Preliminary study on agarwood essential oil and its classification techniques using machine learning

Anis Hazirah 'Izzati Hasnu Al-Hadi[1], Aqib Fawwaz Mohd Amidon[1], Siti Mariatul Hazwa Mohd Huzir[2], Nurlaila Ismail[1], Zakiah Mohd Yusoff[2], Saiful Nizam Tajuddin[3], Mohd Nasir Taib[1,4]
[1]School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Shah Alam, Malaysia
[2]School of Electrical Engineering, College of Engineering, Universiti Teknologi MARA, Kampus Pasir Gudang, Malaysia
[3]BioAromatic Research Centre of Excellence (BARCE), Universiti Malaysia Pahang, Gambang, Malaysia
[4]Malaysia Institute of Transport (MITRANS), Universiti Teknologi MARA, Shah Alam, Malaysia

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ABSTRACT

Using essential oils derived from trees for pharmaceutical purposes, incense, aromatherapy, and other areas has expanded its popularity on the international market. However, since human sensory evaluation is still the primary technique used to grade essential oils in Malaysia, the classification technique for determining their grade is still below standard. Nonetheless, prior studies established new approaches for classifying the grade of essential oils by studying their chemical compounds. Therefore, agarwood essential oil was selected for the suggested model due to the increasing demand and the high cost of the world's natural raw materials. The support vector machine (SVM) using one versus all (OVA) approach was selected as the classifier for agarwood essential oil. This study provides an overview of essential oils and their prior research techniques. In addition, a review of SVM is conducted to demonstrate that the technique is appropriate for future studies.

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

Essential oils are highly potent, fragrant oils that are extracted from plants using pressure, hydrodiffusion, or steam distillation [1], [2]. Almost every significant end-use industry, including food and beverage, cosmetics, personal care, and aromatherapy, has seen continuous and rapid expansion in the worldwide essential oils market [1]-[4]. Essential oils are often used as raw ingredients for other goods and to remove unpleasant fragrances [2]. Traditionally, the grade of essential oils is determined and evaluated manually using a sensory evaluation based on its physical characteristics. According to a trained human panel (sensory) with experience in a range of oil compositions, the highest-grade essential oils have a significant amount of resin, oil purity of its numerous compositions, a potent fragrance, geographic origin, and aroma intensity [4]-[8]. The current findings determined manually by sensory evaluations differ according to whether the testers have a keen feel for judging the grades of essential oil or not. Thus, similarly to the earlier approach, limited dependability is projected since it relies on the human nose, which cannot maintain a high number of samples due to quick fatigue, zero consistency and time-consuming process [5], [6], [9], [10].

Due to its highly valuable resin-impregnated heartwood, Aquilaria species are one of the most valuable trees in the world, particularly in Asia. It belongs to the Thymelaeaceae family [8]. Agarwood essential oil, often known as oudh oil, is obtained from agarwood trees. Agarwood production in the wild is frequently brought on by unavoidable natural occurrences like lightning strikes, broken branches from strong winds, and pest and disease infections. These issues may result in wounds or other openings that allow pathogenic germs to enter and start the tree's defences. Some researchers referred to the openings or wounds as an infected areas [7], [11], [12]. Agarwood essential oil is well-known among manufacturers and retailers for its aroma as a base for fragrances, ritual purposes and for its pharmaceutical purposes [5], [7], [8], [12], [13]. Agarwood essential oil has become a widespread goods among consumers in present-day society because of its potent fragrance, high resin content, and dark colour [4]-[8]. Agarwood essential oil needs to have a global grading system and price according to its grades due to demand on the worldwide market from China, Japan, India, and the Middle East. Grading is crucial for classifying goods according to their marketable grades and determines trade transparency and pricing decisions [8]. The grades of agarwood essential oil can be totally identified by their chemical compounds. This enables the classification of essential oils into different classes (low, medium low, upper low, medium high, high and, upper high grade), and precise findings can be evaluated. This study is presented to review the capabilities of support vector machine (SVM) using one versus all (OVA) as a good classifier to be used as future classifier for agarwood essential oil to be grading into low, medium low, upper low, medium high, high, and upper high grade.

2. LITERATURE REVIEW

2.1. Extraction techniques of essential oil

Essential oils can be extracted by a variety of extraction techniques. Distillation (hydro-distillation, steam distillation and water distillation) and solvent extraction are currently employed often to extract essential oil from plants [1], [3], [5], [6], [13]-[19]. Distillation is an early technique used to separate chemical compounds that is widely employed in the petroleum, natural gas, and petrochemical industries. Distillation is defined as the heating of a liquid solution or vapor-liquid mixture. The outcomes of the vapour will be collected and condensed [5], [6], [13], [14]. In solvent extraction, which is used with delicate plant matter that cannot withstand the distillation process, known chemical affinities for lipid or hydrophilic solutions are exploited to remove aromatic chemicals; the concern of whether introducing solvents to facilitate extraction can alter the components of the extracted essential oil has been the topic of discussion, and this technique has been discredited by some researchers [1], [3], [20].

