

RESEARCH ARTICLE

Case Modelling Odour Profiles and Temperature Intensity of Water: A Comparative Analysis using Case-Based Reasoning and K-Nearest Neighbours

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ABSTRACT - Water, a vital resource for human life and global economic activities, prompts ongoing water quality studies in Malaysia due to excessive usage. This study investigates Malaysia's water resources condition, focusing on identifying water through its odor profile relative to temperature intensity. Clean and pure drinking water is crucial for global human health, necessitating knowledge of water source content to mitigate health risks from water quality degradation caused by inorganic contaminants, heavy metals, and microbial pollutants. Recent interest in water quality stems from the high demand for clean water and population growth. This research employs E-Anfun, mimicking the human nose, to establish a case library profile for tap and lake water samples based on odor attributes. Using Case-Based Reasoning (CBR) and K-Nearest Neighbour (KNN), the study classifies water odor profiles and evaluates performance. The E-nose simplifies the process with gas sensors of varying odor sensitivity. Samples collected based on temperature intensity are managed using Microsoft Excel and MATLAB for normalization. CBR, utilizing four cycles, intelligently classifies by solving new problems based on prior successful solutions. KNN enhances CBR by classifying data samples based on proximity to learning data. Evaluation using a recognized confusion matrix indicates 100% accuracy, sensitivity, and specificity for CBR. For KNN, the accuracy increases with the ratio, starting at 97.056% for k=3 with a 10:90 ratio, accompanied by 84.833% sensitivity and 98.369% specificity. Both CBR and KNN successfully classify tap and lake water odour profiles.

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1.0 INTRODUCTION

Water is a fundamental component of practically all forms of production, including agriculture, industry, power, and transportation (Baleta et al., 2019); water is a source of life, livelihood, and prosperity. It is a vital component of life and essential to the existence of all living things (Khan et al., 2020). (Sharma et al., 2020) It has been acknowledged for millennia that human survival and ecological protection depend on the dependable availability of abundant water of adequate quality.

The World Health Organization (WHO) (Mishra et al., 2021) states that access to safe drinking water is a fundamental human right. Since 1990, 2.6 billion people have gained access to improved drinking water, with 96% residing in urban areas and 84% living in rural regions (WHO and UNICEF 2015). 663 million people continue to rely on unimproved tap water sources, including as unprotected wells, springs, and surface water, according to (Hirai et al., 2019). Almost half of the population resides in Sub-Saharan Africa, while one-fifth is in Southern Asia.

Malaysia is a tropical nation that receives abundant rainfall throughout the year, but the nation continues to struggle with water scarcity and water quality issues. Over 63.94 percent (144) of Malaysia's 477 rivers are classed as Class II, while 30.19 percent (144) are classified as Class III, citing the Department of Environment's 2017 Annual Report. Biochemical oxygen demand (BOD) from sewage, agriculture, and manufacturing, ammoniacal nitrogen from animal farms and domestic sewage, and suspended particles from earthwork and land clearing activities are the principal pollutants in rivers (Ismail et al., 2021). The remaining 1% is sourced from groundwater (Mridha et al., 2020). In Malaysia, tap water, bottled water, and bottled mineral water are the most common sources of drinking water (Praveena et al., 2023). On the West Coast of Peninsular Malaysia, Sungai Langat, Sungai Selangor, and Sungai Kinta are among the most regularly used water sources for drinking water (Mohtar et al., 2019). In contrast, states such as Kelantan, Terengganu, Pahang, Perlis, Kedah, Sabah, and Sarawak rely on groundwater as a supply of drinking water (Jones et al., 2021). Although extensive research on drinking water quality has been undertaken in Malaysia, no comprehensive study of the situation of drinking water quality has, to our knowledge, been conducted yet. While some studies have evaluated

microbiological, chemical, elemental, and physical parameters in treated water, filtered water, ground water, and mineral water, it is difficult to draw conclusions regarding the nation's drinking water quality.

