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A preliminary study on the intelligent model of k-nearest neighbor for agarwood oil quality grading

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ABSTRACT

Essential oils extracted from trees has various usages like perfumes, incense, aromatherapy and traditional medicine which increase their popularity in global market. In Malaysia, the recognition system for identifying the essential oil quality still does not reach its standard since mostly graded by using human sensory evaluation. However, previous researchers discovered new modern techniques to present the quality of essential oils by analyse the chemical compounds. Agarwood essential oil had been chosen for the proposed integrated intelligent models with the implementation of k-nearest neighbor (k-NN) due to the high demand and an expensive natural raw world resource. k-NN with Euclidean distance metrics had better performance in terms of its confusion matrix, sensitivity, precision accuracy and specificity. This paper presents an overview of essential oils as well as their previous analysis technique. The review on k-NN is done to prove the technique is compatible for future research studies based on its performance.

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1. INTRODUCTION

Essential oil is a commodity that captures volatile aromatic essences extracted from different parts of the trees. 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], [2]. Recently, it is valued in many cultures where it is being used to treat various illnesses, perfumery and incense for religious and spiritual ceremonies purposes [3]-[5]. Currently, essential oil quality was measured and graded manually using sensory evaluation based on physical properties. Based on human perception and experience, an essential oil with the greatest grade has a lot of resin, dark oil color, strong odor and long-lasting aroma [3], [6], [7]. 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 essential oils. 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 [8]-[10]. As a result, several methods have been proposed and implemented to verify essential oil quality using intelligent techniques [8], [9], [11]-[17].

Agarwood oil is commonly used for medical purposes, ritual and fragrances. In today's modern society, agarwood oil become a hot topic among customers due to the strong odor, high content of resins and

dark color [18]. The volatile aromatic compounds concentrated from agarwood oil are also one of the factors of consumer attraction. As the high demand throughout the world market from countries of middle east, China and Japan, agarwood oil quality should be graded fairly to match with the pricey cost [19]. Chemical profiles can be used to classify essential oils into each classes (high, medium high, medium low or low quality) and the precise grade can be determined. The compounds will have fed to the k-Nearest Neighbor (k-NN) model by evaluate the accuracy of high percentage with Euclidean distance metric. This paper is presented to review the abilities of k-NN as a good classifier to be used as future classifier for agarwood essential oil to be grading into high, medium high, medium low and low quality.

2. LITERATURE REVIEW

2.1. Extraction methods of essential oils

Several techniques have been employed in essential oils extraction such as water distillation (hydro distillation), steam distillation, supercritical fluid extraction (SFE) and soxhlet extraction. Each method has its own unique strengths and weaknesses [5], [20]-[26]. A conventional Soxhlet extractor is used to convert a solid to a liquid form which has been performed on lemongrass oil. The results of the extracted oil-solvent mixture will be collected and distilled to obtain solvent-free oil [24], [25].

SFE has been used to extract the citronella essential oil using supercritical carbon dioxide. Supercritical fluid extraction does certainly allow the removal of polluting organic solvents, resulting in [20] solvent-free extract that concentrates on the active components of the essential oil. The continuous modulation of supercritical fluid's solvent selectivity had been practiced in the SFE method. The temperature of the heating bath will be adjusted and carbon dioxide was fed at a specific volumetric flow rate during the extraction time. The results found that essential oils that are concentrated in the active main components are purer [5].

Steam distillation and hydro distillation method have been performed on Kaffir Lime. Several researchers mostly use the distillation method for extracting the essential oil due to the low cost and friendly environment [21], [27]-[29]. The distillation process has created a layer of oil and hydrosol when the steam and oil mixture evaporates and condenses (mixture of oil and water). Water temperature was initially set to a particular degree Celsius and then gradually increased to 100 °C. The components were soaked in distilled water throughout the extraction using the hydro distillation process and the yield collected was only hydrosol. Both methods that generated hydrosol needed to be isolated. Finally, the extracted oil sample is analyzed using gas chromatography-mass spectrometry (GC-MS). The findings revealed that the steam distillation method was shown to be superior to hydro distillation because of the high percentage yield for essential oil extracted [5], [21].

