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Sensing fermentation degree of cocoa (Theobroma cacao L.) beans by machine learning classification models based electronic nose system

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Abstract

Cocoa bean fermentation is an important postharvest process that develops aroma and processing properties. Although the cocoa fermentation is of high complexly, farmers are employing empirical methods to determine the fermentation degree of cocoa. Researchers, on the other hand, are using expensive equipment such as high-performance liquid chromatography and gas chromatography-mass spectrometry to study cocoa fermentation. In this study, machine learning based electronic nose system, a fast measuring and affordable method, was developed to determine the fermentation degree of cocoa beans. Six machine-learning methods (bootstrap forest, boosted tree, decision tree, artificial neural network (ANN), naïve Bayes, and k-nearest neighbors) were conducted to classify the fermentation time of cocoa beans. Bootstrap forest algorithm achieved a misclassification rate as low as 9.4%. ANN and boosted tree achieved 12.8 and 13.6% misclassification rate respectively. However, other methods failed to do classification for cocoa beans.

Practical applications

The electronic nose system can be used by cocoa farmers to monitor cocoa fermentation and ensure the quality of cocoa beans. The method is relatively inexpensive and easy to operate.

1 | INTRODUCTION

Chocolate is one of the most profitable merchandise of the global confectionary industry. The chocolate market worth 98.3 billion dollars in 2016 and the retail sale of chocolate in United States alone is estimated to be 22.4 billion for 2017 (Tan & Balasubramanian, 2017). Cocoa bean (Theobroma cacao L.) is the major raw material in chocolate products (Tan & Kerr, 2018a). Globally, the production of cocoa bean was 4.031 million tons in 2016. Consumers are willing to pay more money for better quality chocolate, which creates big price gaps between mediocre chocolates and fine making chocolates. In most cases, the quality of cocoa bean is pivotal to the value of the final the chocolate products (Afoakwa, Paterson, Fowler, & Ryan, 2008).

The quality of cocoa bean is influenced by its variety, soil, climate, crop management, and mainly by postharvest processing (Sukha, 2009). Fermentation is a prerequisite for the development of cocoa flavor precursors and better processing properties (Hue et al., 2016). After harvest, farmers open the cocoa pods, then extract the cocoa seeds along with pulp and fill up wooden boxes or containers to start fermentation (Lima, Almeida, Rob Nout, & Zwietering, 2011). The fermentation of cocoa bean is a process that involves microbial, physiochemical, and enzymatic effects. Although, the microbial ecology of cocoa bean fermentation has been studies for more than 100 years, fermentation remains empirical and does not give rise to beans of consistent quality, which obliges processors continuously to make changes of their formulations (Ho, Zhao, & Fleet, 2015).

To date, cocoa fermentation degree determination still remains empirical, even though some requirements, such as temperature, cut test, and pH have been recommended by scientists and manufacturers (Senanayake, Jansz, & Buckle, 2002). In addition, the control of cocoa fermentation is challenging because the fermentation environment is difficult to control. Even in two adjacent fermentation boxes with same cocoa bean, the progress of fermentation may still different. Therefore, it is useful to develop a fast and affordable method by which farmers can determinate the fermentation degree of cocoa beans. Currently, the standard methods for determining the fermentation degree of cocoa bean is cut test. This method consists in longitudinally cutting and counting the proportion of purple and brown beans on a representative dried sample of 300 beans (Wood & Lass, 2008). However, cut test is relatively time consuming and it requires special training. Sensory evaluations on cocoa bean fermentation have been conducted by previous study (Crafack et al., 2013), indicating that there are significantly changes in the profile of free amino acid, peptide-N, sugar, and pyrazine. However, sensory-based determination methods involve many professional trainings, which can only be conducted by specialists.

Some chocolate manufacturers quantify the ammonia nitrogen (NH_3) content by the Conway technique and use nitrogen as an indicator for cocoa fermentation (Conway & Byrne, 1933). Some researchers have applied techniques such as gas chromatography-mass spectrometry (Grün et al., 2008), high-performance liquid chromatography (Sandhya et al., 2016), and near infrared spectroscopy (Hue et al., 2014) to determine the fermentation degree of cocoa beans by tracking the profile of compounds such as ammonia nitrogen, free amino acids, and volatile compounds. Those methods were reported to have achieved high accuracy of determination, however, the equipment and the corresponding analytical are relatively expensive for manufacturers and farmers. In addition, the methods are time consuming and unable to be conducted on site or remote controlled.