The rising costs of water and wastewater treatment, as well as the increasing demand for safe drinking water, have led businesses and governments around the world to study innovative water-saving technology. Electronic Nose (E-Nose) is a device that compares and identifies gaseous samples (or emissions from liquid or solid samples) using non-specific chemical sensors and statistical pattern recognition algorithms (Naquuddin et al., 2020). Using a collection of such non-specific sensors, the relative responses of the sensors can be used to generate a unique odour profile (Tan et al., 2020). The odour profile can then be further analyzed (Viejo et al., 2020) using pattern recognition techniques and/or neural network algorithms. Thus, the recent availability of commercial E-Noses for detecting and evaluating headspace odours may provide a more quick and practical technique for monitoring the purification process and the quality of potable water than laboratory-based conventional methods.

Electronic noses offer a wide range of commercial applications in fields such as agriculture, biomedicine, cosmetics, the environment, food, industry, the military, regulatory science, and pharmaceuticals (Zhuang et al., 2023). The role of the e-principal nose is to detect odours created as gases or vapour (Park et al., 2019), which is ideal for water because it contains a variety of volatile odour-profiles and temperature intensities (Casco et al., 2023). Several intelligent classification methods, such as case-based reasoning (CBR) (Zahari et al., 2022), k-nearest neighbours algorithm (k-NN) (Hanif et al., 2021), and artificial neural network (ANN) (Rasekh et al., 2021), have been mentioned. CBR is one of the mentioned intelligent systems that does not require training and is only applicable to a limited domain area (Guo et al., 2021).

2.0 METHODS AND MATERIAL

The overall flowchart of the study is presented in Figure 1. The classification of tap and lake water based on temperature intensity involves four main steps. The first step is data collection, which is performed using the E-Nose device. Following data collection, the next step involves data pre-processing to extract the odor features from each sample. The extracted features are then subjected to classification using intelligent techniques such as k-Nearest Neighbours (k-NN) and case-based reasoning (CBR).

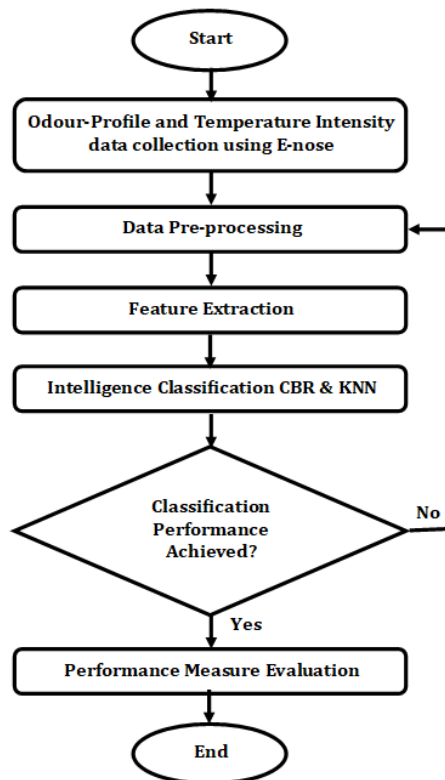


Figure 1. Overall flowchart for tap and lake water odour-profile classification.

2.1 Water Sample

This study selected two types of water, namely tap water and lake water, for investigation. The tap water samples were collected from the Bio Aromatic Lab at UMPSA Universiti Malaysia Pahang Al-Sultan Abdullah Gambang, while the lake water samples were obtained from UMP Pekan. To maintain sample integrity, all supplied samples were carefully

stored in closed containers, ensuring no contamination occurred. During the data collection process, each sample was contained within a 400mL bottle and processed in a closed room.

2.2 Electronic Nose Setup

Figure 2 illustrates the water sample used for E-Nose data collection. The E-Nose setup used to measure odour data is depicted in Figure 3. Within the E-Nose chamber, there are four sensor arrays positioned in parallel. The E-Nose incorporates an internal pump that facilitates the controlled intake of gas from both water samples. The sensors integrated in the E-Nose have the capability to detect various gases, including carbon monoxide (CO), LPG, CH₄, natural gas, propane, methane, i-butane, alcohol, hydrogen, and smoke. During the experiment, the odour data captured by the four sensor arrays are transmitted to a computer equipped with Arduino software for further analysis.



Figure 2. Electronic nose experimental setup.