Alcohol-soluble extraction has been used to extract essential oil while GC-MS was used for analyze chemical compounds in agarwood oil [18]. The yield show to have less than 10% and the yield value is reduced from 15%. The high-quality agarwood proved to have over 66.47% of 2-[2-4-methoxyphenylethyl] chromone and 2-(2-phenylethyl) chromone [18]. The 1-gram agarwood sample with ether was added and the solution was filtered and at a low temperature ultrasound for 30 min. Agarwood sample was undergoing alcohol-soluble extract process and analyzed by GC-MS. Findings show that fungi of T. marchalianum, S. podzolica, H. grisea, G. butleri and C. bulbillosum were the species with high oil content and high quality [30].

A furnace with an adjustable microwave power has been implement to study the rosehip essential oil [31]. Microwave-assisted hydro distillation (MAH) methods are proved to have the least time for extraction and give the highest yield percentage. It was found that using a high-frequency electromagnetic field and the ethyl alcohol is much better in resulting high amount of oil [32]. It is a good alternative for extracting essential oils of rosemary [31] and fresh ginger root [33] since it can reduce cost, be energy-saving and environmental friendly. Agarwood oil [19] was analysed using support vector machine (SVM) modelling of radial basics function (RBF) and multilayer perceptron (MLP) as kernel evaluation. The important parameters that have been considered were the performance of accuracy, precision, confusion matrix, sensitivity and specificity. The RBF tuned kernel parameter is better compared to MLP.

Hydro distillation has been used because it is offer the best price (cheapest), safest and friendliest environment method of extracting the agarwood oil [27]. Furthermore, hydro distillation is a popular method for extracting essential oils in the industry [29]. The review on method extraction of agarwood oil is summarized and tabulated in Table 1.

Table 1. Extraction of agarwood oil

Extraction methods	Review and summary	Ref.
Alcohol-soluble extract	Method of alcohol-soluble extract is used to extract essential oil while GC-MS is used for analyze chemical compounds in agarwood oil. Results: The yield show to have less than 10% and the yield value is reduced from 15%. The high-quality agarwood proved to have over 66.47% of 2-[2-4-methoxyphenylethyl] chromone and 2-(2-phenylethyl) chromone.	[18]
	Researcher used 1g agarwood sample with ether added. Solution was filtered and at a low temperature ultrasound for 30 min. Agarwood sample was undergoing alcohol-soluble extract process and analyzed by GC-MS. Results: Results obtain that fungi of T. marchalianum, S. podzolica, H. grisea, G. butleri and C. bulbillosum were the species with high oil content and high quality.	[33]
Steam Distillation	The essential oil extracted from A. sinensis leaves using steam distillation and separated using capillary column chromatography. Results: - Hexadecenoic acid (48.86%) - 6, 10, 14-trimethy 1-2-pentadecanone (8.22%) - Tetradecanoic acid (7.22%) - (E)-9-octgadecenoic acid (6.04%) - Pentadecanoic acid (2.58%) - 4, 8, 12, 16-tetramethylheptadecan-4-olide (2.31%) - Phytol (1.91%) - Nonanoic acid (1.73%) - Isophytol (1.38%) - Octadecanoic acid (1.31%)	[5]
	The agar pieces are chipped into very small pieces and placed in water for one to five weeks. Fermented agar chips were then taken to a distillation plant to extract oil. Results: Results obtain in order to make incense light after grinding was used the low-quality agarwood.	[19]
Distillation	In a 1:5 (weight/volume) ratio, agarwood chips and water were fed to the distiller. It was left overnight to ensure that all of the agarwood chips were wet and completely soaked in the water. Results: The chips demonstrate structural degradation due to long term heat exposure during the water distillation process. It is required 14 days to obtain the maximum oil yield for soaked agarwood chips.	[34]
Hydro distillation	A study in investigated agarwood oil by hydro distillation. Results: It is found that fatty acid, hydrocarbon sesquiterpene, oxygenated sesquiterpene and monoterpene were the high chemical compound produced in hydro distillation. All of those chemical profiles in agarwood oil samples contribute to the sweetness of fragrant wood aroma and the unique odor of oil. The agarwood extraction also shows a high percentage of yield even though it is time and energy-consuming.	[35]
Supercritical carbon dioxide	GC–MS technology is being used to determine the agarwood metabolite composition generated either naturally or artificially, with an emphasis on the volatile components of agarwood, particularly sesquiterpene derivatives from essential oils. Results: The substituted PEC derivative agarotetrol has been proven to have a favourable connection with agarwood quality and is utilised as a biomarker to evaluate agarwood quality.	[31]