Nor *et al.* [5], the researchers did an experiment to find the best extraction technique using standard hydro-distillation and modified hydro-distillation. The findings found that the modified hydro-distillation extracts maximum yield 0.78% of agarwood essential oil compared to standard hydro-distillation extracts only 0.68%. Nasardin *et al.* [15] made a study to compare the extraction technique between hydro-distillation and steam distillation. The steam distillation technique took no less than 7 days to complete the process of extracting the agarwood essential oil while, the hydro-distillation technique only took no less than 5 days. The findings found that the hydro-distillation produced more agarwood essential oil with 150 ml and steam distillation produced only 100 ml. To conclude, the study in [15] showed that the hydro-distillation is more practical technique to produce the agarwood essential oil. Pornpunyapat *et al.* [13], Rahim *et al.* [16] also extracted the agarwood essential oil using hydro-distillation but to improve the technique, they experimented using various temperatures, different pre-treatment technique, different size of agarwood samples, various duration of shaking time and many more. Kasuan *et al.* [19] did the same experiment as in [15] but the researchers used kaffir lime. The findings found that the extraction of kaffir lime essential oil using stream distillation yield more than 0.25% for leaves and 1.18% for peels compared to hydro-distillation. The study found that the steam distillation is the efficient technique to produce kaffir lime essential oil.

Zakaria *et al.* [20], Kahar *et al.* [21] had done a study on solvent extraction used in extracting agarwood essential oil. Zakaria *et al.* [20] used methanol, ethanol and water while, [21] used hydrosol. Different extracting solvents that have been utilised in various agarwood extraction techniques have been the subject of limited studies. The solvents such as methanol, ethanol, hydrosol, and water have their own role in extracting agarwood. Most of them are used in pharmacological, nutraceutical and medicinal purposes. Hence, the usage of methanol, ethanol, hydrosol, and water as solvent extraction is safe for human consumption [20], [21]. There is a new technique has been approached by few researchers to improve the extraction of essential oil by using hydro-distillation technique which is microwave assisted hydro-distillation also known as microwave assisted extraction (MAE) [6]. MAE has been used to extract *Rosmarinus officinalis L.* often called as rosemary [18]. Elyemni *et al.* [18], the extraction of rosemary essential oil using conventional technique of hydro-distillation has been compared with the microware assisted hydro-distillation by calculating the yield of the rosemary essential oil. The chemical compounds produced using microwave assisted hydro-distillation are almost like the conventional technique of hydro-distillation, but the extraction time reduces significantly. The microwave assisted hydro-distillation took 20 minutes while, the conventional technique hydro-distillation took 180 minutes. Mollaei *et al.* [17], the extraction of an important medical plant from Iran named *Ferulago angulata* has been done with the microwave assisted hydro-distillation technique. The yield of Ferulago angulata essential oil has been compared with the conventional technique of hydro-distillation to measure the effective technique to extract the essential oil. Radzi and Kasim [6] did the same experiment as in [17], [18] but they were using agarwood. From [6], [17], [18], it is stated that the microwave assisted hydro-distillation is an effective technique to extract essential oil since it can give high percentage of yield, reduce the extraction time as well as reduce the release of carbon dioxide (CO_2). Kusuma *et al.* [14], the experiment to compare between extraction of agarwood essential oil using microwave hydro-distillation also known as MAE and solvent-free microwave extraction (SFME) had been conducted. The researchers concluded that the SFME technique is effective compared to MAE since SFME took only 6 hours to extract the agarwood essential oil and produced a yield of 5.95 times more than MAE, which took 12 hours to extract the agarwood essential oil. Furthermore, the SMFE uses lower electric consumption and emits lower CO_2 compared to MAE. Hence, the SMFE can be used as a new green technique to improve the environmental sustainability.

2.2. Grading techniques of essential oil

Even though United States (US) distributors have recommended a specific grading system, there are currently no specific standards for grading essential oil [1]. Presently, the techniques for grading essential oil are both traditional and modern grading systems. The traditional grading system is graded based on physical characteristics such colour intensity, resin content, and odour by human sensory panels. The modern grading system is graded using mathematical modelling of GC-MS including computer algorithms such as artificial neural network (ANN), K-nearest neighbor (k-NN), linear discriminant analysis (LDA), electronic nose (E-nose), Z-Score and SVM [7], [9]-[12], [22]-[27].

