



THE APPLICATION OF ELECTRONIC NOSE COUPLED WITH 80:20 K-NEAREST NEIGHBORS CLASSIFICATION TECHNIQUE FOR AGARWOOD OIL QUALITY INDEX ESTABLISHMENT

(Kombinasi Aplikasi Hidung Elektronik Bersama Teknik Klasifikasi 80:20 K-Nearest Neighbors Untuk Pembangunan Indek Kualiti Minyak Gaharu)

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Abstract

Agarwood oil is highly valued with numerous uses and benefits to the user. However, traditional agarwood grading techniques are subjective, time consuming and labor intensive with poorly reproducible results, in our study, a commercial Fox4000 electronic nose (EN) with AlphaSOFT software was evaluated as a substitute for human nose sniff assessment. Eight pure agarwood oil samples were used: the JBD sample that was selected as the initial high-grade reference sample based on previous research, and seven samples new to the FRIM collection. All samples were subjected to the EN tests and the seven new samples compared with the JBD sample using the non-parametric Wilcoxon's signed-rank test. The REG sample that was closest in aroma profile to JBD was then chosen as the high-grade reference sample for subsequent tests. Varying volumes of REG were blended with gurjun balsam and sandalwood pure oils to produce nineteen blended samples containing increasing percentages of REG. The 19 samples were then used in the EN tests for database establishment. All 19 blended samples were subjected to the EN tests and resulting data transformed using a z-score scale to generate an Agarwood Oil Quality Index (AOQI) that was classified into three levels based on percentage volume of agarwood oil in the oil blend. The EN significant sensor selection process was conducted using Spearman's rho correlation (SRC) and stepwise multi linear regression (SMLR). Finally, the 80:20 k-Nearest Neighbors (kNN) classifier was used to evaluate the AOQI model with the confusion-matrix based performance measure (CMBPM) as the classifier performance evaluator. The results showed SRC with 11 selected sensors outperformed SMLR with 80:20 k-NN test accuracy equal to 89.5%.

Keywords: agarwood oil grading, electronic nose, 80:20 k-NN classifier

Abstrak

Minyak gaharu dikenali mempunyai harga yang tinggi dengan pelbagai kegunaan dan manfaat kepada pengguna. Walau bagaimanapun, teknik penggredan gaharu secara tradisional adalah sangat terhad dari segi subjektiviti, keboleholungan yang rendah, penggunaan masa, dan kos buruh yang mahal. Dalam kajian ini, Hidung Elektronik (EN) Fox4000 komersial dengan perisian AlphaS OFT telah digunakan bagi menggantikan penilaian menghidu menggunakan hidung manusia. Lapan sampel minyak gaharu tulen telah digunakan. Sampel JBD telah dipilih sebagai sampel rujukan bergred tinggi berdasarkan kajian terdahulu. Semua sampel teraklukkan kepada eksperimen EN dan dibandingkan dengan sampel JBD menggunakan ujian peringkat-bertanda Wilcoxon bukan parametrik untuk pemilihan sampel rujukan gred tinggi yang baharu. Sampel REG telah dipilih dan dicampur dengan sampel minyak keruing dan cendana tulen. Kesemua 19 sampel campuran telah melalui ujian EN untuk penubuhan tiga tahap utama Indeks Kualiti Minyak Gaharu (AOQI) menggunakan skala skor-z. Proses pemilihan sensor EN yang signifikan telah dijalankan menggunakan teknik Spearman Rho Correlation (SRC) dan Stepwise Multi Linear Regression (SMLR). Akhirnya, teknik klasifikasi 80:20 k-Nearest Neighbors (k-NN) telah digunakan untuk menilai model AOQI dengan teknik Confusion-Matrix Based Performance Measure (CMBPM) sebagai penilai prestasi pengelasan. Keputusan menunjukkan SRC dengan 11 sensor terpilih mengatasi prestasi SMLR dengan ketepatan ujian 80:20 k-NN bersamaan dengan 89.50%.