Electronic nose is an array of many gas sensors, mimicking the discrimination of the mammalian olfactory system for smells (Persaud & Dodd, 1982). Different gas sensor gives a fingerprint response to given odors, and the response pattern of gas sensors can be recognized by certain algorithms and then performs odor identification and discrimination (Arshak, Moore, Lyons, Harris, & Clifford, 2004). Typical electronic nose systems that comprise gas sensors, reaction chamber, air pumps, and data acquisition (DAQ) devices were reported by previous studies (Zhang & Tian, 2014; Zhang & Zhang, 2015, 2018). Many researchers have established e-nose based quality measurement systems to predict the fermentation time of wine (Buratti et al., 2011) and cheese (Drake, Gerard, Kleinhenz, & Harper, 2003); the oxidization of olive oil (Cosio, Ballabio, Benedetti, & Gigliotti, 2007); the shelf life of meats (El Barbri, Llobet, El Bari, Correig, & Bouchikhi, 2008); and fruits (Torri, Sinelli, & Limbo, 2010). However, the applications of e-nose in cocoa quality and processing controls were barely reported. Only few studies (Olunloyo, Ibidapo, & Dinrifo, 2011; Tan & Kerr, 2018b) have reported using artificial neural network (ANN) based electronic nose to determine cocoa bean qualities. Chocolate conching can be monitored by kernel distribution model based e-nose was reported recently (Tan & Kerr, 2019). No study has reported the application of e-nose in controlling cocoa fermentation, which plays an important role in developing cocoa bean aroma and processing qualities. The fermentation of cocoa beans is a complex postharvest process that can be influenced by bean variety, climate, insect, and handling. Therefore, developing a universal, affordable, and fast measuring methods for cocoa bean fermentation is potentially useful.

The existing feature recognizing algorithms being investigated include ANN, decision tree, random forest (RF), support vector machine, and subspace learning. ANN is one of the main tools used in machine learning, mimicking the neuronal structure of the mammalian cerebral cortex but on much smaller scale. In a most basic mathematical model of the ANN, the effects of the synapses are represented by connection weights that modulate the effect of the associated input signals, and the nonlinear characteristic exhibited by neurons is represented by a transfer function. The neuron impulse is then computed as the weighted sum of the input signals, transformed by the transfer function. ANN has been reported to be useful in pattern recognition, shelf life prediction, quality discrimination, and classification in food industry (Goyal & Goyal, 2011). E-nose using ANN has been used to detection abnormal odors was reported and good performance was obtained (Zhang & Deng, 2017).

A decision tree represents a decision procedure for determining the class of a given instance based on previous instances. Each node of the tree specifies either a class name or a specific test that partitions the space of instances at the node according to the possible outcomes of the test. Each subset of the partition corresponds to a classification subproblem for that subspace of the instances, which is solved by a subtree.

RF is constructed by multiple decision trees and when a new object is to be classified, each decision tree will "vote" for the class of the object. The object is assigned to a certain group based on majority votes (Liaw & Wiener, 2002). The bootstrap forest is an RF approach that uses an ensemble of classification trees by averaging many decision trees each of which is fit to a bootstrap sample of the training data. Each split in each tree considers a random subset of the predictors. In other words, given a training set S of n examples, a new training set S_0 is constructed by drawing m examples uniformly (with replacement) from S (Ripley, 1996). On the other hand, the boosted tree (gradient boosting) approach maintains a set of weights over the original training set S and adjusts these weights after each classifier is learned by the base learning algorithm. The weights of examples that are misclassified are increased by the base learning algorithm and the weight of examples that are correctly classified are decreased (Elith, Leathwick, & Hastie, 2008). Currently, few studies have reported the use of RF algorithm combining with electronic nose in food quality control and evaluation.

Naïve Bayes (NB) classifier is a machine learning algorithm that greatly simplify learning by assuming that features are independent given class, that is, $P(X|C) = \prod_{i=1}^{n} P(X_i|C)$, where $X = (X_1, \cdots, X_n)$ is the vector of features and C is the class. Naïve Bayes classifiers assign the most likely class to a given subject depending on its feature vector. Although, its unrealistic assumption, NB is considered remarkably successful in practice compares to other more sophisticated algorithms. Its application

includes medical diagnosis (Mitchell, 1997) and food quality classification (Cen, Lu, Zhu, & Mendoza, 2016).

k-Nearest neighbors (KNN) algorithm is a nonparametric method used for classification. It is among the simplest of all machine learning algorithms. This algorithm assigns a subject with a feature $X = (X_1, \cdots, X_n)$ to a class C based on the sum of the distance between its KNN $d = \sum_{i=1}^{n} \sum_{j=1}^{k} | X_i - Y_{ij} |$, where $Y_k = (Y_{k1}, \cdots, Y_{kn})$ is a feature vector of a training sample among the nearest neighbors.