To ensure consistency, a heating system was implemented to maintain the sample temperature at five different levels, ranging from 10°C to 50°C, for each water sample. As depicted in Figure 3, the experimental setup involved a measurement phase lasting 2 minutes, followed by a cleaning phase lasting 3 minutes. In the cleaning phase, the sample was removed from the E-Nose chamber while the system and pump continued to operate, effectively eliminating residual odour from the previous sample prior to initiating the subsequent experiment. This cleaning phase was deemed necessary to minimize reading errors.

For each experiment, a total of 200 data points were collected. The experiment was repeated five times for each water sample. All the acquired data were systematically tabulated in Table 1. In Table 1, the designations S1, S2, S3, and S4 correspond to sensor 1, sensor 2, sensor 3, and sensor 4, respectively, while DM represents the data measurement. The subscript number associated with DM indicates the specific odour reading and sensor number. For instance, DM1,1 denotes the first data measurement captured by sensor 1.

Table 1. Data measurement table for tap and lake water odour-profile.

Data Measurement	S1	S2	S3	S4
1	DM1,1	DM1,2	DM1,3	DM1,4
2	DM2,1	DM2,2	DM2,4	DM2,4
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
N	DMN,1	DMN,2	DMN,3	DMN,4

2.3 Data Preprocessing

Reference During the data processing stage, the collected data will undergo normalization using Equation 1, as depicted below:

$$R' = \frac{R}{R_{max}} \quad (1)$$

where: R' represents the normalized data, R_{max} is the highest odor data within each row, and R corresponds to the odor data for each sensor. Table 2, presented below, showcases the normalized data obtained from both water samples.

To achieve normalization, all the data points in each row are divided by the largest value within that row. The primary objective of normalization is to rescale the data within the range of zero to one (0 to 1). In Table 2, ND denotes the normalized data, while S1, S2, S3, and S4 correspond to sensor 1, sensor 2, sensor 3, and sensor 4, respectively. The subscript number associated with ND represents the specific odor reading and sensor number. For instance, ND11 signifies the first normalized data measurement captured by sensor 1.

Table 2. Data normalization table for tap water correlation of odour-profile and temperature intensity.

Normalized Data	S1	S2	S3	S4
1	ND1,1	ND1,2	ND1,3	ND1,4
2	ND2,1	ND2,2	ND2,3	ND2,4
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
N	NDN,1	NDN,2	NDN,3	NDN,4

2.4 Feature Extraction

Each sample's characteristics were determined using the normalized value. Normalized values will be classified according to the degree of tap water deterioration. The mean of the normalized values produced ten instances in each category. For the categorization procedure, the examples from each category were tabulated and placed into the CBR memory as "stored cases" or "past experiences". The use of boxplots to validate the data of feature extraction is crucial in ensuring that the data is suitable for use in CBR and KNN algorithms, as it provides a visual representation of the data's distribution and highlights any potential outliers that may affect the accuracy of the algorithms.

2.5 Intelligent Classification

The method that will be used for classification are K-Nearest Neighbours (KNN) and Case-based Reasoning (CBR), this is to compare which one is the best method for classification.