Mainly, the grading for essential oil is using human sensory panels. The findings of the old approach differ according to whether the testers have a keen feel for judging the grades of oil or not. Thus, as with the prior approach, limited dependability is predicted since it is based on the human nose, which cannot sustain many samples due to quick exhaustion [5], [6], [9], [10]. This technique is also performed based on the human's health and at the end of the day, it will affect the human's health due the hazardous work by smelling the essential oil continuously in a large number of samples [7], [9], [10], [28]. Kaleri *et al.* [28], researchers concluded that the natural agarwood tree's smoke is damaging the health and artificial agarwood tree's smoke can cause poisonous damage to the health. The traditional technique of grading essential oil based on its resin content [4]. The forest research institute malaysia (FRIM) used this technique to determine the resin content of gaharu essential oil also known as agarwood essential oil. A high proportion of resin content is required for an essential oil to be rated as high grade. According to the findings in [4], gaharu essential oil contains a significant percentage of resin, which is classified as Grade A when it exceeds 30%.

A modern grading system has been applied on grading the maturity of oil palm fresh fruit bunches [23]. The study has implemented LDA as the classification technique. It has different classes which are raw, under-ripe and ripe. To conclude the findings in [23], accuracy value for the LDA technique's performance evaluation was successfully reached at 98.89%. Alfatni *et al.* [24] grades real-time oil palm fresh fruit bunches using ANN, KNN and SVM. The study classifies oil plam fresh fruit bunches into under ripe, ripe, and over ripe. It has been concluded that the performance of ANN technique achived an accuracy value of 93% [24]. Another existing study has done a classification of agarwood essential oil using E-nose and ANN [10]. It is found that the E-nose classification of agarwood essential oil can produce fast and precise findings. Additionally, ANN was effectively used to forecast unidentified agarwood essential oil samples [10]. Another study using E-nose, LDA and SVM has been done in [26]. The study aims to classify *Rosa damascena* Mill. into the three classes which are C1, C2 and C3. From the study, it has been concluded that LDA has 95% accuracy value while, SVM has increased the accuracy value to 99%. These findings show that an E-nose can be utilised as a quick, simple, accurate, and low-cost approach for categorising the content of essential oils in *Rosa damascena* Mill [26].

Z-score technique has been applied in [27], [29]. It was used to identify the significant compounds of kaffir lime oil and agarwood essential oil respectively from various compounds extracted by GC-MS. Both studies concluded that z-score technique gave a good performance in identifying the significant compounds [27], [29]. k-NN technique has been applied in [30] to grade agarwood essential oil into low and high grade. According to the findings [30], the k-NN technique passed the accuracy, confusion matrix, sensitivity, precision, and specificity performance evaluations. SVM has been applied in [11] to classify agarwood essential oil into low and high grade. The result has been concluded that the accuracy was 89.47%, while two samples that were meant to be of high grade were incorrectly classified [11].

2.3. Support vector machine

The concepts of classification and regression are the core topics covered by SVM, which are an implementation of the supervised learning paradigm. The support vector machine was created by Vapnik and

Chervonenkis [31]-[33]. SVM has proven to be a potent approach for tackling actual binary classification issues. SVM has been demonstrated to be more effective than other supervised learning techniques [32], [33]. SVM can be categorized into linear and non-linear. SVM classify data for nonlinear differently than linear support vector machines [22], [32], [33]. When classifications of data can be separated linearly using a hyperplane, the linear SVM is utilised; in contrast, the non-linear SVM employs non-linearly separable data that cannot be separated linearly using a hyperplane [32], [33].

SVM decision function is trained by finding a recurring hyperplane that maximises the margin or distance between the support vectors of the two class labels [22], [31]-[34]. In other words, the classification abilities of SVM and other strategies differ significantly, especially when the number of input data is small. This classification strategy reduces the classification errors of the training data and achieves a higher generalization performance. SVM acquires using a subset of support vectors-often just a small portion of the initial data set-which gives them a distinct advantage. For example, this small data collection was used to create a set of support vectors that represents a specific classification task [22], [31]-[33].

Performance of SVM is significantly impacted by kernel function and parameter. Non-linear modelling can be learned using a mapping called a polynomial kernel. The polynomial kernel, a kernel function frequently employed with SVM and other kernelized models, represents the similarity of vectors (training data samples) in a feature space over polynomials of the original variables, enabling the learning of non-linear models [33]. SVM has been used in a variety of fields, including text classification, including hypertext [35], [36], image classification [37], [38], cancer classification [39], [40], character recognition in writing [41], [42], face recognition [43], [44], plants classification [45], [46] and many more.

