International Journal of Electrical and Computer Engineering (IJECE)
Vol. 12, No. 6, December 2022, pp. 6716~6723
ISSN: 2088-8708, DOI: 10.11591/ijece.v12i6.pp6716-6723

Intelligent grading of kaffir lime oil quality using non-linear support vector machine

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Article Info

Article history:

Received Sep 29, 2021
Revised Jul 18, 2022
Accepted Aug 10, 2022

Keywords:

High/low quality
Kaffir lime oil
Non-linear support vector machine
Radial basis function kernel

ABSTRACT

This paper presents kaffir lime oil quality grading using the intelligent system classification method, a non-linear support vector machine (NSVM). This method classifies the quality kaffir lime oil into two groups: high and low quality, based on their significant chemical compounds. The 90 data of kaffir lime oil were used in this project from high to low quality. The abundance (%) of significant chemical compounds will act as the input and high or low quality as an output. The 90 data will be divided into two sets: training and testing data sets with a ratio of 8:2. The radial basis function (RBF) optimization kernel parameters in NSVM. Using the implementation of MATLAB software version R2020a, all data and analysis work was performed automatically. The results showed that the NSVM model met all performance criteria for 100% accuracy, sensitivity, specificity, and precision.

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1. INTRODUCTION

Kaffir lime, known by its scientific name *Citrus Hystrix*, which comes from Rutaceae family, is very famous in Asian countries [1]. Nowadays, kaffir lime is in high demand in industrial sectors such as aromatherapy, perfume, beauty products, and the medical field [2]–[5]. Kaffir lime oil can be obtained from its fruit or leaves. This oil has also been widely sold in the market at different prices. However, the higher prices do not guarantee the higher quality of oil products. Currently, kaffir lime oil quality grading is evaluated using human sensory organs and human perception based on the long-lasting aroma, odor and color of this oil. This method is less accurate because every human has different perceptions, and their noses are prone to getting fatigued [6]–[8]. To overcome this problem, the quality of kaffir lime oil can be grad by using significant chemical compounds.

Chemical compounds of kaffir lime oil contain almost hundreds and complex compounds. The significant compound of kaffir lime is monoterpene components, including citronellal, β-pinene and limonene [9]–[12]. The significant compound can be used as a marker compound to identify the quality of kaffir lime oil. This project proposes a new technique for classifying important compounds in kaffir lime oil using a non-linear support vector machine (NSVM) to avoid conflicting and time-consuming oil classification results. NSVM is a supervised learning technique commonly used in a classification system. NSVM can overcome classification and regression problems for linear or non-linear data [13], [14]. NSVM is utilized when a straight line cannot simply separate the data. It requires using a kernel to convert

inseparable data into separable data. Data from input vectors can be mapped into high-dimensional vector spaces by using kernels [15]. The abundances (%) of significant chemical compounds are used as input and high or low quality as an output of NSVM model developed by tuned radial basis function (RBF) kernel. So, the oil quality and grading of kaffir lime will be classified using an automated intelligent NSVM regarding their chemical compounds and reduce the time-consuming grading process.

2. THEORETICAL WORK

2.1. Non-linear support vector machine

A support vector machine (SVM) is a supervised classifier technique that finds the best hyperplane between two classes with the least distance. The ideal hyperplane is defined as a hyperplane that can divide a dataset into two classes without causing the class error and the distance between the nearest vector and the greatest margin [16]. SVM contains linear and non-linear. In general, real-world problems are not linearly separable. NSVM is updated to handle the non-linear problem by adding a kernel function. The function in NSVM maps the X data to a higher dimensional vector by the function Φ(X). A hyperplane can be constructed to separate these two classes. Cores help form hyperplanes in higher dimensions without adding complexity.

$$y = \Phi(X) \tag{1}$$

Figure 1 shows an illustration of this concept. The data in the input space is mapped by the function Φ(X) to a new vector space with a higher dimension. So that two data classes can be separately linearly by a hyperplane [17]. According to Mercer's theory, the dot product computation is substituted with the kernel function $K(X_i, X_j)$, which implicitly defines the transformation Φ. Also known as the kernel trick, it is written as (2) 18 [18].

$$K\ (X_i\ .X_j) = \Phi\ (X_i)\ .\Phi(X_j) \tag{2}$$

Kernel trick provide a variety of convenience. In the process of learning NSVM, to determine the support vector, just enough know the kernel function used, and it is not necessary to know the existence of a non-linear function Φ. Several kernel functions commonly used are linear, polynomial, and RBF [19]. The advantages of the NSVM method compared to other computer algorithm classification are its stability, classification, generalization, and ability to process non-linear data have made NSVM a reliable classification method [14].