In previous studies, the application of subspace learning and support vector machine algorithms in electronic tongue (Zhang, Wang, Huang, Liu, & Tan, 2019) and electronic nose (Zhang, Liu, & Deng, 2017) have been investigated, and good prediction (98% accuracy) was achieved. However, detection and of cocoa fermentation in natural condition using e-nose was not reported. Fast and accurate detection methods for cocoa fermentation degree are not available. In this study, the fermentation of cocoa (Theobroma cacao L.) beans was monitor by self-built electronic nose system. Compares to e-nose developed in previous studies, the selected of gas sensors of this e-nose was based on the volatile profiles of cocoa beans, so that the features of the volatiles can be captured. The responses of the e-nose were processed by several machine learning methods including decision tree, bootstrap/boosted tree RF algorithm, and ANN. Simple classification methods include NB and KNN were also conducted for comparison. In previous studies (Güney & Atasoy, 2012, 2015; Li, Gu, & Wang, 2017; Yu, Wang, Yao, Zhang, & Yu, 2008), ANN, RF algorithm, KNN, and NB were used to conduct pattern recognition for e-nose. However, the performance of the algorithms was not compared in one study. No previous study has reported the determination of cocoa bean fermentation time using e-nose. The performance of the algorithms in recognizing odors were not compared in any studies. The temperature and pH of cocoa beans during fermentation were recorded and cut tests were conducted as reference.

2 | MATERIALS AND METHODS

2.1 | Cocoa fermentation

Seventy-five kilograms of fresh cocoa beans (Theobroma cacao L.) were harvest at Trinidad and kindly provided by Montserrat Cocoa Farmer's Cooperative Society Limited. The beans were evenly distributed to three Styrofoam coolers (60 × 30 × 30 cm). The three coolers were placed adjacent to each other in a fermentation room with ambient temperatures varied from 20 to 30°C. The fermentation room provided shade for rain and sunshine, but humidity was not controlled and insects (mostly fruit fly) had access to the cocoa beans. The beans were turned and mixed in the fourth and sixth day of fermentation. Longer fermentation time results in greater fermentation degree. At different fermentation day, cocoa beans have distinct combination of pH, temperature profile, dominant microorganism, and most importantly, volatiles profile. Therefore, in this study, different fermentation time, in terms of the number of days after the beginning of fermentation, was considered has different fermentation degree.

2.2 | Temperature/pH measurements and cut test

Temperature, pH measurements, and cut tests were taken every day (Days 0–7) after the first electronic nose reading was obtained. A thermometer (model EW-94469-40, Cole-Parmer, Vernon Hills, IL) was inserted at three different depths (top, middle, and bottom) in each of the three Styrofoam coolers in order to obtain three replicates of readings for each treatment. pH measurements were carried out using an Oakton Acorn series pH meter (model WD-35613-70, Oakton, IL). The testa was separated from the cotyledons and placed in separate ceramic mortars. Ten milliliters of distilled water was added to each and then the mixture was grounded using a ceramic pestle. The pH probe was then inserted into the mixtures to obtain a reading. Cut tests were conducted by randomly selecting 30 beans from each composite sample. Each bean was cut along the longitudinal axis and placed on a cut test template. The cut beans on the template were then photographed for physical assessment purposes.

2.3 | E-nose system

Three e-noses for the three fermentation boxes were built following the design in previous study with some modification (Tan & Kerr, 2018b) and the diagram was showed in Figure 1. The system consisted of five major components, including a micropump (NMP830, KNF, Trenton, NJ), a two-way solenoid valve (225T031, NR, Caldwell, NJ), an Arduino board microcontroller (Uno, Arduino), e-nose (gas sensors and chamber), and data collection boards. The e-nose chamber was built from a 10 × 10 × 5 cm nylon box with a 1.5 cm thick Teflon top. The sensor sockets were inserted into the outer top of the chamber, while the gas sensors were inserted into the sockets from inside the chamber. Nine gas sensors were purchased from Figaro USA, Inc. (Arlington Heights, IL) and the specifications of each gas sensors were shown in Table 1. The e-nose was turned on and equilibrated for 3 hr before the measurements every day.