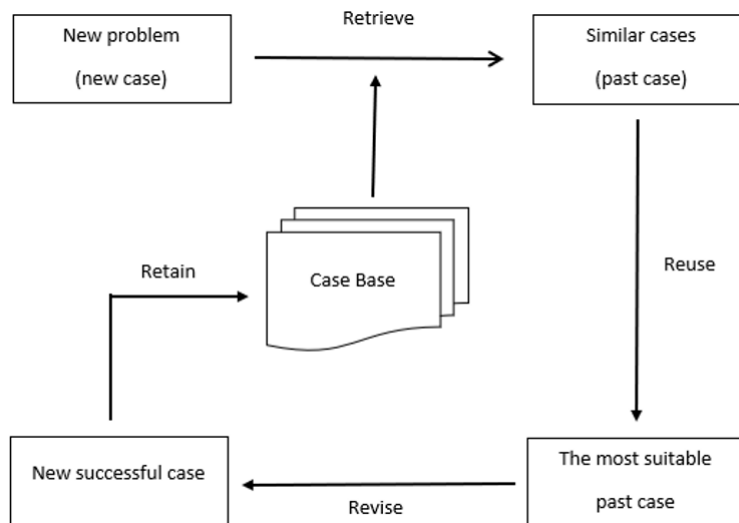


Figure 3. CBR cycle system

2.5.1 K-NN Classification Technique

KNN classifier is one of intelligent classification techniques that can be run in MATLAB software as there are the setting algorithm for this function in software. To complete classification technique in this system, the distance of data was measured by applying selective rule. The measured data was compared between training and testing data. This system was started with input and output assignment. In this step, input and output of the system was clearly declared. The input the mean of cluster data for each sample and output is the class for each sample. The value assigned for input and output remains the same. The second step was data preparation. To find the best performance of intelligent classification using KNN, it undergoes data splitting or split sample technique. Total data is subsample to 'training' data and the remaining data is subsample to 'testing' data which is prepared accordingly to training to testing ratio. This practice approach is accepted by Cool et al, 1987 and already practice by other researchers using statistical measures 70:30, 60:40 and 50:50 (Surendiran & Vadivel, 2011). In this step, the total data was split from ratio 10:90 until 90:10 before it was inserted into the system. The next step was assigning the training and testing prepared data. The data of the training was assigned first in the system and continued with testing data. The system has automatically calculated the class of the testing data based on training data. Consequently, the confusion matrix was done to measure true and false case from result of classification.

Lastly, performance measures of water classification using KNN was evaluated. The three distance that being used are Euclidean, Minkowski and Cityblock.

$$d(x, y) = \sqrt{\sum_{i=1}^k x_i - y_i^2} \quad (2)$$

$$(d(x, y) = \sum_{i=1}^k (|x_i - y_i|^2)^{1/q} \quad (3)$$

$$d(x, y) = \sum_{i=1}^m |x_i - y_i| \quad (4)$$

2.5.2 CBR Classification Technique

CBR terminology, a case usually denotes a problem situation. A previously experienced situation, which has been captured and learned in a way that it can be reused in the solving of future problems, The Case-Based Reasoning, has marked its existence in the field of decision-making in diverse areas, with a standing success rate. Case based reasoning (CBR) is the technique, which involves the process of solving new problems based on the solutions of similar past problems, i.e., it works on the basis of previously experienced and stored problem-solution case set. Retrieve, Reuse, Revise, and Retain are the four key steps involved in the CBR process to solve or predict an optimal solution for new problems or cases. If the sample has a high similarity percentage with a previously stored sample, the system will use the information from the previously stored case to decide or provide an answer. In the CBR retrieval cycle, one case out of 100 stored examples was chosen to calculate the similarity percentage between two examples. The remaining 99 cases are then left as the remaining stored cases. The similarity % was calculated using Equation. If the percentage of similarity between two cases is the largest, it indicates that the distance between the two examples is small, and they belong to the same group.

$$\text{Similarity } (T, S) = \frac{\sum_{i=1}^n f(T_i, S_i) \times W_i}{\sum_{i=1}^n W_i} \quad (5)$$

In this equation, T and S represent the target and source cases, respectively, n is the number of attributions for the tap and lake water sample, i is the single attribution for each case, f is the formulation of the similarity function for the tap water sample, and w is the weight of each attribution.

2.5.3 Performance Measure

The result of the CBR Classification was evaluated using a confusion matrix. Equations (2)-(4) were utilized to calculate the overall sensitivity, specificity, and accuracy of the tap water sample in the categorization process.

$$\text{Sensitivity} = \frac{TP}{TP + FN} \quad (6)$$

$$\text{Specificity} = \frac{TN}{FP + TN} \quad (7)$$

$$\text{Accuracy} = \frac{TP + TN}{P + N} \quad (8)$$

The classification's sensitivity was calculated by dividing the true positive value of the classification result by the sum of the classification's true positive (TP) and false negative (FN). The classification's specificity was calculated by dividing true negative (TN) by the sum of false positive (FP) and true negative (TN). While the classification accuracy was calculated by dividing the sum of true positive and true negative with the total case (P+N).