The NSVM has been used to classify lemons based on the spice in the lemon juice, and the results show the accuracy is 100%. In addition, it is also used to determine the quality of agarwood oil, whether low or high quality and provides 100% accuracy [20], [21]. It shows NSVM are the best classifier with high robustness and prediction accuracy.

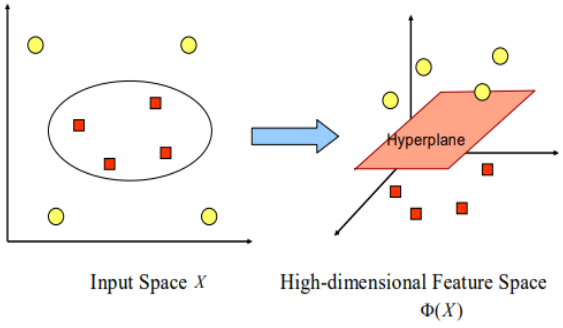

Figure 1. Function Φ(X) maps the data to a higher-dimensional vector space [22]

2.2. Radial basis function kernel

The RBF kernel is one of the most used because of its similarity to a Gaussian distribution. In general, RBF kernels are a good place to start. This kernel non-linearly maps samples to a higher-dimensional space, so it can handle cases where the relationship between class labels and attributes is non-linear, unlike linear kernels [23]. Since the linear kernel also has a kernel with some parameters (C, γ), it

is a special case of RBF [24]. Furthermore, the sigmoid penalty parameter performs similarly to the RBF kernel and behaves similarly to RBF for certain parameters [17]. Another reason is the set of hyperparameters that affects the difficulty of model selection. Polynomial kernels have more hyperparameters than RBF kernels. Finally, RBF kernels are less numerically challenging. A key point is that $< K_{ij} \leq 1$ as opposed to polynomial kernels, whose kernel values can be infinite $({}_yX_i\mathrm{T}\,X_j + \mathrm{r} > 1)$ or zero $({}_yX_i\mathrm{T}\,X_j + \mathrm{r} < 1)$, with large degrees. Also, we have to note that the sigmoid kernel is invalid under certain parameters (i.e not the inner product of two vectors). In various cases, the RBF kernel is not sufficient. For example, only linear kernels can be used if the number of features is large [25]. This kernel can be mathematically represented in (3) [24], [25]:

$$K(X_i\,.X_j) = exponent\ (-_y||X_i - X_j||2) \tag{3}$$

where γ was gamma and $||\mathrm{X}_i - \mathrm{X}_j||$ was Euclidean distance between X_i and X_j. The kernel scaling parameter corresponds to the γ parameter in the RBF definition. As parameter γ increases, NSVM tends to overfit, which means that all training instances are used as support vectors-assigning a smaller value to γ results in underfitting, causing all instances to be grouped. Therefore, an appropriate value must be chosen for the kernel width [26].

3. RESEARCH METHOD

Figure 2 shows the flowchart of this NSVM model creation. It begins with input and output data collection. The 90 samples of kaffir lime oil used in this project contain high and low quality. After that, data will be pre-processed. The data will be randomized and divided into two datasets: the training and testing data set. Afterwards, the NSVM models were constructed to tune the RBF kernel parameters from the training dataset. Finally, the NSVM model will be validated and evaluated in its performance. The model needs to pass all performance criteria. If the model is not passed, the data will be reprocessed. The requirements that the model needs to pass are confusion matrix, accuracy, sensitivity, specificity, and precision. The proposed method's performance measures are evaluated in terms of confusion matrix, accuracy, sensitivity, precision and specificity, and mean squared error (MSE).

