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Ensemble machine learning approach for electronic nose signal processing

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Abstract

Electronic nose (e-nose) systems have been reported to be used in many areas as rapid, low-cost, and non-invasive instruments. Especially in meat production and processing, e-nose system is a powerful tool to process volatile compounds as a unique 'fingerprint'. The ability of the pattern recognition algorithm to analyze e-nose signals is the key to the success of the e-nose system in many applications. On the other hand, ensemble methods have been reported for favorable performances in various data sets. This research proposes an ensemble learning approach for e-nose signal processing, especially in beef quality assessment. Ensemble methods are not only used for learning algorithms but also sensor array optimization. For sensor array optimization, three filter-based feature selection algorithms (FSAs) are used to build ensemble FSA such as reliefF, chi-square, and gini index. Ensemble FSA is developed to deal with different or unstable outputs of a single FSA on homogeneous e-nose data sets in beef quality monitoring. Moreover, ensemble learning algorithms are employed to deal with multi-class classification and regression tasks. Random forest and Adaboost are used that represent bagging and boosting algorithms, respectively. The results are also compared with support vector machine and decision tree as single learners. According to the experimental results, our ensemble approach has good performance and generalization in e-nose signal processing. Optimized sensor combination based on filter-based FSA shows stable results both in classification and regression tasks. Furthermore, Adaboost as a boosting algorithm produces the best prediction even though using a smaller number of sensors.

Keywords: e-nose, ensemble, feature selection, beef quality

1. Introduction

In the last decades, e-nose systems have been utilized in many areas including food processing, agriculture, medical, etc. Low cost of a single analysis, rapid, simplicity of measurement, non-invasive, and suitability for real-time analysis, make it a high potential for application in many areas [1]. E-noses have been reported for analytical instruments such as beef quality assessment and monitoring [2–5], meat cuts identification [6], prediction of bacterial population [7], pork adulteration in beef [8–10], non-invasive diabetes detection [11,12], etc. In addition, non-invasive methods are needed to avoid the patient's pain due to the invasive pricking process which generally occurs several times a day. Therefore, in many cases already mentioned, e-nose can be potentially developed as a non-invasive instrument. E-nose imitates the function of the human olfactory system to detect odor information in the air or sample chamber. There are two main parts to an e-nose system such as gas sensor array and pattern recognition algorithm. The gas sensor array consists of several gas sensors with different selectivity. Each gas sensor works individually and simultaneously converts the chemical information associated with various gas mixtures into a measurable signal. Multivariate responses are generated by a series of gas sensors according to the selectivity and sensitivity of each gas sensor. Furthermore, these signals are processed by a pattern recognition module to perform classification or regression tasks.

In a particular application, a sample can produce different volatile profiles than others. It leads to a different combination of gas sensors in the sensor array. For example, a combination of gas sensors to classify tea will be different from a gas sensor array to distinguish coffee samples. In other words, each sample has a different biomarker which means it requires a different combination of gas sensors. Utilizing a large number of gas sensors to cover all gas selectivity is not a wise solution for building a cost-efficient and robust e-nose system. This causes several problems including overlapping selectivity, large electrical power requirements, network communication traffic, computational overhead, etc. In contrast, the use of a smaller amount of sensor gas can save production costs, save electric power, and more compact device size. Thus, sensor array optimization procedure is necessary for e-nose system development. Several studies addressed this problem and proposed sensor array optimization methods. FSAs are common methods to deal with many sensor array optimization problems. A proper learning algorithm is also needed to build a classifier or regressor model. A weak machine learning model is susceptible to be failed to produce accurate predictions. In the last few years, ensemble methods have been reported for favorable performance in the various data set. The ensemble method refers to the combination of multiple models or algorithms to produce improved results. It usually yields better performance than a single model. Hence, in this study, we have several motivations as follows:

1. The majority of existing studies related to sensor array optimization only utilized a single FSA to determine the best sensor combination in a sensor array. It leads to bias results and not a general gas sensor combination. Therefore, in this study, the most stable FSAs according to our previous study are used to build ensemble FSA such as reliefF, chi-squared, and Gini index [13].
2. For the machine learning models, ensemble learning algorithms are applied to e-nose signals for beef quality monitoring data sets to improve the performance of the single model. They include bagging and boosting algorithms to build a strong model for classification and regression tasks to differentiate beef quality and predict microbial

population in the beef samples, respectively. To the best of our knowledge, the utilization of ensemble learning is considered rare and new in e-nose signal processing.

According to the above explanation, the contribution of this study is to propose an ensemble approach for electronic nose signal processing including ensemble FSA for sensor array optimization and ensemble learning algorithm for classification and regression tasks. The ensemble method combines the output of several algorithms to get better and general results than using one algorithm. In recent years, ensemble approaches have been reported to deal with various cases [14–17]. Typically, the ensemble method is used for classification tasks, but it is also possible to apply it to feature selection problems with satisfactory performances [18–20]. In detail, the signal processing methods that we propose are the noise filtering process, the FSA ensemble, the ensemble model for classification and regression, and evaluation.

The remainder of this paper is structured as follows: Section 2 discusses related studies. Section 3 explains materials and methods including experimental setup, data set, and our proposed method. Section 4 demonstrates the results and discussion. Finally, section 5 is the conclusion of this study.

2. Related works

In many e-nose applications, sensor array optimization and building models for classification or regression tasks are considered as two main problems. Numerous methods have been studied to solve the problem of sensor array optimization. As an example, the use of sensor combination in the several heterogeneous data sets is enhanced by using Genetic Algorithm (GA) [21], wrapper FSA is built by using heuristic algorithms, and optimization for multi-objective purposes is employed on larger heterogeneous data sets [22]. Furthermore, the individual sensor weight, continuous value from 0 to 1, in the sensor array is analyzed using particle swarm optimization (PSO) dan GA combination to detect wound infection. However, there is no reduction in sensor number [23]. The other study discusses sensor optimization in tea quality detection [24]. The classification rate increases higher than 3% that can reduce the sensor array from 30 to 14 even up to 7 sensors. The optimization of sensor array, in this case, was solved using filter-based FSAs. Furthermore, the number of sensor array reductions is up to 5 sensors using analysis of variance (ANOVA). The advantage of the low number of sensors is more accurate in predicting the period to store wheat [25]. In a different study case, ANOVA combined with Wilks statistic and loading analysis decrease up until 6 gas sensors [26]. Wilks statistic method is used to classify wound infection diagnosis [27] and vinegar [28]. Furthermore, sensor array optimization to classify black tea using rough-set is studied [29]. This method can lower up to 4 gas sensors while maintaining its accuracy. The other idea to reduce the number of sensor array is analyzing feature selection algorithm based on filters [30]. The beef quality classification case uses a fast correlation filter-based to find the optimum gas sensor combination [31]. This method can decrease up to 4 gas sensors. This method is combined with neural networks [32] and random forest [33] to pick gas sensors. Moreover, cluster analysis is used in the subarray of gas sensor minimization [34]. Gas sensor selection in the indoor air contaminants was done by using linear discriminant dan kernel principal component [35]. This method can reduce one of the four gas sensors. In the other case, regression task performance is improved by using non-searching FSA [36]. Furthermore, the use of a sensor array in the strawberry freshness selection has been optimized by using a response surface [37]. Nearly all studies state that a lower number of gas sensors increases system performance. On the other hand, principal component analysis (PCA) has been used in many e-nose applications and meat spoilage detections [8,26,38–41]. It was reported for favorable results. However, PCA is utilized for data dimensional reduction. Hence, the number of sensors is actually not changed.