Kata kunci: penggredan minyak gaharu, hidung elektronik, pengelasan 80:20 k-NN

Introduction

The wood and essential oils of agarwood (*Aquilaria* spp.) command very high prices of up to USD90,000/kg for grade AAAAA wood and USD14,000/kg for super grade essential oil on the global market. In Malaysia, grade A agarwood is priced at MYR18,000/kg [1]. Grading methods traditionally used by traders involve assessing the color (shine and resin content estimation), size, shape, fragrance, thickness and density of the raw materials. These grading methods are subjective and can leave the harvesters' product undervalued [2]. To address this problem, better techniques used to grade and classify agarwood woodchips and essential oils have been developed based on wood colour scale template (grades A through C) [3], intended usage (aroma, block, classic, dust, extractable wood and fragrance) [4], wood extractive resin content (A, B, C and D), and electronic nose (EN) grading (high and low grades) for wood [1].

Not as easily accessible are scientific grading or quality assessment techniques offered to the agarwood industry as technical services, such as gas chromatography (GC), gas chromatography–mass spectrometry (GCMS), solid phase micro extraction (SPME) and EN approaches. These methods are typically used separately to identify the selected predefined quality of agarwood oils (pure and in oil blends) and for low and high grade classifications [5-13]. To date, no research has evaluated the use of EN combined with chemistry inputs in quantifying agarwood oil percentages in oil blends for export regulation (taxation or tax exemption) or for use

by agarwood traders as an evaluation standard. This study proposes a technique to evaluate the established three levels of the agarwood oil quality index (AOQI) using the 80:20 k-NN classifier with Spearman's rho correlation (SRC) and stepwise multi linear regression (SMLR).

Materials and Methods

The overall research flow outlined in Figure 1 includes agarwood oil sample collection, EN tests, statistical analysis for selection of a high-grade reference sample, sample blending, EN features extraction, data scaling for AOQI and the 80:20 kNN classifier. The detailed methods for each step are described below.

Agarwood oil collection and high-grade reference sample selection

Eight agarwood oil samples and two common essential oils i.e., gurun balsam (*Dipterocarpus* sp.) and sandalwood (*Santalum album*) were collected or purchased from local reputable traders of agarwood oil. The Johor Baharu Deluxe (JBD) agarwood sample was selected as the high-grade oil benchmark and reference sample (REFF) as it reportedly contains all significant chemical compounds found in high-grade agarwood. A new high-grade agarwood oil reference (B1) was selected based on its EN fingerprint aroma, from seven new samples in the Forest Research Institute Malaysia (FRIM) collection (EXQ-OUDO30, HER-OUDO35, MAL1-OUDOI9, MAL2-OUDOI10, MAL3-OUDOI11, MAJ-OUDOI12 and REG-OUDOI13), and using statistical cor

relation of EN data with JBD EN data.

Sample blending processes and EN tests

Pure samples of the three selected reference oils: agarwood (B1), sandalwood (B2) and gurjun balsam (B3) were blended by volume in ratios as given in Table 1. A total of 19 samples (S1–S19) were blended. The blending formula in Table 1 was based on fixed volumes of B2 and B3 while the volume of B1 varied from 0% to 90%. S12 had an equal volume ratio for B1, B2 and B3 (33%:33%:33%). The percentage value of agarwood oil was represented by the percentage value of its volume in the blended oil samples. A commercial FOX4000 EN (Alpha-MOS, Toulouse, France) containing an 18-sensor array of metal oxide semiconductor (MOS) chemical sensors, bundled with AlphaSOFT version 12 data analysis software were used. The EN sensor chambers were divided into three types of high performance (HiP) chambers: chamber A containing doped metal oxide sensors (T30/1, P10/1, P10/2, P40/1, T70/2 and PA2), chamber B containing doped metal oxide sensors (P30/1, P30/2, P40/2, T40/2, T40/1 and TA2) and chamber CL2 containing undoped metal oxide sensors (LY2/AA, LY2/G, LY2/gCT, LY2/gCTI, LY2/Gh and LY2/LG). The carrier gas used was purified air grade ($P = 5$ psi). For each EN test, the sample was first prepared, heated, then injected via an injection port into the EN sample inlet, which recorded sensor response data into a main database. The EN was used to capture the uniqueness of each sample's scent and transform that information into sensor response data. The headspace generated from each heated sample was injected manually into the injection port using a gas-

tight syringe. The system allowed the purified air as the headspace carrier gas to carry the sample headspace through all three chambers in the system and exit at the exhaust port. Simultaneously, the AlphaSOFT software recorded all EN raw data in the database. A total of 135 sample vials were used in the EN tests in developing the database.