The sampling for the tests were achieved by the solenoid valve, the micropump, and the microcontroller. The valve has two inlets and one outlet. The outlet was always open and connected to the pump, while the two inlets were connected to the headspace of the beans

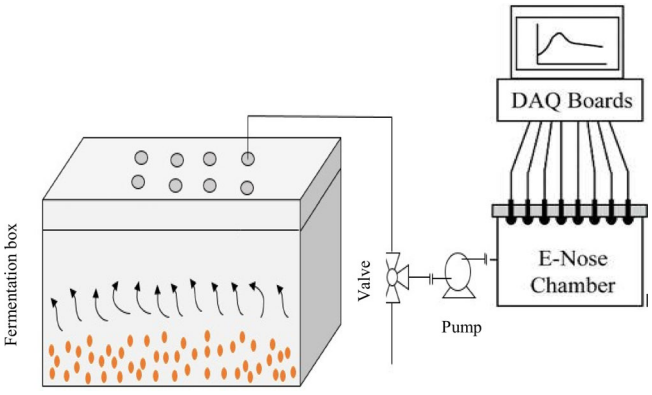

FIGURE 1 Schematic diagram of the e-nose system used to determine cocoa fermentation time

TABLE 1 Gas sensors used for the e-nose system and their specifications

Sensors	Features and specification
TGS821	Hydrogen
TGS826	High sensitivity to ammonia and ethanol
TGS813	High sensitivity to methane, propane, and butane
TGS2602	High sensitivity to VOCs and odorous gases
TGS822	High sensitivity organic solvent vapors such as ethanol
TGS2610	High sensitivity to LP and its component gases (e.g., propane and butane)
TGS2620	High sensitivity to alcohol and organic solvent vapors
TGS830	R11, R113, and other halocarbons
TGS823	High sensitivity to organic solvent vapors such as ethanol

Abbreviations: VOC, Volatile organic compound; LP, liquid petroleum gas.

and open environment, respectively, through rubber tubes. However, only one of the two inlets was open at one time. By opening the inlet that connected to one random location of the headspace, the pump provided suction to drive the cocoa headspace gas to the e-nose chamber at flow rate 0.9 L/min and the gas reacted with the gas sensors for 300 s. The pump was closed for 30 s after the reactions began. The signals (output voltage as a function of time) were collected by three DAQ boards (Model NI9219, National Instruments, Austin, TX). A program was developed using LabView software (Version 2015, National Instruments) to collect data from the DAQ boards and to provide a visual representation of voltage versus time for each channel. Then, the inlet connected to environment was opened and the pump was started, directing compressed air to wash the e-nose chamber before next sampling cycle begin. Each cleaning process took 100 s at flow rate 1.8 L/min and next sampling started 10 min after cleaning.

Based on previous studies (Arshak et al., 2004; Vergara et al., 2012; Yan & Zhang, 2015), three characters (relative peak, relaxation time, and rising time) of the responses of each gas sensor were extracted. The "relative peak" was defined as absolute value of the output peak value minus the baseline values of each sensor. Some sensors have negative peak during the measurements because of the dilution of their target gases. The "relaxation time" was defined as the time that the output voltage decreased from the peak value to 80% of its relative peak value. The "rising time" was defined as the time needed before the responses of each sensor reached its relative peak. The exacted features were used as training sets for all the algorithms. A typical diagram of one gas sensors of this e-nose was showed in Figure 2.

2.4 | ANN setup

The three characters of each sensor were scaled to 0–1 before being used as training data for all machine learning methods. The ANN were conducted by neural network toolbox from MATLAB (R2017a, MathWorks, Natick, MA). The number of hidden layers was one and the number of neutrons in the hidden layer was 17, which gave the highest classification successful rate. There were 72 repetitions at each day of fermentation and 504 sets of e-nose measurements, of