2.2. Quality grading system of essential oils

Essential oil compounds are susceptible to high temperatures and degraded which affects their qualities. Hence, liquid extraction with a solvent is a suitable process to solve those compounds properties instead of distillation [24]. The current method to grade oil qualities is commonly using sensory evaluation which refers to its physical appearance of consumer perception, color, odor and high fixative. In other words, a grading system for essential oil still no approval for oil grading standards that are consistent to be practices in the industry [4], [12]. It's quite impossible to spot with the naked eye. Grading the essential oil according to its chemical properties is one of the advanced techniques that had been introduced to counter the manual technique of sensory evaluation [36]. The grading system of agarwood oil data produced using GC-MS involves graphical analysis was used in [21], [35], [37]. The general flow of data analysis as illustrated in Figure 1 [35].

Missing values ratio was used for dimension reduction while correlation matrix was computed to select data with the best missing values. The samples will be removed if samples have equal or more than 75% of missing values. The results showed only 19 compounds were left to have the best data from 106 compounds of 22 agarwood oil samples.

Z-score technique and GC-MS has been conducted in a research study as data transformation and normalization. This study consists of 11 samples of Kaffir lime oils from various Malaysian product [3]. The application of Z-score technique was discovered to have the advantages of being sensitive to data outliers as well as robust and effective in the normalization process. [11]. The significant compounds of Kaffir lime oil samples were clarified to have six compounds in total which are Limonene, Citronellal, β –pinene, terpine-4-ol, E-caryophyllene and terpinolene [11]. These compounds can be used as a guideline to classify the kaffir lime oil as two qualities which high and low [11]. A modern grading system of agarwood oil using a linear regression model was discussed to be fed into feed forward neural network (FFNN) [8]. The best regression line of hidden neurons will be identified to discriminate the quality of Gaharu oil from high to low quality. Levenberg Marquadt (LM) algorithm was implemented for the trained dataset because it is the most commonly used optimization algorithm in many research studies [13], [38], [39]. The findings strongly showed that a best fit linear regression line with a value of R exactly 1 at hidden neurons number 2 which is the lowest compared to other neurons [40]. Regression analysis is used to study the interdependence of multiple variables while stepwise regression analysis is frequently used to discover the ideal appropriate regression model to study the interdependence of variables in more depth [41], [42].

In a research study, the performances of k-NN and artificial neural network (ANN) were measured for both intelligent techniques [8]. The input and output measured in the research included the abundances of significant chemical compounds (%) and agarwood oil qualities which are high and low. Sensitivity, precision, confusion matrix and specificity were used to test the training performance and testing data of k-NN classification system. Based on the result, the accuracy of k-NN model was in the range of 81-86% while the ANN model showed excellent accuracy of 100%. These high accuracies can be a solid reason to develop the technique further for intelligent application for agarwood oil quality classification [43].

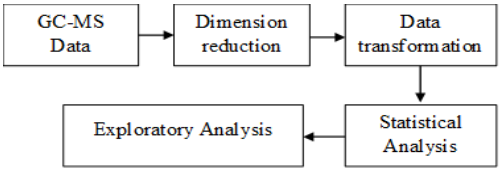

Figure 1. General flow of data analysis

2.3. K-nearest neighbor

K-NN is a non-parametric classification algorithm [44]. The k-NN classifier model is widely implemented as one of the best-known algorithms and is easy to use in analyse the solving classification problems as well as identify the sample [13], [15], [45]. The algorithm requires ‘k’ value to find the closest data based on distance computation and determine the class of the new data. It also works by looking for a class of ‘k’ values that are related to objects in new data or data testing in the nearest training data [23], [46].