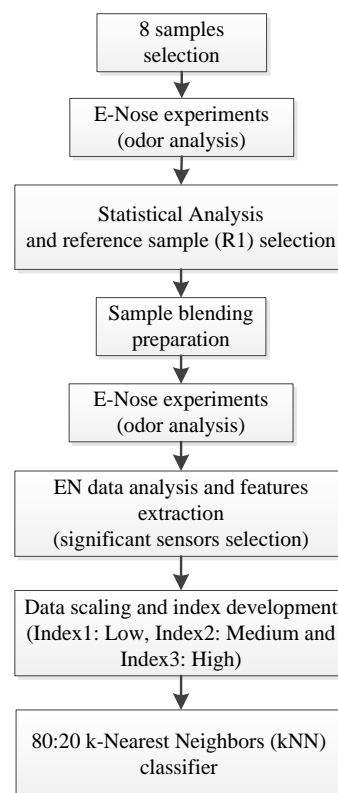


Figure 1. Overall research flowchart showing progression of samples in the electronic nose (EN) tests

Table 1. Ratios (by volume) of essential oil blends for samples used in the study; agarwood oil being the main reference

	Essential Oil Blend Ratio																			
	Sample No.	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19
Sandalwood, B3 (fixed)	%	50.0	49.5	49.0	48.0	47.0	46.0	45.0	42.5	40.0	37.5	35.0	33.3	32.5	30.0	25.0	20.0	15.0	10.0	5.0
	Gram (mg)	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00
Gurjum balsam, B2 (fixed)	%	50.0	49.5	49.0	48.0	47.0	46.0	45.0	42.5	40.0	37.5	35.0	33.3	32.5	30.0	25.0	20.0	15.0	10.0	5.0
	Gram (mg)	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	150.00	0.15	0.15	0.15	0.15
Agarwood, B1 (variable)	%	0.0	1.0	2.0	4.0	6.0	8.0	10.0	15.0	20.0	25.0	30.0	33.3	35.0	40.0	50.0	60.0	70.0	80.0	90.0
	Gram (mg)	0.00	3.00	6.10	12.50	19.10	26.10	33.30	52.90	75.00	100.00	128.00	150.00	161.00	200.00	300.00	450.00	0.70	1.20	2.70
TOTAL (mg)		300.00	303.00	303.12	312.50	319.10	326.10	333.30	352.90	375.00	400.00	428.00	450.00	461.00	500.00	600.00	750.00	100.00	150.00	300.00

Agarwood oil quality index (AOQI) scaling and 80:20 k-nearest neighbors' classifier (kNN)

The AOQI scale is based on the conversion of B1 values (of 0% to 90%) in the sample blends (S1-S19) into a z-score scale using the z-score transformation. The z-score is a standard score method that normalises each score to its standard deviation from the mean score. For the z-score data scaling process in our study, the main EN database data were converted into x-scale values using Equation 1.

$$Z_{\text{score}} = \frac{X - \mu}{\sigma} = \frac{X - \text{mean}}{\text{standard deviation}} \quad (1)$$

Z-score conversion values (Table 2) produced two main threshold values that fell between -0.55 and -0.37 (closest to -0.5) and between 0.34 and 0.70 (closest to 0.5), which corresponded with 20% and 50% B1 volumes in the original data for the blended samples, respectively. Three indices were selected for AOQI with z-score and actual values as illustrated in Figure 2. As a result, three values for AOQI were established as represented in Equation 2.

$$\text{Agarwood oil quality index (AOQI)} = \begin{cases} \text{INDEX 3: HIGH \% VOLUME} \geq 50\% \\ 20\% < \text{INDEX 2: MIDDLE \% VOLUME} < 50\% \\ \text{INDEX 1: LOW \% VOLUME} \leq 20\% \end{cases} \quad (2)$$

Table 2. The Agarwood Oil Quality Index (AOQI) three scales based on z-score conversion values

		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	
B1 (Variable)	%	0.00	1.00	2.00	4.00	6.00	8.00	10.00	15.00	20.00	25.00	30.00	33.33	35.00	40.00	50.00	60.00	70.00	80.00	90.00	
	z-score	-1.09	-	-	-	-	-	-0.73	-0.55	-0.37	-0.20	-0.02	0.10	0.16	0.34	0.70	1.05	1.41	1.77	2.12	
			1.05	1.02	0.95	0.87	0.80														
		INDEX 1 _{z-score} ≤ -0.37									-0.37 < INDEX 2 _{z-score} < 0.34					INDEX 3 _{z-score} ≥ 0.34					
		INDEX 1 _{real} ≤ 20%									20% < INDEX 2 _{real} < 50%					INDEX 3 _{real} ≥ 50%					

K nearest neighbor (kNN) is one of the simplest machine learning algorithms with a robust statistical-based supervised machine learning classification technique. The kNN classifier assigns samples that are unclassified to the class that most of its k-nearest neighbors belong to. Furthermore, it is a classifier that uses distance between a point and all its neighbors in an image to find nearest neighbors. The core idea of the kNN algorithm is to select the category of the sample with the most same categories among the K nearest samples in the feature space as the classification of the sample to be tested [14-18].