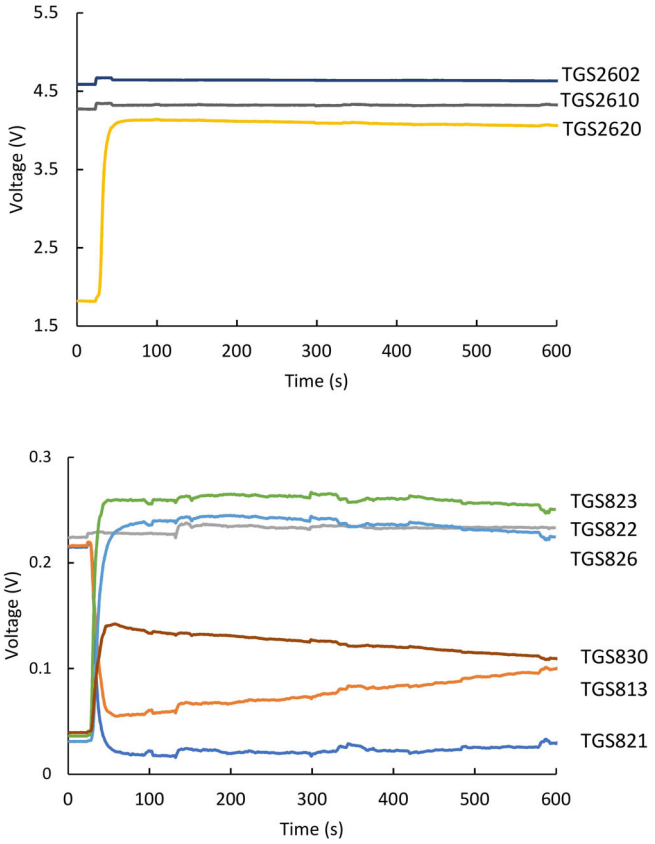

FIGURE 2 Example of typical signal response diagrams for selected gas sensors of the e-nose

which 66 % of the measurements were used for training the ANNs, respectively, while the rest were used for prediction validation. The target data were then scaled for the degree of roasting with 0, 0.13, 0.28, 0.42, 0.57, 0.71, 0.85, and 1 representing fermentation times of 0, 1, 2, 3, 4, 5, 6, and 7 days, respectively. The network was a feed-forward type with back propagation. Mean square error (*MSE*) and R^2 values were recorded. During training, initial weights between 0 and 1 were randomly assigned. Training was done using a backpropagation function, which updates weight and bias values according to the Levenberg–Marquardt optimization. Target termination *MSE* was 0.0005. Settings for the routine are: mu = 0.001, mu-dec = 0.1, mu-inc = 0.1, iteration = 1000, validation check: 5000. The parameter "mu" is part of the training function and is used to tune how roots of differentiable equations are determined. The values of "mu-dec" or "mu-inc" specify how this factor can be decreased or increased, allowing it to be adjusted to most quickly reach an optimized solution. Hyperbolic tangent sigmoid ("tansig") functions were used for hidden layers and output layers. The "validation check" parameter allows the training to be stopped early if the network performance fails to improve.

2.5 | Decision tree, RF algorithm, NB, and KNN settings

Same data used for training/validating the ANNs were used for the algorithm described in this section. Decision tree and two type of RF algorithms (bootstrap forest and boosted tree) were conducted by JMP

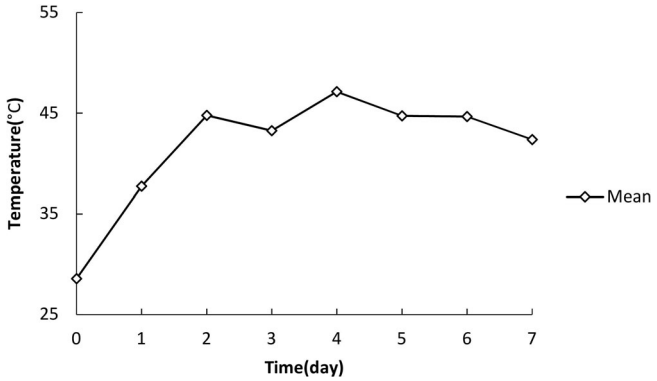

FIGURE 3 The mean temperature of cocoa beans as a function of fermentation time

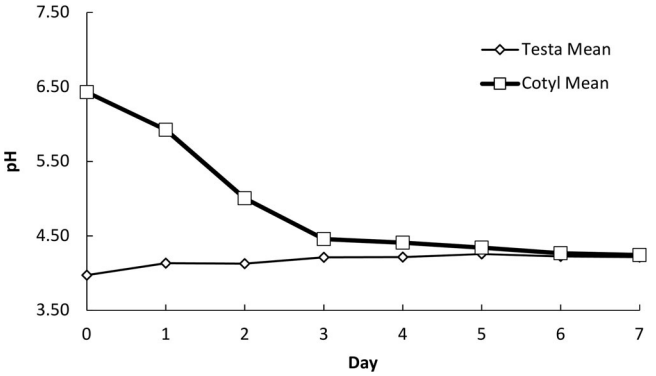

FIGURE 4 The averaged pH of cocoa testa and cotyledons as a function of fermentation time