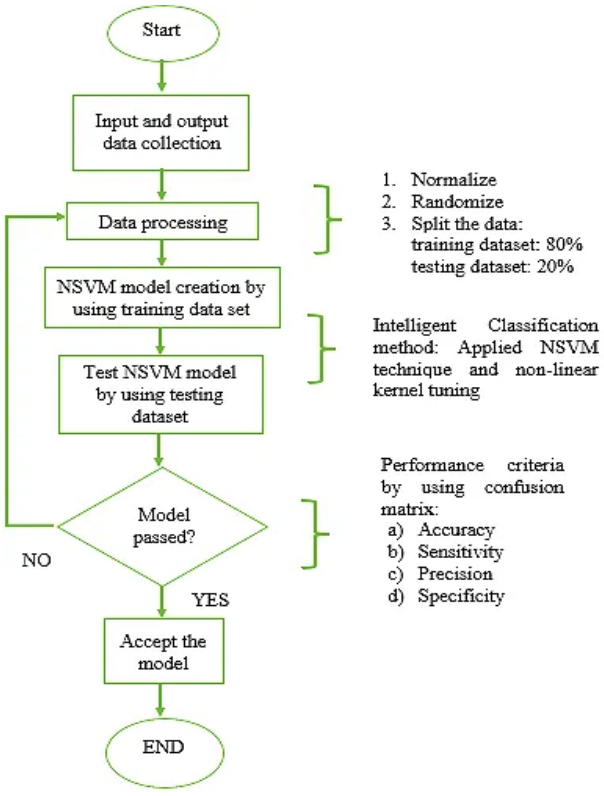

Figure 2. Flowchart of NSVM model creation

All analytical work was done automatically using MATLAB software R2020a. This experiment starts with uploading and pre-processing data, as shown in Figure 3. The 90 data of kaffir lime oils were saved in a file name "90data.xlsx". The file contains the abundances (%) of the significant chemical compounds that act as input, and the output will be high '1' and low '2' quality. The 6 significant used in this project were β-pinene, citronellal, limonene, terpinolene, terpinene-4-ol, and caryophyllene. After uploading the data, the data will be randomized and divided into two datasets were training dataset and testing dataset, with ratio 8:2 [15], [21], [27]. The large number of training datasets were needed to train and develop the NSVM model with higher accuracy [20].

```
clc, close all, clear all

RandStream.setGlobalStream(RandStream('mt19937ar','seed',1));

data= importdata('C:\Users\SYAHIRA\Documents\MATLAB\90data.xlsx');
data1=(data.data);
xdata = data1(:,1:6);
group = data1(:,7);
P = cvpartition (group, 'Holdout', 0.20);

inptrain = xdata(P.training,:);
outtrain = group(P.training);
inptest = xdata(P.test,:);
outtest = group(P.test);
```

Figure 3. Uploading and pre-processing data MATLAB script

The training data is used for model building, while the test data is executed as model output predictions, as shown in Figure 4. This figure shows MATLAB script for NSVM model by using RBF kernel. The command *fitcsvm* was used for model creation and the *predict* command for output prediction. Analyze the performance of the NSVM model using the confusion matrix. Figure 5 shows the MATLAB script for confusion matrix.

```
SVMStruct = fitcsvm(inptrain,outtrain,'KernelFunction','rbf');
outtestpredicted = predict(SVMStruct,inptest);
```

Figure 4. NSVM with RBF kernel MATLAB scripts

```
conMat = confusionmat(outtest,outtestpredicted);
tp = conMat(1,1);
fp = conMat(2,1);
fn = conMat(1,2);
tn = conMat(2,2);
```

Figure 5. MATLAB script for confusion matrix

4. RESULTS AND DISCUSSION

As a result, NSVM model with tuning RBF kernel parameter contains 63 support vectors from training dataset was tabulated in Table 1. The support vectors belonged 6 compounds labeled as C1 until C6. The minimum and maximum vector values of C1 are 0-18.90. Next, the minimum and maximum vector values of C2 are 0-51.38. After that, the minimum and maximum vector values of C3 are 0-11.41. Then, the minimum and maximum vector values of C4 are 0-79.67. Besides, the minimum and maximum vector values of C5 are 0-11.32. Finally, the minimum and maximum vector values of C6 are 0-19.72.

From this finding, kaffir lime oil can easily be classified using RBF tuned kernel parameter in NSVM. Table 2 shows the confusion matrix for testing dataset. It is shows only true positive (TP) and true negative (TF) have values, but false positive (FP) and false negative (FN) have not. That means, when the quality oil classified as high, the actual also high (TP) while when the quality oil classified as low, the actual also low (TN).