In our study, the 80:20 kNN was optimized with training and testing datasets constructed from 80% and 20% data partitioned from total EN data, respectively. Three AOQI indices represent three different classes (Figure 2) and the three indices previously defined with the z-score method therefore show 8, 6 and 5 samples falling under Index 1, 2 and 3, respectively.

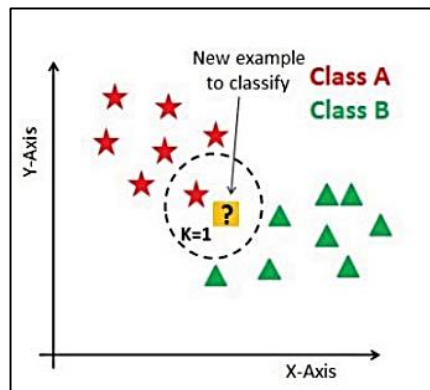


Figure 2. K-nearest neighbor (kNN) classifier illustration [17]

The 80% training dataset consisted of 64 data from Index 1, 48 data from Index 2 and 40 data from Index 3 for a total of 152 data (Table 3). All unique data patterns related to each index group were recorded in the kNN model. The remaining 20% testing data consisted of 16 data from Index 1, 12 data from Index 2 and 10 data from Index 3.

for a total of 38 data. After that, the 20% testing data were projected to the kNN classifier training database to find the nearest matching index group. Finally, classifier accuracy was calculated using the confusion-matrix based performance measure (CMBPM; Equation 3) where TP = true positive, TN = true negative, FN = false

negative and FP = false positive. The highest classifier accuracy is 100%.

$$80:20\ k-NN\ Accuracy\ (\%) = \frac{TP + TN}{TP + TN + FN + FP} \quad (3)$$

Table 3. The agarwood oil quality index (AOQI) three scales with electronic nose (EN) data distribution for 80:20 kNN classifiers

INDEX 1 _{real} ≤ 20%								20% < INDEX 2 _{real} < 50%						INDEX 3 _{real} ≥ 50%				
S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19
Data matrix size = [18 sensors x 5 vials x 8 samples] + 100% synthetic data = [80 x 18]								Data matrix size = [18 sensors x 5 vials x 6 samples] + 100% synthetic data = [60 x 18]						Data matrix size = [18 sensors x 5 vials x 5 samples] + 100% synthetic data = [50 x 18]				
Training _{80%} = 64 samples								Training _{80%} = 48 samples						Training _{80%} = 40 samples				
Testing _{20%} = 16 samples								Testing _{20%} = 12 samples						Testing _{20%} = 10 samples				

Results and Discussion

For the normal data distribution test, all samples were not normally distributed as all p and h values were < 0.05 and 1, respectively (Table 4). Thus, a non-parametric statistical test was selected. For EN data comparison between JBD with seven selected samples using the Wilcoxon rank sum test, REG had the highest p-value =

0.78293 and h = 0 indicating REG had almost the same odor data in continuous distribution as JBD (Table 5). The REG sample was then selected as the reference agarwood oil (B1) mixed with B2 and B3 to produce 19 oil blend samples. All 19 samples were subjected to EN testing and were stored in the main EN database.