Ensemble methods have been implemented in various areas. The combination of long-short term memory (LSTM) neural network with bagging ensemble learning shows the effectiveness to improve forecasting accuracy [42]. In the medical field, ensemble classifiers were utilized for arrhythmia detection based on ECG signals with 99.37% of classification accuracy in detecting 17 arrhythmia classes [15]. Moreover, several ensemble methods are implemented and evaluated to predict diabetes mellitus type 1 [43]. Furthermore, the Ensemble method was also used for air quality prediction. The experimental results show that it outperforms a single model [17]. For sound recognition, an ensemble classifier has been reported as an effective way to improve the accuracy score of classification by using a selected feature subset in feature selection [44]. Furthermore, the ensemble concept was not only utilized for learning purposes but also for feature selection. The stability issue is a major reason why ensemble FSA needs to be developed. Several studies also demonstrate the effectiveness of ensemble FSA for high dimensional data [19,45,46]. Ensemble FSA is recommended to build more robust, more stable, and more accurate than a single FSA [47–49]. It still becomes a hot topic in machine learning researches [18]. In the e-nose community, only a few studies have discussed the implementation of ensemble concept. For example, the Adaboost model was used to identify Chinese herbal medicine [50]. The experimental results show that it produces better performance than a single classifier. Moreover, the soft-voting approach as an ensemble approach was employed to estimate several odor classes and concentrations [51]. Multivariate logarithmic regression, multilayer perceptron, and support vector machine (SVM) were combined for the approximation model. Also, boosting method was reported to classify two groups of coffee based on an e-nose data set [52]. The application of ensemble learning was demonstrated for classification and regression tasks for beef quality assessment. It used SVM as a base classifier and regressor [53]. SVM was also used to recognize air contaminants as a base classifier for ensemble [16]. The results show that ensemble classifier can significantly improve recognition accuracy and get better generalizations than a single classifier. In addition, ensemble classifier was potentially used to compensate for gas sensor drift [54]. These existing studies demonstrate the potential implementation of ensemble method in e-nose data. However, these applications are quietly limited to build classification or regression models. Different from them, our study proposed an ensemble approach not only to build a classification or regression model but also to determine the best sensor combination in the sensor array using ensemble FSA.

3. Materials and methods

3.1 Experimental setup and Data sets

The detailed components of the proposed e-nose box can be seen in FIGURE 1. This box consists of two chambers. In the first chamber, the sensor box contains 11 gas sensors and the detailed specification of them is shown in Table 1. In the second chamber, the control box contains a wireless communication module. Each minute, the gas sensor signal from the box is sent to the workstation. Raw data is stored continuously for about 2220 minutes in each experiment round. This duration represents the beef quality from fresh or excellent to spoiled. The mechanism to neutralize each round is needed. The first step is flushing both chambers in the e-nose box by using a high-speed fan. The second step is to leave the box for about 3 to 6 hours to remove any lingering odor residue caused by previous experiments. Each beef cut measurement is about 2220 points, so the total is 26640 from 12 types of beef cut. The weight of meat observed for each scenario was the same, that is 125 grams. It consists of various types of beef cut such as clod/chuck, fat, round, brisket, top sirloin, short loin, tenderloin, flap meat, rib eye, inside/outside, skirt meat, and shin. The difference in beef quality is known by using the total number of bacteria inside the beef cut. Therefore, quantification of optical density by using a spectrophotometer with 1000x dilution is implemented. Furthermore, the microbial population inside beef cut is known by using a hemocytometer. The integration among classical and two-hour methods construct the experiment [55]. The baseline to standardize beef quality is based on four sensory classes according to total viable count (TVC) by the Agricultural and Resource Management Council of Australia and New Zealand. The detail for each standard can be seen in Table 2 [56]. Based on those characteristics, this case can be classified as homogenous data sets. An identical pattern of the result is the reason. However, fluctuations in humidity levels produce noise that obscures the pattern. Furthermore, the stability of the result depends on the small sample size and variance of the feature selection algorithm [49]. Therefore, the experiment of e-nose in beef quality monitoring produces data sets that have several characteristics such as noisy, homogenous, and nearly low dimension. Noisy data means obscurity because of humidity's fluctuation in the sample chamber. This topic has been solved by the noise filtering framework [57,58]. The homogenous data sets mean different analyses to the data sets but in the same environment. Moreover, data dimension plays important role in the number of sensors used in the experiment. Eleven gas sensors generate eleven features that can be classified as low. Nevertheless, the sensor's number in the sensor array eventually be a sensitive topic in the optimization problem. The higher number of sensors used lead to higher electrical consumption, data storage/traffic, and production cost. In this experiment, twelve data sets are used. It reflects twelve number of variance meat's cut produce 26640 measurement points. This value is acceptable in dealing with small data set problem. In addition, using a different variant of sensor combination to monitor different meat cuts will need more effort in building each variant of the sensor array. Therefore, one solution to deal with sensor array optimization problems is assessing the stability of FSA. The data sets used in this experiment can be found at [59].

Table 1. Gas sensors specification

Gas sensor	**Selectivity**	**Detection Range**
MQ2	Alcohol, i-butane, hydrogen, liquefied petroleum gas (LPG), smoke, methane, propane,	200 – 5000 ppm LPG and propane, 300 – 5000 ppm butane, 5000 –

		20000 ppm methane, 300 – 5000 ppm H2, 100 – 2000 ppm alcohol
MQ3	Alcohol, methane, benzine, LPG, carbon monoxide, hexane	25 – 500 ppm alcohol
MQ4	Methane	300-10000 ppm natural gas / methane
MQ5	Alcohol, carbon monoxide, hydrogen, LPG, methane	200 – 10000 ppm
MQ6	Iso-butane, Propane, LPG,	300 –

		10000 ppm
MQ8	Hydrogen	100 – 10000 ppm
MQ9	Carbon monoxide, methane, and propane	20 – 2000 ppm carbon monoxide, 500 – 10000 ppm CH_4, 500 – 10000 ppm propane
MQ135	Alcohol, ammonia, benzene, carbon dioxide, smoke, NOx	10 – 300 ppm NH_3, 10 – 1000 ppm benzene,

		10 – 300 ppm alcohol
MQ136	Hydrogen sulfide	1 – 200 ppm
MQ137	Ammonia	5 – 500 ppm
MQ138	Alcohols, aldehydes, ketones	10 – 1000 ppm benzene, 10 – 1000 ppm alcohol, 10 – 3000 ppm NH_3