Table 1. Support vector from C1 to C6

Vector	C1	C2	C3	C4	C5	C6
1	0.00	0.00	0.00	52.27	0.00	13.15
2	1.42	0.52	0.00	60.06	0.99	0.00
3	0.00	0.00	0.00	51.05	0.00	18.58
4	0.60	0.46	0.00	54.73	0.62	0.65
5	18.13	22.70	10.98	0.00	11.15	0.00
6	10.47	15.06	2.87	28.32	5.98	0.65
7	1.16	0.42	0.00	60.65	0.85	0.96
8	0.00	4.55	0.00	0.00	0.00	0.00
9	0.19	18.49	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00
11	0.85	0.97	1.68	51.59	0.26	13.63
12	0.42	0.52	0.09	59.96	0.15	0.04
13	0.08	0.99	0.08	51.31	0.70	18.81
14	17.81	22.35	11.13	0.21	11.32	0.88
15	0.83	1.85	0.06	77.95	0.52	1.03
16	2.21	50.94	0.16	0.18	0.08	0.33
17	10.43	15.29	4.08	28.02	6.09	0.73
18	16.31	25.13	4.57	0.08	10.87	0.75
19	0.29	0.35	0.11	60.12	1.10	0.06
20	15.76	23.15	3.13	4.37	10.05	0.53
21	0.08	16.55	0.09	0.07	0.09	0.13
22	0.39	18.29	0.06	0.08	0.32	0.06
23	0.00	0.00	0.00	0.00	0.00	0.00
24	0.15	0.32	0.28	52.60	0.41	13.89
25	1.35	1.50	0.51	59.65	1.39	0.55
26	0.11	0.29	1.37	50.43	0.35	19.64
27	1.00	0.69	0.05	54.72	1.08	1.45
28	18.90	22.13	11.00	0.38	10.76	0.54
29	1.04	0.87	0.71	78.21	0.19	1.89
30	2.78	50.94	0.30	0.57	0.21	0.34
31	10.23	15.56	2.83	28.53	5.35	0.05
32	15.99	22.95	3.53	4.33	9.42	1.14
33	0.01	4.61	0.01	0.09	0.17	0.01
34	0.37	0.06	0.74	51.49	1.39	14.45
35	2.09	0.90	0.62	60.30	0.28	1.16
36	0.92	0.47	0.56	51.17	1.14	19.72
37	0.53	0.46	0.09	77.25	1.45	1.17
38	10.15	15.44	3.52	27.01	5.39	0.60
39	16.62	24.75	5.39	0.69	9.90	0.83
40	0.02	4.54	0.16	0.10	0.02	0.00
41	0.06	18.30	0.40	0.01	0.21	0.48
42	0.32	0.62	0.70	59.80	1.47	0.50
43	0.58	0.99	0.26	52.33	0.01	18.69
44	0.56	0.57	0.89	55.30	0.07	0.64
45	18.49	21.80	10.89	0.24	11.19	0.35
46	1.25	1.13	0.42	79.63	0.15	0.00
47	2.07	50.01	0.66	0.20	0.58	0.66
48	0.85	1.31	0.01	59.62	1.88	0.25
49	16.40	23.29	3.69	4.24	9.58	1.76
50	0.53	16.87	0.24	0.13	0.18	0.14
51	0.39	18.45	0.04	0.05	0.01	0.04
52	0.44	0.43	1.41	52.96	0.36	13.16
53	2.01	0.70	0.50	58.52	1.17	0.57
54	0.83	0.58	0.80	51.71	0.42	19.39
55	0.22	0.57	0.56	55.87	0.19	2.03
56	17.94	23.26	11.41	0.09	11.32	0.01
57	0.22	0.43	1.03	79.67	0.73	1.57
58	2.08	51.38	0.99	0.58	1.24	0.47
59	10.75	14.93	2.58	28.06	5.38	1.51
60	16.26	24.21	4.62	0.15	11.21	0.11
61	0.72	0.84	0.46	60.32	0.97	2.26
62	16.32	23.37	3.30	3.95	10.09	0.23
63	0.05	16.95	0.05	0.30	0.13	0.45

Table 2. Confusion matrix

N=18	Classified: HIGH (positive)	Classified: LOW (negative)
Actual: HIGH (positive)	TP=14	FN=0
Actual: LOW (negative)	FP=0	TN=4

Table 3 tabulates the test target, predicted test target, prediction errors and mean square error (MSE). This table shows predicted test target was same with the test target. That means no prediction output error for 18 test data and the mean square error was zero. By using the confusion matrix in Table 2, the performances criteria of NSVM can be measured. Table 4 shows the performance measures of this model. All the performance criteria such as accuracy, sensitivity, specificity, and precision were 100% and the MSE was 0.

Table 3. The test target, predicted test target, prediction errors, and MSE

Number Of Samples	Test Target	Predicted Test Target	Prediction Output Error	Mean Square Error (MSE)
1	1	1	0	0
2	1	1	0	
3	1	1	0	
4	2	2	0	
5	1	1	0	
6	1	1	0	
7	1	1	0	
8	2	2	0	
9	1	1	0	
10	1	1	0	
11	1	1	0	
12	1	1	0	
13	1	1	0	
14	2	2	0	
15	1	1	0	
16	1	1	0	
17	1	1	0	
18	2	2	0	

Table 4. Performance measures

Performance Criteria	RBF kernel (%)
Accuracy	100
Sensitivity	100
Specificity	100
Precision	100
MSE	0

5. CONCLUSION

In conclusion, the present study successfully graded the high and low-quality kaffir lime oil using NSVM. The NSVM model passed all performance measures with 100% accuracy, sensitivity, specificity, and precision. This finding and result are valid and important so that they will be encouraging and provide many benefits for future research, especially in systematic classification.

ACKNOWLEDGEMENTS

A big thank you to this research funder, the Ministry of Higher Education Malaysia, for providing me with financial support through the Fundamental Research Grant Scheme (FRGS) with Grant No: 600-IRMI/FRGS-RACER 513 (115/2019) and 600-RMC/GIP 5/3(152/2021). The authors would like to thank Universiti Teknologi MARA, Cawangan Pulau Pinang and the Faculty of Electrical Engineering, Universiti Teknologi MARA, Cawangan Pulau Pinang for their endless technical support.

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