(Pro 13, SAS Institute, Inc., Cary, NC). Some study defined bootstrap forest as "random forest," while defining boosted tree as "gradient boosting." In this study, the two algorithms were defined as two type of RF algorithm because the working principle of both algorithms were to build more powerful model by training multiple decision trees, while the main difference was the selection of training set. The number of decision trees for both algorithms was 100. Maximum splits per tree was 30. In this study, the ratio of validation samples varied from 0.1 to 0.5 and 0.4 validation ratio yielded highest correct classification rates. Naïve Bayes and KNN were conducted by JMP. The X factors were the sensor response features and Y factors were the fermentation time. The number of nearest neighbors, *K*, was varied from 5 to 10.

2.6 | Statistical methods

Based on the assumptions that observations being tested are independent and there was equal within-group variance across the groups associated with each mean in the test (homogeneity of variance), the influence of fermentation time on the characteristics (peak valve, rising time, and relaxation time) of gas sensors were evaluated by one-way analysis of variance followed by Tukey's HSD at a 95% level of confidence using JMP.

3 | RESULTS AND DISCUSSION

3.1 | Temperature and pH variation during cocoa fermentation

The trendlines in Figures 3 and 4 shows the change of temperature and pH, respectively, during fermentation. Generally, in the fermentation process, the temperature varied between 28 and 50°C, and the peak temperature was observed in the fourth day of fermentation when microbial action on producing ethanol and acids was about to over. The temperature of cocoa beans changes in the fermentation process was due to heat-generated activities of microorganisms which transformed the substances in pulp into alcohol, carbon dioxide, organic acid, and other volatiles. The observations in Figure 3 concurred with the statement made by Schwan and Wheals (2004), who indicated that the peak temperature appeared at around the fourth day of fermentation.

The pH in testa remained relatively constant (~4.4) during fermentation, however, the pH in cotyledon during drastically from 6.5 to 3.2. The observations were due to the organic acids including acetic, oxalic, phosphoric, succinic, and malic acids produced by several yeasts, penetrating the testa, and gradually absorbed by the cotyledon. The observation of pH in cocoa cotyledon were consist with many previous studies (Amin, Jinap, & Jamilah, 1998). However, the pH in the testa of the beans remained relatively constant during the fermentation, that was because the organic acid contacted with the testa and decreased the pH because penetrated it.

3.2 | The responses of e-nose during fermentation

Generally, relative peak value of each sensor is proportional to the overall concentration of target gases. Rising time indicates how sensitive one gas sensor responses to interacting gases and relaxation time shows how strong the "bonding" between the gas sensor and the molecules (Arshak et al., 2004). Although the overall concentration of the target gases of each gas sensor may influence its rising time and relaxation time, other factors such as the combination of nontarget gases and target gases in the environment, the environmental temperature, and air turbulence may also influence the two parameters.

Table 2 shows the scaled relative peak values of each gas sensor at different fermentation time. The relative peak values of sensors 2620 and 826 remained at relative high activity at Days 2, 3, 6, and 7. This observation is due to the sensor's high sensitivity to odorous gases, such as ammonia generated at the late stage of fermentation, and to volatile organic compound, such as ethanol and organic acids which were generated by yeast at early stage of fermentation. Sensors 822, 823, 826, 2620, and 2610 were generally at relatively high activities at the first 4 days of the fermentation due to their sensitivities to organic vapors such as organic acids and ethanol. Sensors 813 and 830 did not underwent fluctuated activity during fermentation because their target gases, such as hydrogen and refrigerants were not generated during the fermentation. Generally, the responses of each gas sensor concurred with the observations reported

TABLE 2 Scaled features (relative peak, rising time, and relaxation time) of each sensor as a function of fermentation time

