Boxplot analysis of 4 grade agarwood essential oil for various grades

Anis Hazirah ‘Izzati H. Al-Hadi¹, Aqib Fawwaz Mohd Amidon¹, Siti Mariatul Hazwa Mohd Huzir², Nurlaila Ismail³, Zakiah Mohd Yusoff², Saiful Nizam Tajuddin¹, Mohd Nasir Taib¹⁴

¹School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Selangor, Malaysia
²School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Johor, Malaysia
³BioAromatic Research Centre of Excellence (BARCE), Universiti Malaysia Pahang (UMP), Pahang, Malaysia
⁴Malaysia Institute of Transport (MITRANS), Universiti Teknologi MARA, Selangor, Malaysia

Abstract

Agarwood essential oil is used in most perfumery ingredients, as an incense and in traditional medical preparations. Agarwood essential oil, called "Black Gold," is extremely valued to the global community due to its numerous benefits. As of now, there is still no standard technique of grading different grades of agarwood essential oil. The current grading technique is inefficient since the agarwood essential oil is graded by using human sensory panel. Different people might have different perspective on grading the agarwood essential oil hence, the technique is not practical to adapt it globally. Due to the current technology, numerous intelligent techniques for verifying the grades of agarwood essential oil have been proposed and implemented. The study has conducted a statistical analysis on 4 grade agarwood essential oil using boxplot. Boxplot analysis summarizes the abundances for each chemical compounds from four different grades of agarwood essential oil with a high grade as a reference. This study shows the analysis of boxplot investigated 10-epi-δ-eudesmol, α-agarofuran, β-agarofuran, δ-eudesmol and dihydrocollumellarin as most important chemical compounds in high grade of agarwood essential oil. The chemical compounds that have been identified in high grade of agarwood essential oil can be a reference for future research studies.

Keywords:
Agarwood essential oil
Boxplot analysis
Chemical compounds
Grade classification
Grading

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1. INTRODUCTION

Agarwood essential oil is famous among producers and merchants for its aroma as a base of perfumes and for medicinal purposes [1]-[14]. Malaysia is one of agarwood essential oil’s producer. Malaysia’s producer extracted agarwood essential oil from wild trees found in the jungles of Terengganu, Perak, Pahang, and Kelantan [14]. The grading of agarwood essential oil is based on its aroma intensity and duration, resin content, geographical origin, and oil purity of its numerous compositions [1]-[18]. At presently, the purity of agarwood essential oil is determined by a trained human sensory experienced with a range of oil compositions. The results of the technique vary depending on whether the testers have a great sense for determining the grades of oil. Grading agarwood essential oil based on human sensory panel does not guarantee their purity or quality. Due to its reliance on the human nose, which cannot tolerate a high quantity of samples due to rapid fatigue, zero consistency and time-consuming process, this technique is projected to be unreliable [14], [15].
Various intelligent techniques for verifying the grades of agarwood essential oil have been proposed and implemented [1], [6], [14], [15], [18]. There is already a platform where agarwood essential oil grades may be determined entirely on the grounds of their chemical compounds, allowing essential oils to be classed according to their various classes (low, medium low, medium high and high grade) and accurate results can be measured using statistical analysis.

This study is to apply the Boxplot Analysis technique in analysing the 4-grade agarwood essential oil chemical compounds according to its abundances from four different grades. 4-grade agarwood essential oil has 660 samples from low, medium low, medium high and high grade. The samples data also consists of eleven chemical compounds. Some researchers have stated that Boxplot Analysis is a standard technique implemented during the early stage of data pre-processing. The data will be summarized according to its minimum and maximum range values, the upper and lower quartiles, and the median [19]-[31]. Hence, this study has implemented boxplot analysis to analyse the difference in chemical compounds abundances (%) for four different grades of 4-grade agarwood essential oil. This study was conducted using MATLAB software version R2020a.