3.0 RESULTS AND DISCUSSION

3.1 Raw Data Measurement

10 samples have been evaluated. Each sample was subjected to five repeated experiments with different temperatures, each with 200 data measurements, for a total of 1000 data measurements per sample. As a consequence, 10000 data measures were gathered from all samples and are summarized to be in data pre-processing.

3.2 Data Pre-processing

We normalized a total of 10000 previously obtained data measurements by dividing each value in each row of data measurements by the highest value in its own row. Following that, we separated the 10000 normalized data points into ten groups, one for each sample. Following that, 1000 normalized data sets were grouped into ten categories consisting of ten cases each. For normalization figure 4.21 summarizes the results of the 10 sample of correlation between odour-profile and temperature intensity of water using 200 data points.

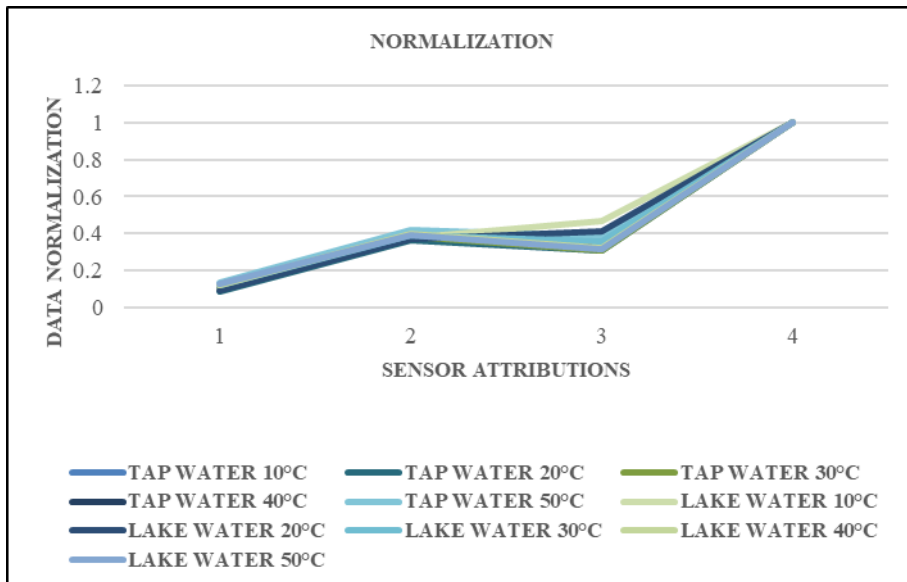


Figure 4. Normalization.

3.3 Data Pre-processing

The crucial aspect of validating the extracted features for subsequent analysis using Case-Based Reasoning (CBR) and k-Nearest Neighbors (KNN) was demonstrated through a unified boxplot graph. This comprehensive visualization integrated temperature-dependent characteristics from 10 samples, combining data from both tap water and lake water sources. The dataset encompassed a temperature range of 10 to 50 degrees Celsius, with 5 samples from each water source. The boxplot graph effectively illustrated the spread, median, and outliers within this amalgamated dataset, providing a robust validation of the feature extraction process. The graphical representation not only assured the statistical integrity of the extracted features but also established the dataset's suitability for subsequent analysis using CBR and KNN. This validation reinforces the confidence in the selected features, ensuring that the patterns observed in both tap and lake water samples across the specified temperature range are well-represented and ready for further in-depth analysis.