Relative peak	813	821	823	822	826	830	2620	2610	2602
0	0.14^{d}	0.09^{cd}	0.57^{e}	0.52^{cd}	0.51^{c}	0.28^{b}	0.91^{c}	0.22^{a}	0.29^{bc}
1	0.09^{cd}	0.05^{b}	0.50^{d}	0.48^{c}	0.46^{b}	0.28^{b}	0.91^{c}	0.54^{c}	0.27^{b}
2	0.08^{c}	0.03	0.55^{de}	0.57^{d}	0.61^{d}	0.25^{ab}	0.87^{b}	0.22^{a}	0.42^{d}
3	0.13^{d}	0.01^{a}	0.53^{d}	0.55^{cd}	0.57^{cd}	0.23^{a}	0.82^{bc}	0.23^{a}	0.41^{d}
4	0.13^{d}	0.08^{c}	0.33^{c}	0.34^{b}	0.35^{a}	0.28^{b}	0.86^{b}	0.40^{b}	0.23^{a}
5	0.04^{b}	0.01^{a}	0.22^{b}	0.32^{b}	0.35^{a}	0.31^{c}	0.82^{bc}	0.36^{b}	0.25^{ab}
6	0.03^{b}	0.10^{d}	0.21^{b}	0.29^{ab}	0.42^{b}	0.25^{ab}	0.78^{b}	0.20^{a}	0.33^{c}
7	0.00^{a}	0.05^{b}	0.10^{a}	0.24^{a}	0.37^{ab}	0.21^{a}	0.74^{a}	0.22^{a}	0.32^{c}
Rising time									
0	0.12^{b}	0.20^{b}	0.15^{cd}	0.25^{d}	0.18^{b}	0.09^{ab}	0.00^{a}	0.04^{c}	0.01^{a}
1	0.08^{a}	0.14^{a}	0.29^{e}	0.17^{c}	0.14^{a}	0.08^{a}	0.28^{e}	0.01^{ab}	0.02^{a}
2	0.12^{b}	0.18^{ab}	0.05^{ab}	0.13^{b}	0.16^{ab}	0.11^{b}	0.18^{cd}	0.01^{ab}	0.03^{ab}
3	0.10^{ab}	0.18^{ab}	0.03^{a}	0.11^{ab}	0.18^{b}	0.11^{b}	0.21^{d}	0.01^{ab}	0.03^{ab}
4	0.23^{c}	0.17^{ab}	0.22^{d}	0.27^{d}	0.30^{c}	0.28^{c}	0.08^{b}	0.02^{b}	0.07^{b}
5	0.10^{ab}	0.19^{b}	0.10^{c}	0.28^{d}	0.20^{b}	0.09^{ab}	0.09^{b}	0.02^{b}	0.07^{b}
6	0.09^{a}	0.25^{c}	0.11^{c}	0.16^{c}	0.16^{ab}	0.11^{b}	0.16^{c}	0.02^{b}	0.06^{b}
7	0.10^{ab}	0.22^{bc}	0.07^{b}	0.10^{a}	0.15^{ab}	0.09^{ab}	0.20^{d}	0.00^{a}	0.03^{ab}
Relaxation time									
0	0.12^{b}	0.20^{b}	0.15^{cd}	0.25^{d}	0.18^{b}	0.09^{ab}	0.00^{a}	0.04^{c}	0.01^{a}
1	0.08^{a}	0.14^{a}	0.29^{e}	0.17^{c}	0.14^{a}	0.08^{a}	0.28^{e}	0.01^{ab}	0.02^{a}
2	0.12^{b}	0.18^{ab}	0.05^{ab}	0.13^{b}	0.16^{ab}	0.11^{b}	0.18^{cd}	0.01^{ab}	0.03^{ab}
3	0.10^{ab}	0.18^{ab}	0.03^{a}	0.11^{ab}	0.18^{b}	0.11^{b}	0.21^{d}	0.01^{ab}	0.03^{ab}
4	0.23^{c}	0.17^{ab}	0.22^{d}	0.27^{d}	0.30^{c}	0.28^{c}	0.08^{b}	0.02^{b}	0.07^{b}
5	0.10^{ab}	0.19^{b}	0.10^{c}	0.28^{d}	0.20^{b}	0.09^{ab}	0.09^{b}	0.02^{b}	0.07^{b}
6	0.09^{a}	0.25^{c}	0.11^{c}	0.16^{c}	0.16^{ab}	0.11^{b}	0.16^{c}	0.02^{b}	0.06^{b}
7	0.10^{ab}	0.22^{bc}	0.07^{b}	0.10^{a}	0.15^{ab}	0.09^{ab}	0.20^{d}	0.00^{a}	0.03^{ab}

Note: Different letter indicates significantly different at 95% confident level.

by previous studies (Schwan & Wheals, 2004) about volatile compounds development during cocoa fermentation.