Table 4. The results of the sample normality distribution test (Lilliefors test) for the eight agarwood oil samples

	JBD	MAL2	MAL3	MAJ	REG	MAL1	EXQ	HER
P-value	0	5.83E-05	0.005966499	6.67E-05	0	0.000617	0	0
h	1	1	1	1	1	1	1	1

Table 5. The Wilcoxon rank sum test comparison of the high-grade reference agarwood oil (JBD) against seven other agarwood oil samples

	JBD-MAL2	JBD-MAL3	JBD-MAJ	JBD-REG	JBD-MAL1	JBD-EXQ	JBD-HER
P-value	0.00424	0.0006	0.61824	0.78293*	0.0006	0.04161	0.0588
h	1	1	0	0*	1	1	0

*Note: P-value > 0.05 & h=0 ----> x1 and x2 are from the same continuous distribution

From Spearman's rho correlation (SRC) test in Table 6, all 11 less correlated sensors with p < 0.05 were selected including T30/1, P10/1, P10/2, P40/1, T70/2, PA/2, P30/1, P30/2, T40/2, T40/1 and TA/2. From MATLAB results in Figure 3, five EN sensors including LY2/LG,

LY2/G, LY2/GH, P10/2 and P10/2 were selected by stepwise multi linear regression (SMLR). Both groups of selected sensors were then tested using the kNN 80:20 classifier and the result with the best classification accuracy was chosen.

Table 6. Spearman's rho correlation (SRC) results for the electronic nose 18-sensor array

		S7	S8	S9	S10	S11	S12	S13	S15	S16	S17	S18
		T30/1	P10/1	P10/2	P40/1	T70/2	PA/2	P30/1	P30/2	T40/2	T40/1	TA/2
S7	T30/1	1.000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
S8	P10/1	FALSE	1.000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
S9	P10/2	FALSE	FALSE	1.000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
S10	P40/1	FALSE	FALSE	FALSE	1.000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
S11	T70/2	FALSE	FALSE	FALSE	FALSE	1.000	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
S12	PA/2	FALSE	FALSE	FALSE	FALSE	FALSE	1.000	FALSE	FALSE	FALSE	FALSE	FALSE
S13	P30/1	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1.000	FALSE	FALSE	FALSE	FALSE
S15	P30/2	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1.000	FALSE	FALSE	FALSE
S16	T40/2	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1.000	FALSE	FALSE
S17	T40/1	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1.000	FALSE
S18	TA/2	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	1.000

```
mdl = LinearModel.stepwise(X_norm,y,'constant','upper','linear')
1. Adding x8, FStat = 31.3251, pValue = 2.19115e-07
2. Adding x9, FStat = 37.4543, pValue = 2.2613e-08
3. Adding x5, FStat = 20.6649, pValue = 1.67939e-05
4. Adding x2, FStat = 30.6164, pValue = 3.0622e-07
5. Adding x1, FStat = 5.6516, pValue = 0.019581
6. Adding x4, FStat = 9.2139, pValue = 0.0031586
7. Removing x5, FStat = 0.52906, pValue = 0.46893

mdl =

Linear regression model:
    y ~ 1 + x1 + x2 + x4 + x8 + x9

Estimated Coefficients:
              Estimate      SE      tStat      pValue
(Intercept)    1.8421    0.045282    40.681    2.7368e-59
x1              0.76541    0.22417     3.4145    0.00096424
x2             -1.9358    0.41402    -4.6756    1.0376e-05
x4              2.906     0.3891     7.4685    5.2772e-11
x8              2.1268    0.22559     9.4277    4.8863e-15
x9             -1.7152    0.22532    -7.6123    2.6927e-11

Number of observations: 95, Error degrees of freedom: 89
Root Mean Squared Error: 0.441
R-squared: 0.723, Adjusted R-Squared 0.708
F-statistic vs. constant model: 46.5, p-value = 2.18e-23
```

Figure 3. Electronic nose sensor selection using stepwise multi linear regression (SMLR) in MATLAB

The highest kNN 80:20 classifier training accuracy values for SMLR and SRC were from $k = 1$ and $k = 2$, respectively, while the highest kNN 80:20 classifier testing accuracy values for SMLR and SRC were from $k = 4$ and $k = 1$ same as $k = 2$, respectively (Figures 4 and 5). Between the two features extraction techniques,

the best k-NN 80:20 classifier training and testing accuracy values were from SRC with values of 100.0% and 89.5%, respectively. While SMLR had a training accuracy of 100.0%, testing accuracy was only 82.5% (Table 7).