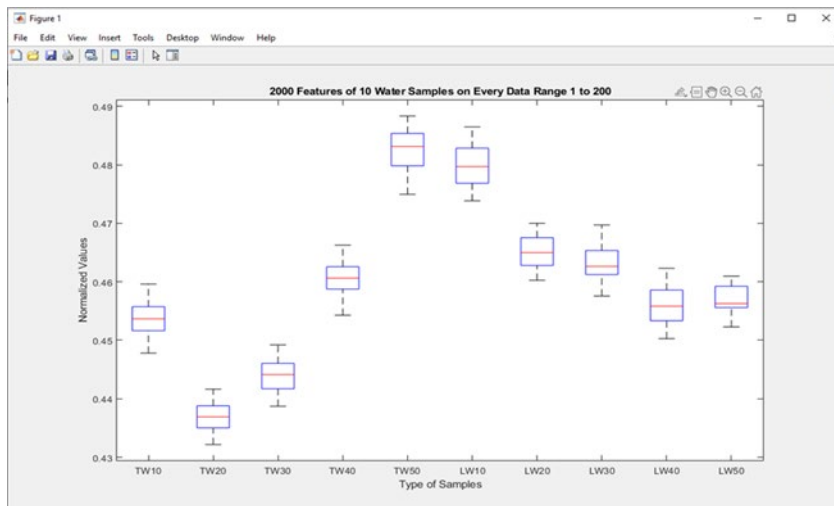


Figure 5. Boxplot = data spread/median/outliers

3.4 Intelligence Classification

3.4.1 K-Nearest Neighbour (KNN)

The K-Nearest Neighbour (KNN) method begins with feature extraction results from tap and lake water samples. A KNN algorithm is implemented to classify odor profiles, utilizing raw data from a Microsoft Excel file via MATLAB's 'xlsread' function. The data is split into 10 sets for cross-validation, maintaining a 10:90 ratio for training and testing. The code defines indices for each set, ensuring representative randomized data. The model is trained and tested for samples 1 to 10, evaluating performance using the Euclidean distance metric. Additionally, the code assesses the impact of different values of k on classification accuracy and visualizes results. The process is repeated for 'Minkowski' and 'Cityblock' metrics, with accuracy presented as a percentage.

3.4.2 Case Base Reasoning (CBR)

The performance evaluation of the CBR classifier for categorizing tap water odour profiles is provided in figure 6. The classification's sensitivity, specificity, and accuracy were determined using Equations (1)–(3).

		sample 1	sample 2	sample 3	sample 4	sample 5	sample 1	sample 2	sample 3	sample 4	sample 5
actual	sample 1	30	0	0	0	0	0	0	0	0	0
	sample 2	0	30	0	0	0	0	0	0	0	0
	sample 3	0	0	30	0	0	0	0	0	0	0
	sample 4	0	0	0	30	0	0	0	0	0	0
	sample 5	0	0	0	0	30	0	0	0	0	0
	sample 1	0	0	0	0	0	30	0	0	0	0
	sample 2	0	0	0	0	0	0	30	0	0	0
	sample 3	0	0	0	0	0	0	0	30	0	0
	sample 4	0	0	0	0	0	0	0	0	30	0
	sample 5	0	0	0	0	0	0	0	0	0	30

Figure 6. Confusion matrix.

By examining the CBR vote results, 30 examples for each sample were identified. Because the vote involves K1, K2, and K3, 10 cases equal 1K, which are resulting in 30 cases per sample (Highest significance value). The cases for samples 1–5 with a result of 1 correspond to an assessment value of 1 in terms of sensitivity, specificity, and accuracy for each tap water sample. Thus, for K = 1, K = 2, and K = 3, each sample's sensitivity, specificity, and accuracy are all 100%. Sensitivity, specificity, and accuracy are all 100% for categorizing tap water samples using the CBR classification methodology

	ACTUAL									
	sample 1	sample 2	sample 3	sample 4	sample 5	sample 1	sample 2	sample 3	sample 4	sample 5
Total Cases	30	30	30	30	30	30	30	30	30	30
Condition Positive(P)	30	30	30	30	30	30	30	30	30	30
Condition Negative(N)	270	270	270	270	270	270	270	270	270	270
True Positive(TP)	30	30	30	30	30	30	30	30	30	30
False Positive (FP)	0	0	0	0	0	0	0	0	0	0
True Negative (TN)	270	270	270	270	270	270	270	270	270	270
False Negative(FN)	0	0	0	0	0	0	0	0	0	0
Sensitivity=TP/(TP+FN)	1	1	1	1	1	1	1	1	1	1
Specify=TN/(TN+FP)	1	1	1	1	1	1	1	1	1	1
Accuracy= (TP+TN)/(P+N)	1	1	1	1	1	1	1	1	1	1
Overall Sensitivity(%)	100									
Overall Specificity(%)	100									
Overall Accuracy(%)	100									

Figure 7. Performance evaluation.

