that the value of the voltage reading is a bit far away but still within the range and acceptable. The result was accepted since the median is around 50% as in the group. However, if there exist '*' in the box plot, it is indicated that there are extremely outside the range. Hence a data cleaning or removing the outliers is needed [13], [17].

B. Stepwise Regression

In multivariable regression analysis, there is a method of selecting the independent variables that can explain the dependent variable very efficiently [18]. The method is known as stepwise regression. The main objective of stepwise regression is to include and exclude the independent variables from the model [19], [20]. Stepwise regression performs two processes which are forward selection and backward elimination [21], [22]. F-test and P-value is common to use in stepwise regression and they are tested using α value [22], [23]. Standard significance of α value in statistics is 0.05 [24], [25]. The advantages of stepwise regression can save time and cost due to only significant parameter is selected [22]. The statistical analysis of Agarwood oil significant compounds is using linear regression [26] by considering the value of correlation coefficient, R and the mean squares error (MSE). Linear regression involves the relationship between single dependent variable and single independent variable [26]. Meanwhile, the significant mechanical properties in [22] used stepwise regression to identify the statistical model with high performance. Instead using linear regression, stepwise regression is a method of selecting multiple independent variables which performs forward selection and backward elimination.

III. METHODOLOGY

A. Data Preparation

The Agarwood oil data consist of 660 samples between low, medium low, medium high and high qualities obtained from previous researcher [27]. There are eleven compounds which are α -guaiane, β -agarofuran, ar-curcumene, β -dihydroagarofuran, γ -cadimene, α -agarofuran, 10-epi- γ -eudesmol, γ -eudesmol, alloaromadendrene epoxide, valerianol and dihydrocollumellarin. Details on this data collection can be found in [8]. The essential oils were extracted from the samples using distillation. Gas Chromatography-mass Spectrometry with a flame ionization detector and a fused silica capillary column was employed for the GC-MS analysis. The identification of chemical components was obtained. All simulations were carried out with the MATLAB software version R2015a. This research involved 660 oil samples of data from four different qualities as tabulated in Table 1.

Table 1. Number of samples based on quality classes

Quality Grading Classes	Low	Medium Low	Medium High	High	Total
Samples collected	210	90	30	330	660

B. Pre-processing: Boxplot method and Stepwise Regression

The boxplot is start creating by sorted the Agarwood oil data into four groups. Each quality's median abundance in percentage has been compared to high quality. The oil data was sorted into two columns:

- x-axis: eleven significant compounds of Agarwood oil as independent variables.
- y-axis: abundances of significant compound (%) as a dependent variable.

The boxplot's performance was then evaluated. In Stepwise Regression method, fewer the design variables that significant to model are needed. It allows detail and systematic analysis of the model. Important parameter likes R^2 , R^2_{adj} , p-value and F-statistic where considered with a strengthened statistical model.

IV. RESULTS AND FINDINGS

In this work, there are eleven significant compounds of Agarwood Oil that consists of 660 samples from high, medium high, medium low and low. The top four candidates were identified based on Stepwise Regression which are γ -Eudesmol, 10-epi- γ -eudesmol, β -agarofuran and dihydrocollumellarin. Summary output of Boxplot analysis is tabulated in Table 2 and Stepwise Regression is tabulated in Table 3.

Table 2. Compilation from boxplot analysis on type of chemical compound for high quality of agarwood oil

Chemical Compounds	High Quality			
	Range	Lower Quartile	Median	Upper Quartile
α -guaiene	0.0100 - 0.9900	0.0100	0.2581	0.4804
β -agarofuran	0.2800 - 0.9250	0.4071	0.5341	0.7592
ar-curcumene	0.0100 - 0.9900	0.0100	0.4961	0.6483
β -dihydro agarofuran	0.0100 - 0.9900	0.0100	0.3256	0.5915
γ -cadinene	0.0100 - 0.4804	0.0100	0.0100	0.0100
α -agarofuran	0.5198 - 0.9900	0.6129	0.6788	0.8410
10- ϵ - γ -eudesmol	0.5269 - 0.9900	0.6857	0.7581	0.8102
γ -eudesmol	0.0100 - 0.9900	0.3117	0.6359	0.7755
allo aromadendrene epoxide	0.0100 - 0.9900	0.0100	0.0100	0.6857
valerianol	0.0100 - 0.9668	0.0100	0.3453	0.6533
dihydrocollumellarin	0.0100 - 0.9250	0.4324	0.6295	0.7631

Based on the highlighted on table 2 shown that high quality of agarwood oils have 9 out of 11 chemical compounds with all the percentage of quartiles compared to other qualities. Chemical compound 10- ϵ - γ -eudesmol and γ -eudesmol are the only chemical compounds that have all lower quartile, median and upper quartile percentage for all the quality of agarwood oil. Based on the stepwise regression results, successfully show that 4 out of 11 compounds show the best performance towards regression value and MSE.

Table 3. Summary output of Stepwise Regression

Root mean squared error (RMSE)	R ²	R ² _{Adj}	P-value
0.756	0.6710	0.755	3.27×10^{-199}

V. CONCLUSIONS

Boxplot Analysis and Stepwise Regression method successfully predict the relationship between actual and target output value of Agarwood oil compounds. The findings successfully show that the agarwood oil with high quality give an output of quartile percentage 9 out of 11 compounds compared to medium high, medium low and low qualities. Then after proceed for stepwise regression method, it found that 4 out of 11 compounds which are γ -Eudesmol, 10- ϵ - γ -eudesmol, β -agarofuran and dihydrocollumellarin had the best performance towards important regression parameters. This technique will give benefits to the Agarwood oil industry and also act as markers for the further grading classification system.

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