Table 2. The standard of beef quality

Class	TVC ($\log_{10}$ cfu/g)
Excellent	< 3
Good	3-4
Acceptable	4-5
Spoiled	>5

*cfu/g: colony forming unit of bacteria in a gram of meat

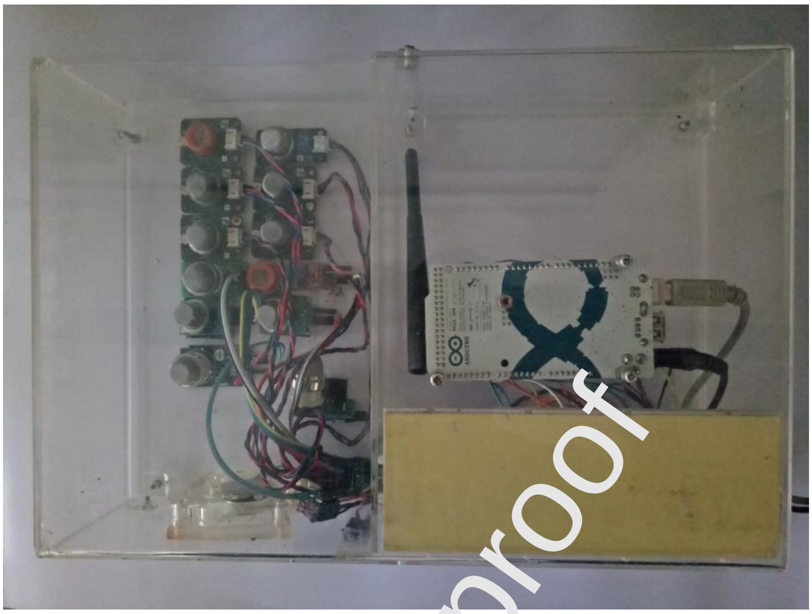


FIGURE 1. E-nose hardware prototype

3.2 Proposed method

The proposed method is described in FIGURE 3. A more detailed explanation of the proposed method can be explained as follows:

1. Noise Filtering

Commonly, e-nose signals are contaminated with noise caused by internal and external sources. Hence, there is necessary to reduce noise level before further processes are conducted. In this study, discrete wavelet transform (DWT) was used and the best-suited parameters were adjusted by using noise-filtering framework [58] and information quality ratio (IQR) [60]. Wavelet decomposition level is determined by the following rule:

$$\frac{F_{sample}}{2^{level+1}} \leq F_{char} \leq \frac{F_{sample}}{2^{level}} \tag{1}$$

where F_{char},F_{sample},level are frequency characteristic, frequency sampling, and decomposition level, respectively. For mother wavelet (MWT) selection, the selected scaled MWT is determined by the largest IQR value between a particular reconstruction signal $y_i^j(t)$ and an original signal $x_i(t)$. The scaled MWT for each signal $(\psi_i((t-2^{v_i}w_i)/2^{v_i})$ is affected by the translation parameter (w_i) and the scaling parameter (v_i) associated with wavelet decomposition. Where, i and j are the index of the signals and the index refers to the MWT used to reconstruct the signal, respectively. Thus, the scaled best suited MWTs for each signal can be associated with argument maxima of IQR function:

$$\psi_i((t-2^{v_i}w_i)/2^{v_i}) = argmax_j\left\{IQR(x_i(t), y_i^j(t))\right\} \quad (2)$$

where,

$$IQR\left(x(t), y(t)\right) = \frac{\sum_{x\in x(t)}\sum_{y\in y(t)} p(x,y)log_2(p(x)p(y))}{\sum_{x\in x(t)}\sum_{y\in y(t)} p(x,y)log_2(p(x,y))} - 1, \quad (3)$$

x, y, $p(x,y)$, $p(x)$, $p(y)$ are element of original signal, element of reconstructed signal, joint probability of x and y, marginal probability of x, and marginal probability of y, respectively. FIGURE 2 shows the e-nose signal sample after the noise filtering process is applied.

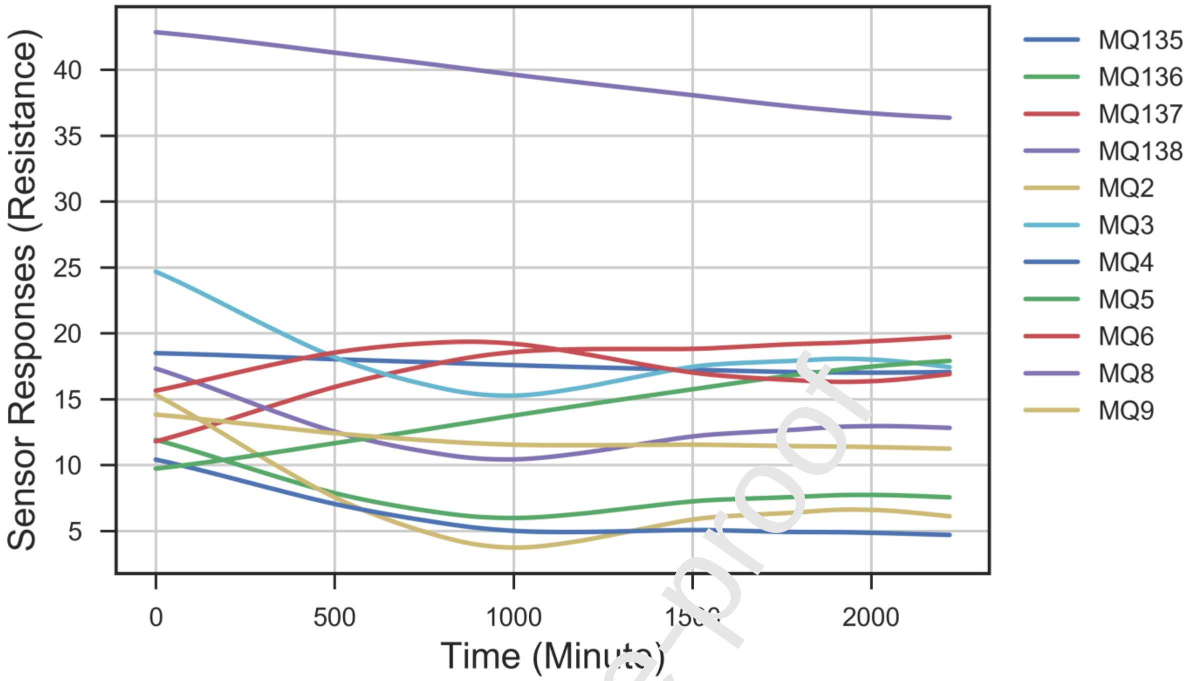


FIGURE 2. Sample of e-nose signals after the noise filtering process

2. Feature selection algorithms

In this experiment, twelve homogeneous data sets correspond to twelve different beef cuts were used. Three filter-based FSAs are used such as reliefF, chi-squared, and Gini index. They have been investigated as the most stable algorithms for these e-nose data sets according to our previous experiment [13].