In artificial intelligence, machine learning permits to evolve through a process of the machine. There are two types of machine learning which are unsupervised and supervised learning. k-NN falls for the supervised learning method categories where labeled datasets were used [15]. The important parameters that had been observed in analysing using k-NN method are distance and classification rules. In a study, k-NN algorithm has been performed to classify breast cancer [44]. To decide how to classify a sample, the different values of ‘k’ for distances (Euclidean and Manhattan) and rules (majority, consensus and random) have been performed to pass all the k-NN performance [44], [47].

k-NN intelligent model has been applied in various fields such as in the medical diagnosis, grading essential oils, fake incense detection and others [30], [48], [49]. The classifier has successfully analyzed the olive oil classification based on their correct group by ‘k’ value equal to 5. The datasets using Euclidean distance and results showed that the k-NN model performed well on the tested classification problems between different quality types of olive oil. Only 5% different when comparing with SVM method for the overall accuracy [15]. The agarwood oil classification was implemented using the k-NN method has been done with high accuracy in the range of 81-86% [13]. The Euclidean distance was also applied for this study. The high accuracy results also indicate the opportunity to develop the technique further for application using dedicated intelligent agarwood oil quality grading [19].

2.4. Criteria of k-NN as a good classifier

A review has been done on k-NN. There is various implementation of distance metrics to measure the performance for Agarwood oil. Some criteria are listed below to show that k-NN application is capable of quality grading classification:

2.4.1. Distance metrics

A distance measures the length of a straight line between two objects for agarwood compounds classification [44]. The distances allow classing the samples either is similar or do not resemble [43]. In agarwood oil grading quality classification, Euclidean distance metric (EU) has been implemented as one of the tuned parameters in the study [43], [50]. The square root of differences between coordinates of pair of objects in [7] as in (1).

$$d_{st} = \sqrt{\sum_{j=1}^{n} \left(x_{sj} - y_{tj}\right)^2} \quad (1)$$

Where Xsj is an object at coordinate sj, ytj is another object at coordinate tj and dst is a distance between them. The advantage of using EU distance metric in k-NN model is the most universal and great for low-dimensional data [50], [51]. Existing work in [43] conducts research on classifying agarwood oil into high and low quality. The accuracy results for both distance variation (Euclidean and city-block) show 100% for testing and training datasets at k=1 until k=5. Results showed that the Euclidean distance metric performs 100% accuracy compared to other metrics which achieved at the range of 78.5% to 100%. Besides, researcher make a comparison between Euclidean distance metric and other metrics such as Cossine and Correlation in k-NN [12]. The researcher found that Euclidean distance metric had better performance in terms of accuracy compared to others due to the greatest efficiency and can be concluded as the most appropriate distance metrics for agarwood oil classification.

2.4.2 The performance measures

Confusion matrix, accuracy, sensitivity, precision and specificity was used in study [19] to describe the behaviour of classifier. A confusion matrix is tabulate in Table 2 [12]. k-NN model was used in [50] for the quality of agarwood oil classification into 2 qualities which are high and low. Euclidean metric was implemented. Based on [13], [43], k-NN resulting that the highest accuracy is yielded Euclidean for training and testing datasets. The sensitivity, specificity precision and accuracy reach 100% for Euclidean distance variation. The KNN classifier can discover the k most comparable trainings and predict the majority class among them. The advantage of using Euclidean distance in k-NN is the efficiency of its implementation [12], [52]. Existing framework in [43] showed the Euclidean distance as a natural benchmark in access the coefficient of dissimilarity because it relates to everyday physical world's typical notion of distance. Besides, researcher in [43] make a comparison between Euclidean, City-block, Cosine and Correlation distance metrics in k-NN. The researcher found that Euclidean and City-block had a better performance in term of accuracy compared to Cosine and Correlation distance.

Table 2. A confusion matrix

Data class	Predicted/classified as positive	Predicted/classified as negative
Positive	True positive (TP)	False negative (FN)
Negative	False positive (FP)	True negtaive (TP)

3. CONCLUSION

The review showed that k-NN model with Euclidean distance metrics can be implemented for grading the quality of essential oil. k-NN technique had been proven to have a good classifier for performance criteria in grading essential oils. agarwood oil becomes in high demand since its benefit not only in medic scope but also in religion and any field. It can be seen that distillation extract is the most common for oil extraction due to the cost and ease to use. As a result, the k-NN technique will be employed in future studies on grading agarwood essential oil.

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