2. THEORETICAL WORK

Boxplot is one of the techniques used for exploratory data analysis. It is a statistical technique for discovering new patterns of data [20]-[25]. Boxplot uses 5-point summary as its standard technique which includes the minimum and maximum values of range, the upper and lower quartiles and the median as shown in Figure 1 [20], [22], [23], [25]-[28]. Each collection of values illustrates the distribution of a dataset quickly. The purpose of median is to identify the data's midpoint, and median typically has two conditions: either half of the values are larger or equal to that value, or half are less. The interquartile range at the central box reflects the 50% scores for the group [20], [23], [25], [27], [29]. When the median is not centred in the box, it demonstrates the sample skewness. Each sample has its unique skewness, which indicates the differences between samples [22]. Interquartile act as a guide for ranges of lower to upper quartile. The third component is lower and upper quartile which is 25% and the lastly is whisker which indicates the scores outside the central 50% [20], [23], [25], [29].

![Figure 1. Boxplot structure](image)

3. METHOD

3.1. Data preparation

The data classification of 660 samples of agarwood essential oil consists of four different grades (low, medium low, medium high and high) acquired from [1], [14] as shown in Table 1. The eleven chemical compounds are known as 10-epi-γ-eudesmol, α-agarofuran, β-agarofuran, Y-eudesmol, dihydrocollumellarin, valerianol, ar-curcumene, β-dihydro agarofuran, α-guaiene, alloaromadendrene epoxide, and Y-cadinene. Information on the data collection can be read in [15]. The samples’ chemical compounds are extracted by gas chromatography-mass spectrometry (GC-MS) employing standard operation procedure (SOP) employed by bio aromatic research centre of excellence (BARCE). The statistical work was carried out using MATLAB software version R2020a.
3.2. Data pre-processing: the boxplot analysis

The agarwood essential oil was divided into four grades using a boxplot. The median abundance (%) of each grade has been compared to high grade. The agarwood essential oil’s data was divided into two axes.

- x-axis: eleven chemical compounds of agarwood essential oil (independent variables).
- y-axis: abundances of chemical compounds (%) (dependent variables).

After that, the performance of boxplot analysis was evaluated.

4. RESULTS AND DISCUSSION

In this section, it is explained the results of the boxplot analysis of eleven chemical compounds of agarwood essential oil in four different grades from 660 samples that has been extracted using GC-MS. The statistical work has been done using MATLAB software version R2020a and the data was set up in two axes. At x-axis, eleven chemical compounds of agarwood essential oil which are 10-epi-γ-eudesmol, α-agarofuran, β-agarofuran, Y-eudesmol, dihydrocollumellarin, valerianol, ar-curcumene, β-dihydroagarofuran, α-guaiene, alloaromadendrene epoxide, and Y-cadinene while at y-axis, the abundances of chemical compounds (%) as shown in Figure 2-5. From the figures, the outliers of eleven chemical compounds are shown to be different in range values.

4.1. Boxplot analysis

The boxplot has been generated with high grade samples from 4 grade (Figure 2) only to see which chemical compounds are the most important to consider the grade of agarwood essential oil is high grade quality to be a reference to grade agarwood essential oil for 5 grade and 6 grade. As shown in the Figure 2, there are 5 chemical compounds (10-epi-δ-eudesmol, α-agarofuran, β-agarofuran, δ-eudesmol and dihydrocollumellarin) considered to be the most important chemical compounds due to the median value is higher than 0.50. The highest median value is 10-epi-δ-eudesmol with the range of 0.53-0.99. For α-agarofuran, the range is 0.52-0.99. For β-agarofuran, the range is 0.28-0.93 For δ-eudesmol, the range is 0.01-0.99. For dihydrocollumellarin, the range is 0.01-0.93.

Boxplot analysis of medium high-grade samples been constructed as shown in Figure 3. β-agarofuran has the highest median value compared to the other most important chemical compounds that have been taken as consideration from the Figure 2. The range value for β-agarofuran is 0.92-0.99. For medium low-grade samples is shown in Figure 4. 10-epi-δ-eudesmol and δ-eudesmol have the highest median value compared to the other most important chemical compounds. The range value for 10-epi-δ-eudesmol is 0.47-0.84. The range value for δ-eudesmol is 0.19-0.88. For low grade samples is shown in Figure 5, dihydrocollumellarin has the highest median value compared to the other most important chemical compounds that have been taken as consideration from the Figure 1. The range value for is 0.01 - 0.99. The other chemical compound that has high median value is ar-curcumene. The range value for ar-curcumene is 0.01-0.99.