ReliefF

The idea of ReliefF is to judge how well certain features differentiate between examples that are close to each other. ReliefF looks for its two closest neighbors: one from the same class, called the nearest hit H, and the other from a different class, called miss M based on randomly selected instances l. The score for quality estimation of feature X_k can be formulated by

$$\llbracket ReliefF_{score(X\rrbracket_k}) = \frac{1}{c}\sum_{j=1}^{l}\left(-\frac{1}{h_j}\sum_{x_r \in NH_j} d(x_{jk} - x_{rk}) + \sum_{y \neq y_j}\frac{1}{m_{jy}}\frac{ratio_y}{1 - ratio_y}\sum_{x_r \in NM_{jy}} d(x_{jk} - x_{rk})\right)$$

, (4)

where c, NH_j, NM_{jy} are the number of classes, the nearest instance of x_j in the same class, and in class y, respectively. h_j, m_{jy}, $ratio_y$ are size of NH_j, size of NM_{jy}, ratio of instances in class y, respectively [61,62].

Chi-squared

The chi-squared feature selection performs an independence test to assess whether the feature depends or not on the class label. A high chi-square score indicates that a feature is relatively important. Given a particular feature f_i with n different feature values, chi-squared value can be computed by

$$chi\_squared(X_k) = \sum_{i=1}^{n}\sum_{j=1}^{c}\frac{(m_{ij}-\mu_{ij})^2}{\mu_{ij}}, \quad (5)$$

where m_{ij} denotes the number of instances with the i^{th} feature value from feature X_k. Furthermore, $\mu_{ij} = \frac{m_{*i}m_{j*}}{m}$, where m_{j*} is the number of instances with j^{th} feature value from feature X_k. m_{*i} is the number of instances in class c [63].

Gini index

Gini index is used as a statistical measure to calculate if a feature is capable to separate instances from different classes [62,64]. Gini index can be formulated by

$$gini\_index(X_k) = min_Z\left(p(Z)\left(1 - \sum_{j=1}^{c} p(C_j|Z)^2\right) + p(\bar{Z})\left(1 - \sum_{j=1}^{c} p(C_j|\bar{Z})^2\right)\right), \quad (6)$$

where $Z, \bar{Z}$ are the set of instances that the feature value smaller or equal to the i^{th} feature value and larger than the i^{th} feature value, respectively. In addition, $p(.)$ and $p(.|.)$ denote probability and conditional probability, respectively.

3. FSA aggregator

Each feature is weighted by their ranking in m data sets $Ds = \{Ds_1, Ds_2, \dots, Ds_m\}$. All of these data sets have the n number of feature set $F = \{f_1, f_2, \dots, f_n\}$. Then, FSAs are applied to determine the feature rankings in each data set by using a weighted appearance of feature. For instance, a weighted appearance feature aggregation (WAFA) of feature f in data set Ds ($w_{Ds,f}$) can be formulated as follows [20]:

$$w_{Ds,f} = \frac{n - rank_{Ds,f} + 1}{n}, \tag{7}$$

where, $rank_{Ds,f}$ denotes the rank of feature f in data set Ds. The minimum weight value equals to $\frac{1}{n}$ if using FSAs with the same cardinality. The frequency with which they appear in the top ranking will result in a higher weight which makes the feature more likely to be selected. In this experiment, three FSAs are used such reliefF, chi-squared, and gini index. The number of feature inputs is twelve and these FSA outputs are feature ranking from 1 to 12. Hence, they have the same cardinality. The selected features are determined using the aggregation rule. Thus, the weighted appearance of features matrix ($\boldsymbol{W}$) produced by a particular FSA from data sets Ds can be computed by

$$\boldsymbol{W} = \begin{bmatrix} w(Ds, f_1) \\ w(Ds, f_2) \\ \dots \\ w(Ds, f_l) \end{bmatrix} = \begin{bmatrix} \sum_{Ds=1}^{m} w_{Ds,f_1} \\ \sum_{Ds=1}^{m} w_{Ds,f_2} \\ \dots \\ \sum_{Ds=1}^{m} w_{Ds,f_l} \end{bmatrix} \tag{8}$$

Hence, we have 3×12 weight matrix from three FSAs and twelve features. Moreover, for the FSA aggregator, the average weight values for every FSA need to be calculated. $\boldsymbol{W^{FSA}}$ denotes a weight matrix obtained from an average of every row.

$$\boldsymbol{W^{FSA}} = \frac{1}{3} \times \begin{bmatrix} \sum_{i=1}^{3} w^{FSA_i}(D, f_1) \\ \sum_{i=1}^{3} w^{FSA_i}(D, f_2) \\ \dots \\ \sum_{i=1}^{3} w^{FSA_i}(D, f_n) \end{bmatrix} \tag{9}$$

The final selected features $\boldsymbol{Y}$ according to a weight matrix $\boldsymbol{W^{FSA}}$ can be obtained by this following rule

$$\boldsymbol{W^{FSA}} \rightarrow \boldsymbol{Y} = \left\{ \forall f_j \in Y \middle| \frac{1}{3} \sum_{i=1}^{l} w^{FSA_i}\left(Ds, f_j\right) > \overline{\boldsymbol{W^{FSA}}} \right\}. \tag{10}$$

Therefore, when $\boldsymbol{W^{Fs}_{f_j}} > \overline{\boldsymbol{W^{Fs}}}$, a feature f_j becomes a member of the selected feature subset.

4. Learning algorithms

In this experiment, several machine learning algorithms were employed to perform both classification and regression tasks. Classification tasks were performed to differentiate four beef sensory classes including excellent, good, acceptable, and spoiled. Moreover, learning algorithms were also used to predict the microbial population in the beef sample as regression tasks. To test the selected sensor, SVM and decision tree (DT) were utilized as a single classifier and regressor. Furthermore, ensemble machine learning approaches were also employed including bagging and boosting algorithms. Bagging stands for bootstrap aggregation. This approach combines multiple estimators in a mechanism to reduce the variance of estimates. Random forest is used as a bagging algorithm to train *M* different DT on different subsets of data and perform voting for the final prediction result. Boosting algorithm consists of a set of the low accurate estimator to build a highly accurate estimator. Boosting algorithms can track models that fail to predict accurately. It is less affected by the overfitting problem. In this experiment, an adaptive boosting (AdaBoost) algorithm is utilized. To determine the best parameters of each learning algorithm, a grid search is performed. Before the learning process is also performed, min-max normalization is utilized as a feature scaling method. Learning algorithms and grid search parameters are demonstrated in Table 3.

