Development of an Electronic Nose for Harmful Gases with Prediction Modeling Using Machine Learning

Ana Antoniette C. Illahi [1], Argel A. Bandala [1], Edwin Sybingco [1], Elmer P. Dadios [1], Ryan Rhay P. Vicerra [1], Ronnie Concepcion II [1], Laurence A. Gan Lim [1], and Raouf Naguib [2,*]

[1] Department of Electronics and Computer Engineering, De La Salle University, Manila, Philippines
[2] School of Mathematics, Computer Science and Engineering, Liverpool Hope University, Liverpool, United Kingdom
*Correspondence: ana.illahi@dlsu.edu.ph (A.A.C.I.)

***Abstract*—Harmful gases can inflict damage, accident, or even death on a human being. The safety and security of human beings are essential to the community. This study aims to develop an electronic nose with prediction modeling using machine learning. With the use of the sensor substitution technique, the system can predict the gas by utilizing a minimal number of sensors. The system, which is designed to predict Ammonia, Ethanol, and Isobutylene, relies on Support Vector Machine (SVM), Gaussian Process Regression (GPR), and Feed Forward Neural Network (FFNN) to ensure the prediction models are accurate. As a result, for Ammonia, Ethanol, and Isobutylene, using SVM, GPR, and FFNN model attain value of 1.00 for R^2. The RMSE and MAE has a low result value indicates that the SVM, GPR, and FFNN model is performing well and can be used to make decisions regarding the concentration levels of harmful gases. This study shows that the system can predict the presence of gases within it using machine learning.**

***Keywords*—machine learning, e-nose, prediction model, support vector machine, gaussian process regression, feed forward neural network**

I. Introduction

Machine learning and biologically inspired engineering technology, such as the electronic nose, play a significant role in the evolution of humanity. Novel technology is significant to society as it assists humans with the instantaneous completion of tasks [1]. The first model of an electronic nose was to copy some simple functionality of the human nose for characterization [2]. In some instances, robots and other related systems can perform even without human supervision. Technology keeps on evolving every day and the development of different applications, systems, equipment, and materials for all industries is of great assistance to society. A device that can detect and classify odors and odorless elements with the use of an array of sensors is labeled as an electronic nose (e-nose). All sensors must be properly calibrated to ensure that the data collected is correct and accurate [3]. Machine learning comprising paradigms, such as AI, Fuzzy Logic, GPR and SVM, is an algorithm to autonomously detect and predict harmful gases/chemicals within the surrounding [4]. E-nose bids fast and constant recognition of odor in the surroundings and, most importantly, it is not invasive. While the human nose is important in everyday life because it is part of the major senses and has the capability to detect and characterize odors, mimicking it is complex. However, advances pertaining to electronic nose technology provide an advantageous solution for this.

The nose is one of the important parts of the face or anterior extremity of the head, consisting of the nostrils and the olfactory system [5]. Olfaction, gustation, and trigeminal senses are the three sensory systems in humans to trigger the sense of smell and taste, and equally react to different types of chemicals [6]. The sense of smell is the leading sensory system of all since the olfactory system can be used alone to identify or profile flavors in some products [7]. While predictions can help to improve the e-nose for detecting and classifying gases [8], the ability to smell emanates from the stimulation of the human olfactory system by odorant molecules emitted from the material. The olfactory system is the sensory system used for smelling or olfaction. The odor enters the nose pathway and reaches the nasal cavity when inhaling or through the throat, when the tongue pushes the air to the back or nasal cavity [9].

An electronic nose, or e-nose is also called an artificial nose, electronic olfactometry, multi-sensor array, odor sensing system, mechanical sensor, aroma sensor, flavor sensor, and odor sensor [10]. The motivation to develop an electronic nose is to mimic the human olfactory system [11]. The olfactory system allows humans to be conscious of their surroundings [12]. The challenge in identifying and classifying an odor is that the odor interaction or chemical mixture bonds naturally [13]. In the past, the concept of electronic nose was not concrete due to limiting early sensor capabilities. The term "electronic nose" was first introduced in the late 1990s [14]. The first structure of an electronic nose was composed of a multisensory array in charge of detecting more than one chemical constituent. With the promising

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potential of the electronic nose in the community, it became popular in the fields of medicine, security systems, agriculture, food, and water industry [15–17]. In an electronic nose, an array of sensors senses the input signal; this is then followed by data analysis, pattern recognition, and machine learning algorithms that detect and identify the odor.