| Classification of Grades | Number of Samples |
|--------------------------|-------------------|
| Low                      | 210               |
| Medium Low               | 90                |
| Medium High              | 30                |
| High                     | 330               |
| Total                    | 660               |

Figure 2. High grade

Figure 3. Medium high-grade
4.2. The median of abundances for each chemical compounds

The 2D graphs represent the median of abundances for each chemical compounds for four different grades are shown in Figures 6-9. All the 2D graphs indicate from the boxplot analysis in 4.1. 5 chemical compounds (10-epi-δ-eudesmol, α-agarofuran, β-agarofuran, δ-eudesmol and dihydrocollumellarin) considered to be the most important chemical compounds. After making a comparison between the 2D graph of high (Figure 6), medium high (Figure 7), medium low (Figure 8) and low grade (Figure 9) for 4 grade agarwood essential oil, 10-epi-δ-eudesmol and δ-eudesmol are found to be the only chemical compounds that have in all quartiles – lower quartile, median quartile, and upper quartile. These two are a must chemical compound in grading agarwood essential oil.

Figure 6. The median of abundances (%) for each chemical compounds–high grade

Figure 7. The median of abundances (%) for each chemical compounds–medium high grade
5. CONCLUSION

This study has successfully constructed the boxplot analysis of 4 grade agarwood essential oil. This technique was used due to its effectiveness on agarwood essential oil classification. The input is eleven chemical compounds: 10-epi-γ-eudesmol, α-agarofuran, β-agarofuran, Y-eudesmol, dihydrocollumellarin, valerianol, ar-curcumene, β-dihydro agarofuran, α-guaiene, alloaromadendrene epoxide, and Y-cadinene while, the output is the four different grades – high, medium high, medium low and low grade of agarwood essential oil. The classification data was done using boxplot technique to illustrate them into 5-point summary – minimum and maximum values of range, the upper and lower quartiles, and the median. The research finding will give a valuable benefit for the future study especially in agarwood essential oil quality grading, its industry, and its research areas. The 5 most important chemical compounds which are, 10-epi-δ-eudesmol, α-agarofuran, β-agarofuran, δ-eudesmol and dihydrocollumellarin that have been considered can be a reference to grade agarwood essential oil for 5 grade and 6 grade.

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**BIographies of Authors**

Anis Hazirah ‘Izzati H. Al-Hadi was born in Malaysia, in July 1998. She is currently pursuing her studies as a postgraduate student majoring in Electrical Engineering at Universiti Teknologi MARA (UiTM) Shah Alam, Selangor, Malaysia. She received her B. Eng (Hons) of Electronics Engineering from Universiti Teknologi MARA (UiTM) Shah Alam, Selangor, Malaysia. She can be contacted at email: anszhrh@gmail.com.
Aqib Fawwaz Mohd Amidon was born in Malaysia, in September 1996. He received his B. Eng. (Hons) of Electronics Engineering from Universiti Teknologi MARA (UiTM) Shah Alam, Selangor, Malaysia. He is currently a Software Engineer at Greatech Technology Berhad and at the same time, he is a full-time postgraduate student at School of Electrical Engineering, Universiti Teknologi MARA(UiTM) Shah Alam, Malaysia. He can be contacted at email: aqibfawwaz.academic@gmail.com.

Siti Mariatul Hazwa Mohd Huzir was born in Malaysia, in May 1997. She is currently pursuing her studies as a postgraduate student majoring in Electrical Engineering at UiTM Cawangan Johor, Kampus Pasir Gudang, Johor, Malaysia. She received her B. Eng (Hons) of Electronics Engineering from Universiti Teknologi MARA (UiTM) Shah Alam, Selangor, Malaysia. She can be contacted at email: mariatulhazwa97@gmail.com.

Ir. Ts. Dr. 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.

Ts. Dr. 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 Mei 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.

Professor Madya Dr. Saiful Nizam Tajuddin received his PhD from Universiti Malaysia Pahang (UMP). He is a senior lecturer at Faculty of Industrial Science & Technology (FIST). He has worked at Universiti Malaysia Pahang since 2005 and was one the members who first founded FIST Faculty in 2007. Later in 2013, he has established BioAromatic Research Center (BIOAROMATIK) and is currently appointed as Director of COE. 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.

Prof. Ir. Ts. Dr. Haji 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.