Table 3. Learning algorithms and grid search parameters

Learning algorithms	**Grid search parameters**
SVM	regularization parameter (C)=[1, 10, 100, 1000], gamma=[0.01, 0.001, 0.0001], kernel = radial basis function (RBF)
DT	criterion=[gini, entropy], maximum tree depth=[5, 10, 15], minimum number of sample to split=[0.1, 1.0, 10], minimum leaf=[0.1, 0.5, 5]
RF	the number of trees in the forest = [50, 100, 150, 200], criterion=[gini, entropy], maximum tree depth=[5, 10, 15], minimum number of sample to split=[0.1, 1.0, 10], minimum leaf=[0.1, 0.5, 5]
AdaBoost	the maximum number of estimators at which boosting is

	terminated=[50, 100, 150, 200], learning rate=[0.1,0.2,0.3]

5. Evaluations

Evaluations are also performed for both classification and regression tasks. For multiclass classification, several performance metrics are used such as accuracy, precision, recall (sensitivity), true negative rate (specificity), and F-measure score. They are computed as macro-average to treat all classes equally. These metrics can be computed by the following equations:

$$accuracy = \frac{tp+tn}{tp+tn+fp+fn} \tag{11}$$

$$precision = \frac{tp}{tp+fp} \tag{12}$$

$$recall = \frac{tp}{tp+fn} \tag{13}$$

$$specificity = \frac{tn}{tn+fp} \tag{14}$$

$$F-measure = 2 \times \frac{precision \times recall}{precision+recall} \tag{15}$$

where, tp, tn, fp, fn are true positive, true negative, false positive, and false negative, respectively. Furthermore, for regression tasks, mean squared error (MSE), R-squared (R^2), bias factor (B_f), and accuracy factor (A_f) are used as performance metrics. MSE is used to measure the error between actual and predicted values. R^2 is utilized to know how much predicted values produced by the regression model can represent the parts of the variance of the actual values. The bias factor indicates whether the prediction result is under or over the estimate of the actual value. B_f equal to 1 indicates an unbiased prediction. $B_f > 1$ means that the prediction result is higher than the actual value (overestimate) and vice versa The accuracy factor measures the accuracy of the regression model. The value of A_f is equal to or greater than one. If the value is greater than one, the prediction results are less accurate [65]. They can be mathematically expressed as follows:

$$MSE(a,p) = \frac{1}{n}\sum_{i=1}^{n}(a_i - p_i)^2 \tag{16}$$

$$R^2(a,p) = 1 - \frac{\sum_{i=1}^{n}(a_i - p_i)^2}{\sum_{i=1}^{n}(a_i - \bar{a})^2} \tag{17}$$

$$B_f(a,p) = \exp\left[\frac{\sum_{i=1}^{L}(\ln(a_i) - \ln(p_i))}{L}\right] \tag{18}$$

$$A_f(a,p) = \exp\left[\sqrt{\frac{\sum_{i=1}^{L}(\ln(a_i) - \ln(p_i))^2}{L}}\right] \tag{19}$$

where a and p mean actual and prediction values.

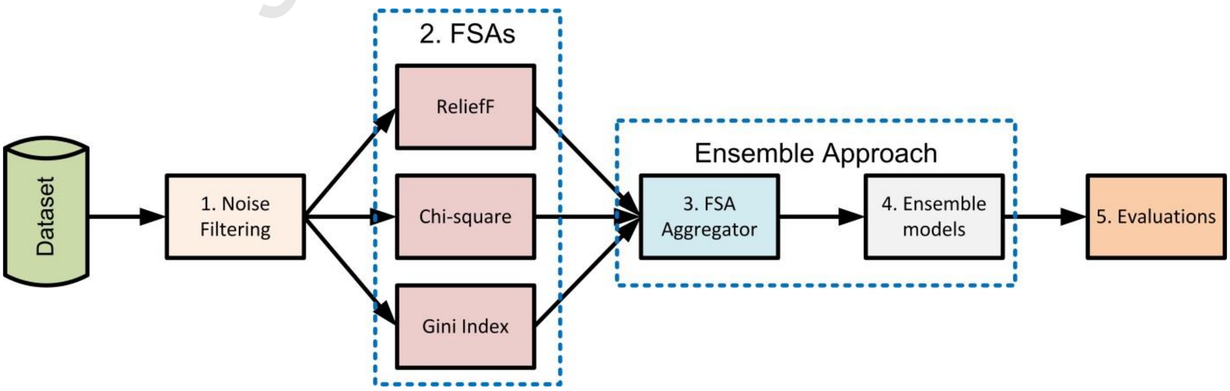


FIGURE 3. Proposed method

4. Results and discussion

In this section, the experimental results including feature selection, classification, and regression results are discussed. First, the results from three conventional FSAs are used and aggregated to build an ensemble FSA. FIGURE 4 shows the WAFA score of ReliefF. The selected sensors represented by the feature subset are determined based on features with scores higher than the average score. According to the aggregation results from twelve homogeneous data sets, the selected sensors are MQ136, MQ137, MQ3, MQ5. With the same mechanism, FIGURE 5 denotes the result of chi-square with selected sensors is MQ136, MQ137, MQ3, MQ4, MQ5. Moreover, the recommendation of selected sensors based on Gini index is shown by FIGURE 6 such as MQ135, MQ137, MQ4, MQ5. Finally, using the soft voting mechanism for result aggregation, the proposed Ensemble FSA produces selected sensors such as MQ136, MQ137, MQ3, MQ4, MQ5. The result summary of sensor array optimization is also shown in Table 4. For this data set, these five gas sensors are recommended to be used for classification and regression tasks.