3.5 Performance Measure

This is the comparison of the KNN and CBR for investigation of classification the correlation of odour profile and temperature intensity. The ratio is to be shown that the KNN needs more data training and testing, the higher the training ratio the greater the classification of the KNN. Furthermore, CBR are more simplified way in the classification that uses of retrieve, reuse, revise and retain. Figure shown the result of KNN and CBR in performance measure that have been use of sensitivity, specificity, and accuracy.

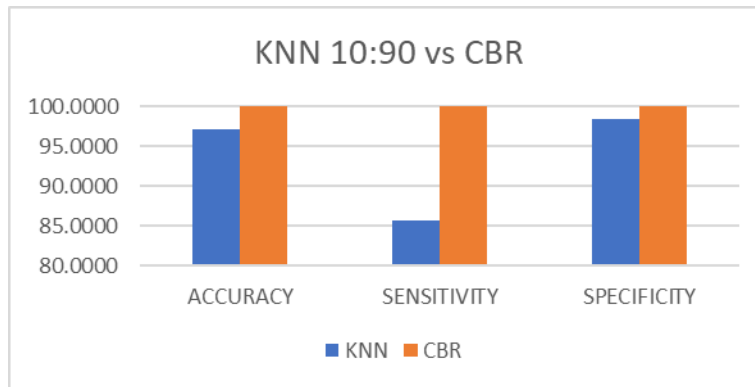


Figure 8. KNN 10:90 vs CBR.

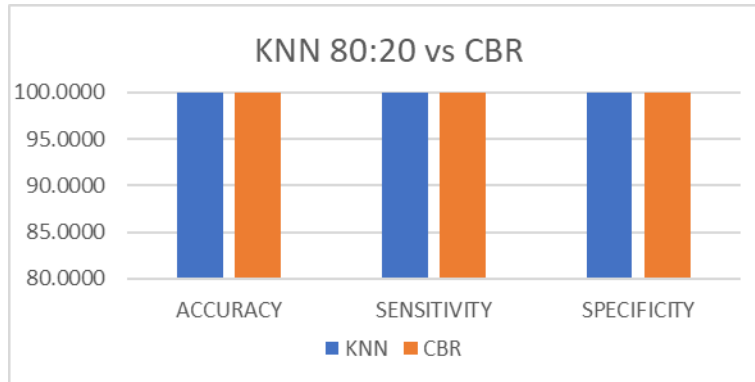


Figure 9. KNN 80:20 vs CBR.

Firstly, it should be acknowledged that CBR offers a simplicity advantage over ML techniques, particularly evident in its ease of implementation and interpretability. CBR relies on the retrieval and adaptation of prior cases, making its decision-making process transparent and understandable to domain experts and end-users.

Conversely, Machine methods, such as k-Nearest Neighbors (k-NN), may require extensive data training and testing. Achieving optimal classification accuracy with ML models often demands a substantial volume of data for training, which can be time-consuming and computationally intensive. The choice of k-NN, in particular, implies a necessity for a sufficient dataset to be effective.

To ascertain the comparative effectiveness of CBR and ML, it is crucial to employ rigorous evaluation criteria and performance metrics tailored to the specific classification problem. These metrics may encompass accuracy, sensitivity, and specificity.

Conducting controlled experiments, preferably within a real-world context or through simulation, will enable a direct comparison of the two approaches. A systematic evaluation should encompass various scenarios, data sizes, and complexities to provide a comprehensive perspective on their respective strengths and weaknesses

4.0 CONFLICT OF INTEREST

In accordance with best practices, the authors of this manuscript have disclosed any financial or non-financial interests that could potentially influence the content. Notably, the authors declare no conflicts of interest.

5.0 AUTHORS CONTRIBUTION

M. Naquiddin (Methodology, Validation, Formal analysis, Data curation, Formal analysis, Investigation, Resources, Software, Visualization, Writing - original draft)

M. Sharfi (Supervision, Funding acquisition, Writing - review & editing, Project administration)

Suhaimi (Supervision) Authorship statements should be formatted with the names of authors first and the author contribution role(s) following, such as

M.M. Rahman (Conceptualization; Formal analysis; Visualisation; Supervision)

W.T. Urmi (Methodology; Data curation; Writing - original draft; Resources)

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