2.4. Multiclass classifier of SVM

SVM were created for binary classification [31]-[33]. The binary SVM technique, on the other hand, can be expanded for multiclass cases that are typical in remote sensing. This is typically accomplished by decomposing the multiclass problem into a series of binary analyses that may be addressed with a binary SVM by employing one of the multiclass techniques, such as the OVA strategy [47]. Most existing multiclass classification methods are either based on binary classifiers or are reduced to them. The fundamental concept behind this data is to employ a series of binary classifiers that have been trained to classify between different groups of objects. Various voting techniques are employed in the classification [47]-[50]. In general, all modern multiclass machine learning approaches may be split into three categories: those that use one-versus-all [47]-[50], or one-versus-one strategies [48], [51], those that use the error correcting output codes (ECOC) approach [49], [50], and those that use the single-machine approach [52].

One-vs-rest (OVR) is a heuristic approach for employing binary classification algorithms for multi-class classification. It is also known as OVA [48], [50]. It involves splitting the multi-class dataset into several binary classification problems. On each binary classification problem, a binary classifier is trained, and predictions are made using the model with the highest confidence [52]. The obvious approach is to utilize a OVR strategy, in which we train C binary classifiers, fc(x), where data from class c is viewed as positive and data from all other classes is viewed as negative [53].

3. CRITERIA OF SVM AS A GOOD CLASSIFIER

3.1. Kernel parameters

Non-linear issues in SVM data mining can be resolved utilising different kernel implementations. As kernel tuning parameters in SVM, polynomial, radial basis function (RBF), multilayer perceptron (MLP), and sigmoid-kernel are frequently employed [7], [12], [22], [26], [32]. Each kernel parameters in SVM [54] have its own equation as shown in (1) to (4). Chen *et al.* [54], RBF is the kernel parameter that research studies most frequently use. Making sure that the mapping function is carried out in input space to feature space is the kernel's primary function. Due to the ability to change the hyperplane for complex issues, employing kernel parameter in SVM has the benefit of increasing accuracy and efficiency in any issues [7], [33]. The study in [7] made a study on classifying agarwood essential oil into low and high grades using RBF kernel parameter. It is shown that all performance measures for RBF were passed by the developed model. The performance measures consist of specificity (%), sensitivity (%), accuracy (%), precision (%), error test and error rates. All the performance measures scored more than 80% and it is proven that RBF show a great performance in classifying agarwood essential oil [7]. The existing study in [22] made a comparison between MLP and RBF on classifying agarwood essential oil into low and high grades. The study concluded that RBF has a better performance in classifying agarwood essential oil compared to MLP [22].

Polynomial : $K(p,q) = (\gamma p^T \cdot r)^d$ (1)

Linear : $K(p,q) = p^T \cdot q$ (2)

Sigmoid $: K(p,q) = tanh(\gamma p^T \cdot q + r)$ (3)

RBF $: K(p,q) = exp\,(-y\|p-q\|^2)$ (4)

3.2. Accuracy in classification and regression

SVM is renowned for its proficiency in cross-validation classifying data with the highest level of accuracy [7], [22], [26]. Laref *et al.* [55] made a comparison between SVM and partial least squares (PLS) for electronic nose to monitor gas concentration. The study concluded that SVM regression provides more higher level of accuracy for estimating gas concentrations in confined spaces compared to PLS regression [55]. Another existing study in [54] made a comparison on SVM, back-propagation neural network (BPN) and linear discriminat analysis (LDA) for equipment fault detection in a thermal power plant. The study has shown that SVM identified the different types of turbine failures in highest level of accuracy (more than 90%) compared to BPN and LDA [54].

3.3. Minimum error

Errors should be kept to a minimum for a technique to be effective in the field. SVM has the capacity to reduce errors by employing a cross-validation technique. Laref *et al.* [55] made a calculation on prediction of root mean square error (RMSE) to identify the best performances model for gas concentraction estimation. The study found that RMSE using SVM regression is much lowered compared to PLS. The RSME for SVM is 0.0346, while the RSME for PLS is 0.0859. Additionally, the study also observed that after 180 samples, the RMSE for the SVM model is very constant whereas the RMSE for the PLS model still exhibits significant volatility [55].

4. CONCLUSION

It is clear from the study above that several techniques are utilised to extract essential oils and classifying their grades. Agarwood essential oil is increasingly in demand because of its advantages in a variety of fields, including pharmaceutical purposes, religion, and other areas. The objective of the SVM methodology review is to demonstrate the SVM's capabilities as a reliable classifier of machine learning in a variety of fields, including the grading of essential oils. Therefore, future studies on grading agarwood essential oil using machine learning especially SVM will be employed.

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BIOGRAPHIES OF AUTHORS

Anis Hazirah 'Izzati Hasnu 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: anshzrh@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.

Associate Professor Dr. Saiful Nizam Tajuddin received his PhD from Universiti Malaysia Pahang (UMP), Malaysia. He is a Associate Professor 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. Mohd Nasir Taib received his PhD from University of Manchester Institute of Science and Technology (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.