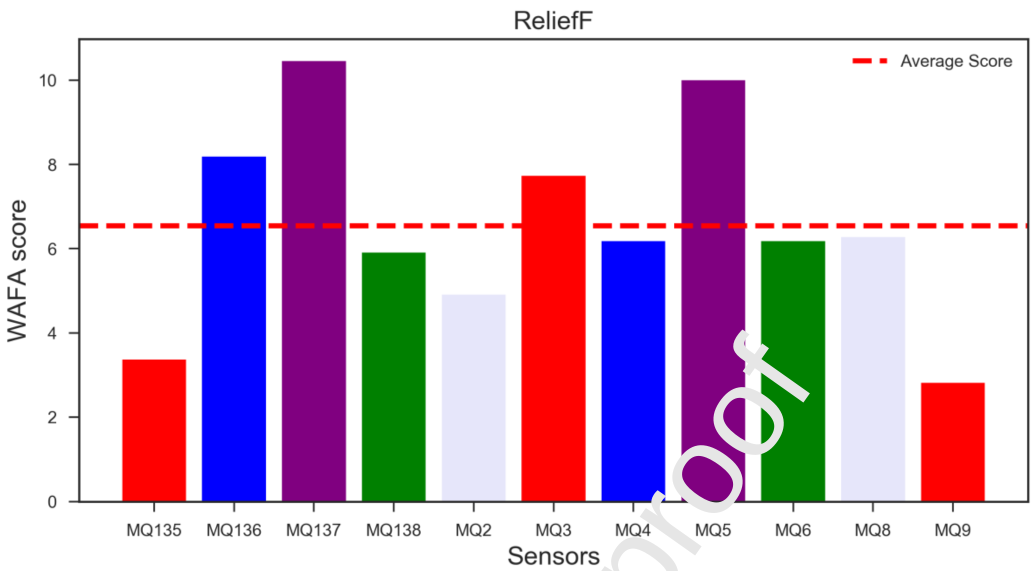


FIGURE 4. Result of ReliefF

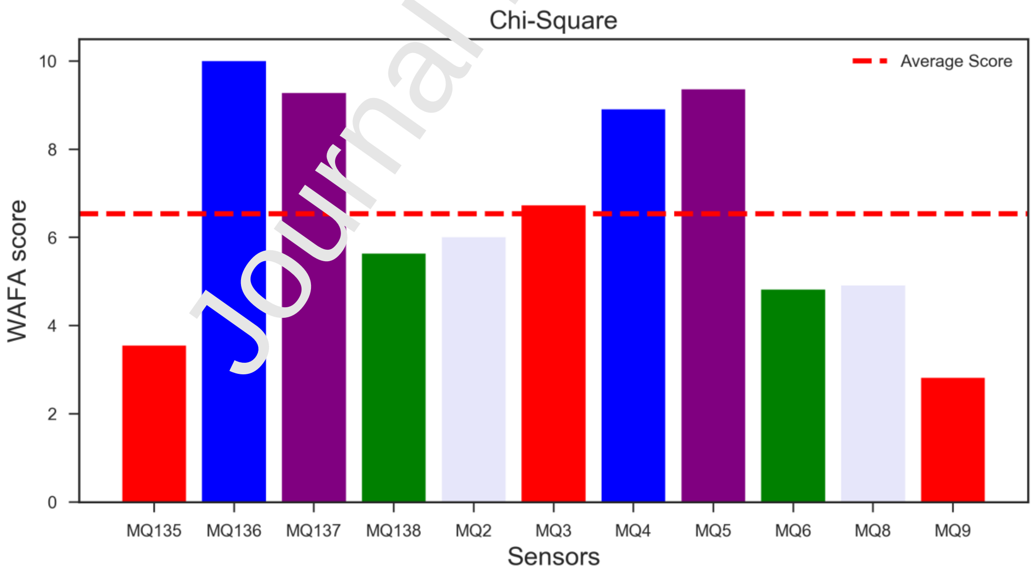


FIGURE 5. Result of Chi-square

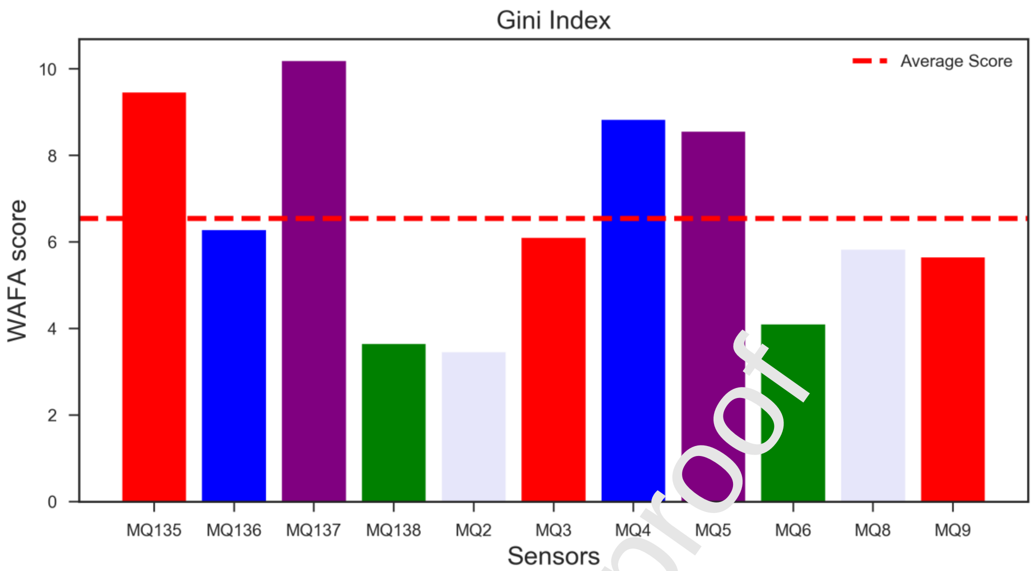


FIGURE 6. Result of Gini Index

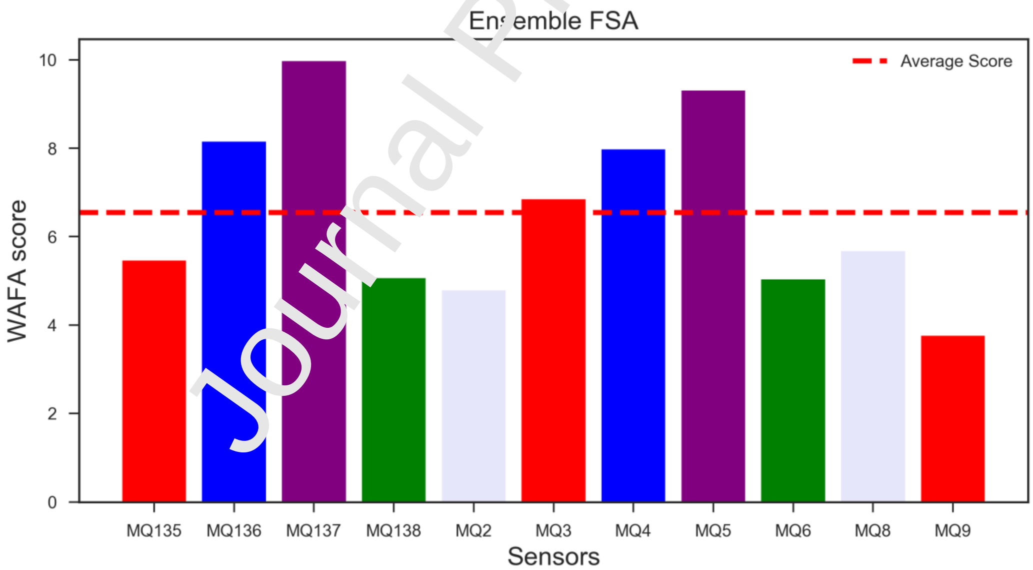


FIGURE 7. Result of Ensemble FSA

Table 4. Selected sensors based on several FSAs

ReliefF	Chi-Square	Gini Index	Ensemble FSA

MQ 136	MQ 136	MQ 135	MQ 136
MQ 137	MQ 137	MQ 137	MQ 137
MQ 3	MQ 3	MQ 4	MQ 3
MQ 5	MQ 4	MQ 5	MQ 4
	MQ 5		MQ 5

After ensemble FSA is performed for sensor array optimization, the next step is using the selected sensors for classification and regression tasks. To built classification and regression models, data set is randomly divided into training data (70%) and testing data (30%). Hence, the number of instances for training and testing data are 18648 and 7992, respectively. Furthermore, the experiment was divided into two scenarios are using all sensors and using optimized sensors from the result of ensemble FSA in the previous step. Using all sensors means machine learning algorithms use 11 input features from 11 sensors. On the other hand, using optimized sensors refers to the utilization of 5 sensors as the output from Ensemble FSA. These scenarios aim to investigate the effect on machine learning algorithm performance associated with the use of fewer sensors. Classification tasks are performed to classify four sensory classes of beef. Furthermore, the microbial population is predicted as regression tasks. For these tasks, single models are employed such as support vector machine classifier (SVC), support vector regression (SVR), and decision tree. In this experiment, two types of ensemble learning algorithms are also utilized such as random forest as bagging and AdaBoost as a boosting approach. Table 5 demonstrates the comparison of classification performance. Ensemble methods have superior performances than single classifiers. SVC gets a higher impact if using optimized sensors. For example, the accuracy score decreases from 0.9970 to 0.9779. Using all sensors, decision trees and random forests have a comparable performance for classification tasks. Basically, the decision tree has better performance than SVC. The good news is decision tree classifier can be potentially used as a base estimator to build ensemble methods. The impact of more trees is felt when the number of features is reduced. Random forest surpasses decision tree when using optimized sensors. The F-measure score shows 0.9966 for decision tree and 0.9974 for random forest. For accuracy, it also produces a better score with 0.9982 against 0.9977. Adaboost has the best performance both using all sensors and using optimized sensors according to precision, recall, specificity, f-measure, and accuracy values. Using optimized sensors, the performance of all machine learning algorithms is slightly lower than using all sensors according to precision, recall, specificity, f-measure, and accuracy score. Normally, this effect is due to fewer features being used as