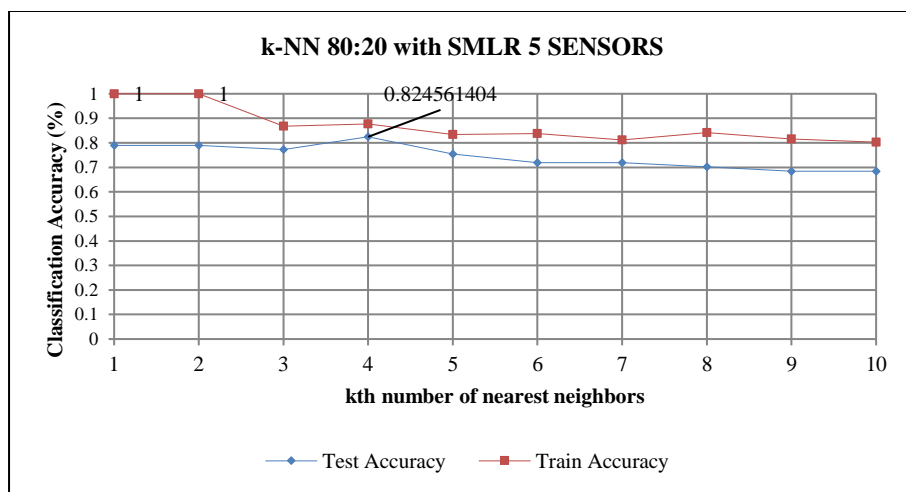


Figure 4. 80:20 k-nearest neighbors (kNN) training and testing classification accuracy with five selected sensors using the stepwise multi linear regression (SMLR) features extraction technique

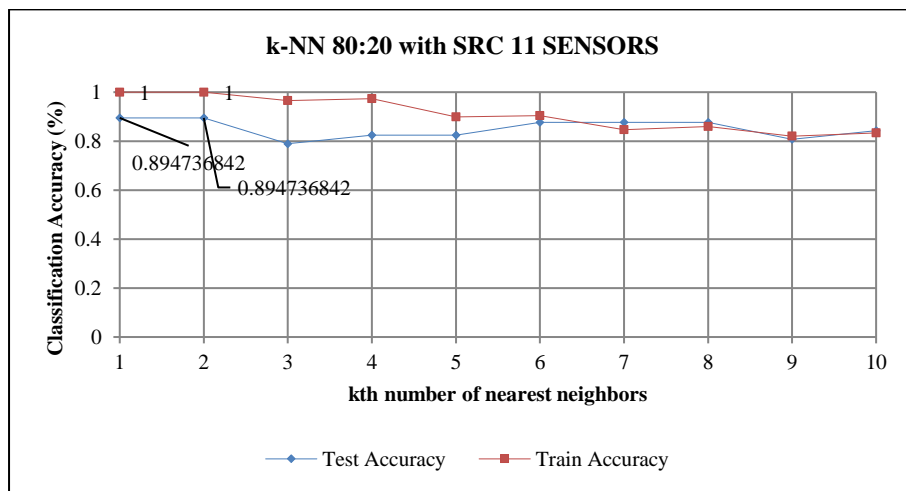


Figure 5. 80:20 k-nearest neighbors (kNN) training and testing classification accuracy with 11 selected sensors using Spearman's rho correlation (SRC) features extraction technique

Table 7. Summary of k-nearest neighbors (kNN) classifier training and testing accuracy for stepwise multi linear regression (SMLR) and Spearman's rho correlation (SRC) features extraction techniques

Classifier	SMLR 5 Sensors		SRC 11 Sensors	
	Train (Accuracy: %)	Test (Accuracy: %)	Train (Accuracy: %)	Test (Accuracy: %)
80:20 kNN	100.0	82.5	100.0	89.5

Conclusions

The REG sample was selected from among seven new samples in the FRIM collection as the high-grade reference (B1) in our study because it had an aroma profile closest to that of the JBD sample. Varying

volumes of B1 were then mixed with B2 and B3 (in fixed, 1:1 ratios) to produce nineteen blended samples containing increasing percentages of B1. The 19 samples were then used in the EN tests for database establishment. The z-score-transformed EN data

successfully indexed the AOQI into three levels. The AOQI with 11 sensors selected by SRC was proven to generate a classification test accuracy that was 7% higher than the SMLR-selected 5 sensors (89.5% vs 82.5% respectively). Lastly, the kNN classifier only needed 11 significant sensors from 18 sensors to produce the best test accuracy. In conclusion, the 80:20 kNN classifier was proven to classify the percentage volume of pure agarwood oil in the oil blend into three groups with Index 1, 2 and 3 denoting AOQI low, medium and high percentage volumes of $\leq 20\%$, $20\% < \text{index} < 50\%$ and $\geq 50\%$, respectively.

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