Table 2 shows the scaled rising time and relaxation time of each gas sensor at different fermentation time. However, as mentioned above, many factors may influence the two parameters in linear or nonlinear way, therefore, little information can be exacted by fitting the fermentation time and the two parameters to multivariate models. As discussed above, the relative peak values of gas sensors provide some information about the changes of concentrations of certain types of volatile compounds generated during the fermentation, however, most of the sensors have very broad sensitivity, which made it difficult to trace the change of one or several compounds which can sever as fermentation indicators by directly looking at the responses of the sensors.

3.3 | Fermentation time determination by ANN, decision tree, and RF

As discussed above, it is difficult to correlate the response of gas sensors to cocoa fermentation time by multivariate models, therefore, some training based-pattern recognition models are potentially feasible to do the classification for cocoa beans. The R^2 and *MSE* of the e-nose-trained ANN were 0.937 and 0.000464, respectively. Table 3 shows the misclassification rate of trained ANN. 12.8% overall misclassification rate was achieved. The ANN misclassified 34% of the first fermentation day's verification samples, this was because microbial reactions did not produce enough discriminating volatiles (ethanol and organic acids) in the first day and the high content of water molecules in the headspace camouflaged other volatiles. In addition, achieving low *MSE* was one of the goals for ANN training, therefore, during the training process, ANN may scarify the accuracy for classifying samples who has great similarity to other group of samples to achieve overall low *MSE*.

The misclassification rates of decision tree and RF models were shown in Table 4. Both the two RF models achieved relatively low misclassification rate (9.4% for bootstrap forest and 13.6 % for boosted tree). The misclassification rate for decision tree was much higher than RF models. As many researchers reported, RF models are more powerful than decision tree in term of classification accuracy because a RF was constructed by many decision trees which decrease the influence of single bad trained decision tree (Liaw & Wiener, 2002). The misclassification rate of boosted tree was higher than bootstrap, which was different from

TABLE 3 Misclassification rates of ANN for determining cocoa bean fermentation time

Fermentation time (day)	Misclassification rate (%)
0	34.0
1	12.8
2	6.4
3	10.6
4	12.8
5	10.6
6	8.5
7	6.4
Overall	12.8

Abbreviation: ANN, artificial neural network.

TABLE 4 Misclassification rates of RF, NB, and, KNN for determining cocoa bean fermentation time

Method	Misclassification rate (%)
Decision tree	18.3
Bootstrap forest	9.4
Boosted tree	13.6
Naïve Bayes	36
k-nearest neighbors	34.1

Abbreviations: KNN, *k*-nearest neighbors; NB, naïve Bayes; RF, random forest.

some researchers (Caruana & Niculescu-Mizil, 2006) who claimed that boosting methods are more likely to achieve lower misclassification rate than bootstrap forest. Because the distribution of gases in headspace of the cocoa was not homogeneous, therefore, samples collected from the edges of the fermentation box may differed from samples collected from other location, which may generate outliers. By using boosted tree algorithm, outliers were more likely to stay in a training set, which can correctly classify the misclassified outliers while misclassifying much more normal samples.

Then performance of NB and KNN were included in Table 4. Generally, the misclassification rates of both algorithms were relatively high (>34%), which were not considered as good performance when comparing to other models. This was because NB made a strong assumption any two features are independent given the output class, however, the features of the samples in this study were strongly depended on each other, for example, the relative peak and relaxation time of one sensor were not independent. In addition, distance-based classification model was not suitable for classifying samples containing too many variables (27) because it is not clear which type of distance to use and which variables to use to produce good results.

4 | CONCLUSION

The application of machine learning based electronic nose system in determining fermentation degree of cocoa bean was proved to be feasible. A misclassification rate as low as 9.4% was achieved by bootstrap forest algorithm. ANN and boosted forest also achieved good classification rate. However, decision tree, KNN, and NB were not able to determine cocoa fermentation time. This observation indicating that with appropriate design of e-nose, sufficient number of training data, and proper machine learning algorithms, cocoa fermentation can be determined at relatively low cost and short time. Although it is realistic to apply the model trained in this study to determine to fermentation time of other varieties and origins of beans, conduct more tests on cocoa beans with different variety, origin, fermentation condition, and so forth, by the same electronic nose and establish an online data library to record to data will make the system more powerful.

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