predictors. This effect can be compensated by using ensemble methods. Using optimized sensors, ensemble learning algorithms have the best performance with 0.9982 of classification accuracy. In general, the experimental results show a stable machine learning algorithm performance. In other words, performance does not really decrease when using a smaller number of sensors from the result of ensemble FSA. This shows that the ensemble approach has good performance and generalization in e-nose signal processing.

Table 5. Comparison of classification results

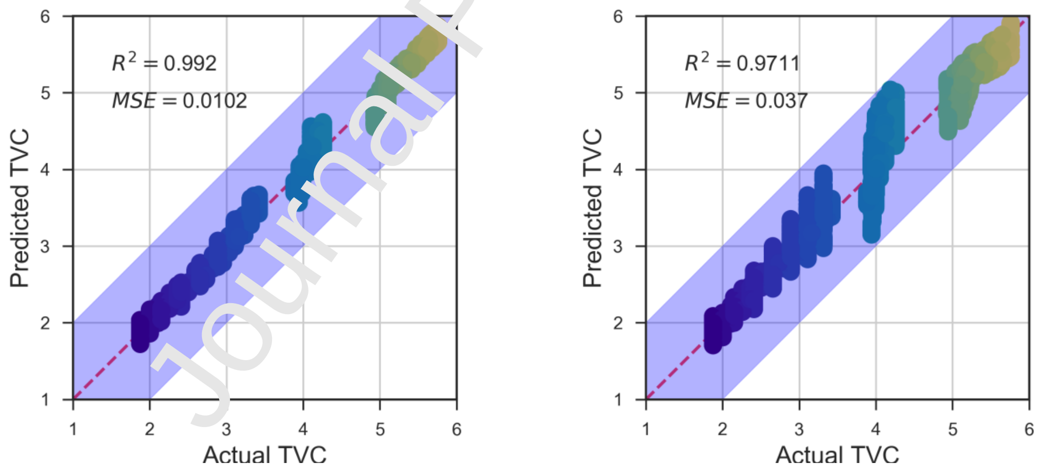
Classifiers	**precision**	**recall**	**specificity**	**f-measure**	**accuracy**
SVC using all sensors	0.9959	0.9949	0.9970	0.9954	0.9970
SVC using optimized sensors	0.9672	0.9606	0.9779	0.9638	0.9779
Decision Tree using all sensors	0.9986	0.9979	0.9987	0.9983	0.9987
Decision Tree using optimized sensors	0.9972	0.9960	0.9977	0.9966	0.9977
Random Forest using all sensors	0.9984	0.9980	0.9987	0.9982	0.9987
Random Forest using optimized sensors	0.9977	0.9970	0.9982	0.9974	0.9982
AdaBoost using all sensors	0.9989	0.9982	0.9990	0.9986	0.9990

AdaBoost using optimized sensors	0.9979	0.9971	0.9982	0.9975	0.9982

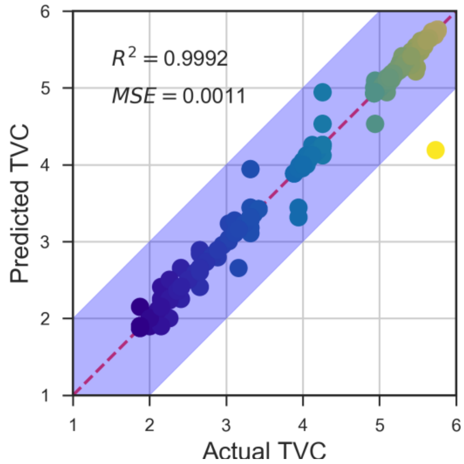
Table 6 shows the comparison of regression performance to predict the microbial population in the beef sample according to MSE and R^2 score. Similar to classification tasks, SVR has the lowest performance with MSE = 0.0102 and R^2=0.992 when using all sensors and it was worse when using optimized sensors with MSE = 0.037 and R^2=0.9711. Decision tree produced better results than SVR even though it uses optimized sensors (MSE = 0.0032 and R^2=0.9975), which means it also can be potentially utilized as a base regressor for the ensemble method. Furthermore, random forest and Adaboost regressors with a decision tree as a base estimator are used. The utilization of these ensemble methods can significantly give performance improvement on regression tasks, especially when using optimized sensors. For instance, random forest reduces MSE value (0.0032 becomes 0.0012) as well as increases R^2 (0.9975 becomes 0.9991) when compared by a decision tree. Adaboost regressor also produces a satisfactory performance even though using optimized sensors with MSE = 0.0005 and R^2=0.9996. This result is better than using all sensors MSE = 0.0006 and R^2=0.9995. These performances can be also visually observed in FIGURE 8. Compared with FIGURE 8 (a), FIGURE 8 (b) shows the performance degradation of SVR when using a smaller number of sensors. The decision tree has better performance even though it has quite a big mistake at some point when using optimized sensors as shown in FIGURE 8 (c) and (d). FIGURE 8 (e) and (f) show that the random forest algorithm as bagging ensemble method gets smoother prediction. Furthermore, Adaboost produces the best prediction when using both all and an optimized number of sensors. The prediction can smoothly follow the line of equity (x=y) as shown in FIGURE 8 (g) and (h).

Table 6. Comparison of regression results

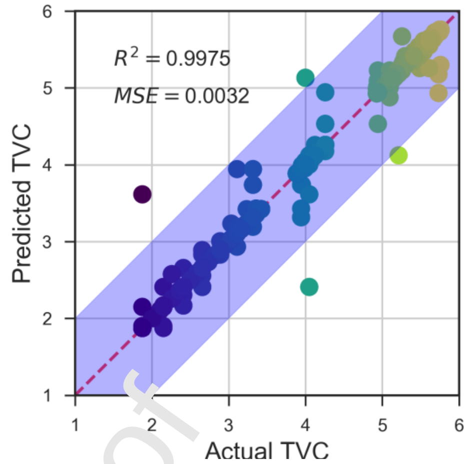
Regressors	**MSE**	**R^2**	B_f	A_f
SVR using all sensors	0.0102	0.992	0.9998	1.0261
SVR using optimized sensors	0.037	0.9711	0.9972	1.0467
Decision Tree using all sensors	0.0011	0.9992	1.0000	1.0104
Decision Tree using optimized sensors	0.0032	0.9975	0.9998	1.0173
Random Forest using all sensors	0.0005	0.9996	0.9999	1.0070
Random Forest using optimized sensors	0.0012	0.9991	0.9998	1.0108
AdaBoost using all sensors	0.0006	0.9995	0.9999	1.0070
AdaBoost using optimized sensors	0.0005	0.9996	0.9999	1.0063



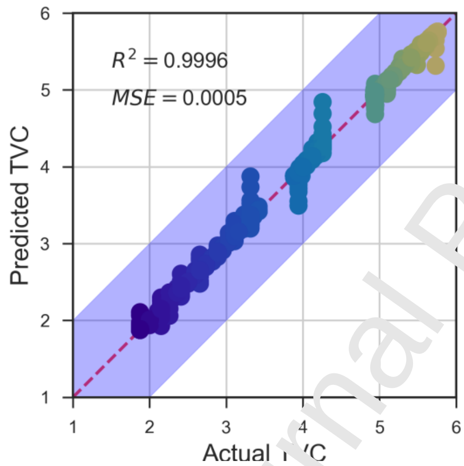
(a) (b)


$R^2 = 0.9992$
$MSE = 0.0011$
Predicted TVC
Actual TVC

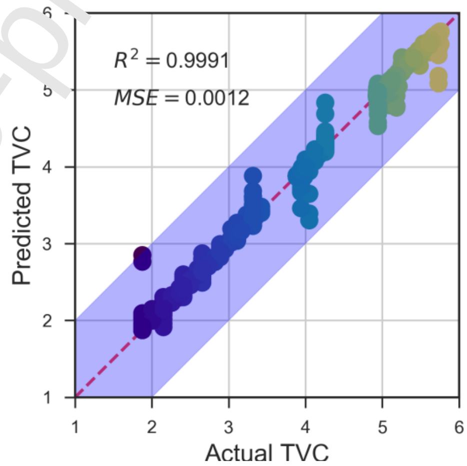
(c)


$R^2 = 0.9975$
$MSE = 0.0032$
Predicted TVC
Actual TVC

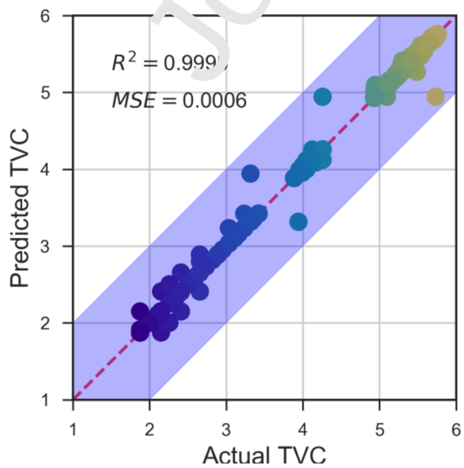
(d)


$R^2 = 0.9996$
$MSE = 0.0005$
Predicted TVC

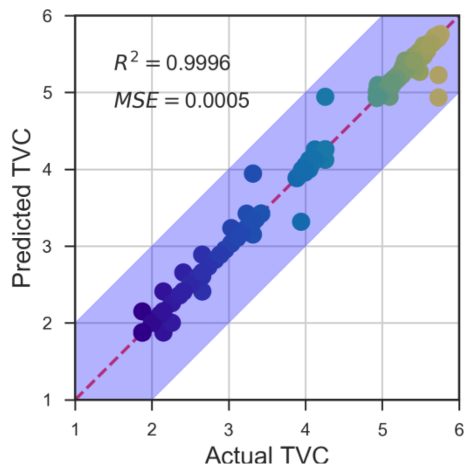
(e)


$R^2 = 0.9991$
$MSE = 0.0012$
Predicted TVC
Actual TVC

(f)


$MSE = 0.0006$
Predicted TVC
Actual TVC

(g)


$R^2 = 0.9996$
$MSE = 0.0005$
Predicted TVC
Actual TVC

(h)

FIGURE 8. (a) SVR with all sensors; (b) SVR with optimized sensors; (c) DT with all sensors; (d) DT with optimized sensors; (e) RF with all sensors; (f) RF with optimized sensors; (g) AdaBoost with all sensors; (h) AdaBoost with optimized sensors

5. Conclusions

This study demonstrates an ensemble machine learning approach for e-nose signal processing. For sensor array optimization, ensemble FSA is employed to determine the best combination of the gas sensor in the sensor array. The utilization of ensemble FSA aims to make sure generalization of gas sensor combination and avoid unstable results when using single FSA on homogeneous data set. Furthermore, ensemble learning algorithms such as bagging and boosting are used to improve the performance of a single learning algorithm in classification and regression tasks. According to the experimental results, decision tree can produce better results than SVC/SVR with 0.9987 of classification accuracy and 0.0011 of MSE. Hence, it is prospective to be used as a base estimator for ensemble learning. Decision tree algorithm is used as a base estimator for the random forest as the bagging algorithm and Adaboost as boosting algorithm. Ensemble learning algorithms are superior to single learning algorithms in e-nose data set for both using all sensors and an optimized number of sensors. The best results can be obtained by Adaboost in that it has a comparable result when using all sensors and optimized sensors. In classification tasks, Adaboost got 0.9990 and 0.9982 of classification accuracy when using all sensors and optimized sensors, respectively. Moreover, in regression tasks, it only got 0.0006 and 0.0005 of MSE when using all sensors and optimized sensors, respectively. Performance doesn't really drop when using a smaller number of sensors using the FSA ensemble results. This shows that the ensemble approach has good performance and generalization in e-nose signal processing. Hence, it can be potentially used for e-nose signal processing. For future works, more advanced boosting algorithms will be developed, especially for e-nose signal processing.

CRediT authorship contribution statement

Dedy Rahman Wijaya: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing - original draft, Writing - review & editing, Visualization.

Farah Afianti: Resources, Writing - Review & Editing, Project administration

Anditya Arifianto: Software, Writing - Review & Editing

Dewi Rahmawati: Funding acquisition

Vassilis S. Kodogiannis: Validation, Writing - Review & Editing

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CRediT authorship contribution statement

Dedy Rahman Wijaya: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing - original draft, Writing - review & editing, Visualization.

Farah Afianti: Resources, Writing - Review & Editing, Project administration

Anditya Arifianto: Software, Writing - Review & Editing

Dewi Rahmawati: Funding acquisition

Vassilis S. Kodogiannis: Validation, Writing - Review & Editing

Declaration of interests

☐The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Highlights:

- An ensemble approach for e-nose signal processing is proposed
- Ensemble FSA is developed for sensor array optimization
- Performance of single, bagging, and boosting algorithms were investigated
- Adaboost as a boosting algorithm produces the best results.
- Ensemble approach has good performance and generalization