Ammonia, Carbon Monoxide, Methane, Toluene, Isobutylene, and Ethanol are explosive gases, explosive chemicals or toxic/hazardous chemicals which are particularly focused on in this research. Table I shows the chemical explosive limits of each substance, including the parameters pertaining to LFL/LEL, UFL/UEL, chemical composition, and flash point. The Lower Flammable Limit (LFL) and Lower Explosive Limit (LEL) are the lowest end of the concentration range of the chemical substances in the air and can be ignited at each temperature and pressure; normally it is expressed by volume percentage. Whereas Upper Flammable Limit (UFL) and Upper Explosive Limit (UEL) is the highest concentration of gas or vapor in the air that can produce a flash of fire in the presence of an ignition source. The Flashpoint is the lowest temperature at which the gas vapors ignite.

TABLE I. CHEMICAL EXPLOSIVE LIMITS

Chemical	Chemical Composition	LFL/LEL in % by volume of air	UFL/UEL in % by volume of air	Flash point (°C)
Toluene	C7H8	1.1	7.1	4.4
Methane	CH4	4.4	16.4	−188
Carbon Monoxide	CO	12	75	−191
Ammonia	NH3	15	28	11
Isobutylene	C_4H_8	1.8	9.6	−76.1
Ethanol	C_2H_6O	3.3	19	12.78

The aim of this research is to design and develop an electronic nose for the detection of harmful gases, such as Ammonia, Carbon Monoxide, Methane, Toluene, Isobutylene, and Ethanol, using a computational intelligence system. With population safety being a global priority, the Development of an e-nose that can detect harmful gases can prevent any form of chemical or biological attack or threat in a given area. By developing advanced models and applying machine learning, e-nose technology can greatly improve its performance. To this end, several models, such as Artificial Neural Networks (ANN) [5, 8], Support Vector Machine (SVM) Regression [9–10], and Gaussian Process Regression (GPR) prediction models are studied. However, it should be noted that using multiple sensors in an e-nose is costly and impractical for implementation in a natural set up in society. The implementation of sensor substitution can reduce the cost and data processing within the system.

This study seeks to address the various challenges present in e-nose technology using the sensor substitution technique. Sensors for Toluene, Methane, and Carbon Monoxide can predict gases, such as Ammonia, Ethanol, and Isobutylene using the sensor substitution technique. The aforementioned model types are used to enhance the computational cost of the e-nose by eliminating/reducing the use of sensors in the system, while still detecting the target gas. This additionally assists in reducing the power/energy consumption of the e-nose in comparison to the sensor substitution technique.

II. MATERIALS AND METHODS

A. Electronic Nose Structure

The design phase of the electronic nose will consist of hardware and software designs that are needed in the system. This phase establishes how the electronic nose functions. Fig. 1 shows the typical input-process-output of an electronic nose.

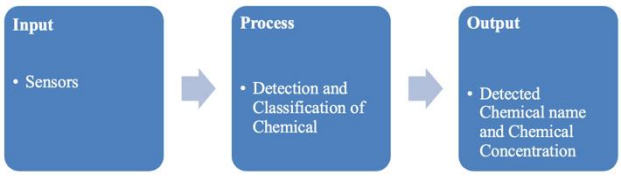


Figure 1. Input-process-output diagram of electronic nose.

The stimulus is the odor from the surrounding environment, and the chemical sensor is responsible for detecting the chemical property and measuring the concentration. A Metal Oxide Semiconductor (MOS) sensor is the type of sensor that will be used in this system. As previously mentioned, the sensor data consist of Ammonia, Carbon Monoxide, Methane, Isobutylene, Toluene, and Ethanol. A computational intelligence system will be used for correcting sensor drift and detecting and classifying chemicals. The output of the system is the name and concentration of the chemical.

Fig. 2 shows the electronic nose process diagram. The following are the system process requirements that need to be considered: a) Data Classification — an algorithm for classification must be utilized to detect sensor data and produce data for the end user; b) Data Processing — an algorithm for data processing must be utilized because sensor data should be processed before it can be used; c) Reliability — the device must receive sensor data in a short period of time, process data, and classify at the same time without compromising the overall performance of the system; d) Connectivity — a tool that establishes a wireless connection to secure the interchange of data in the entire system; and e) Portability — packaged in a small size that is useful in the outside environment.

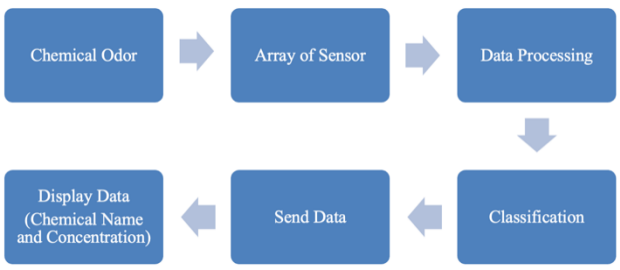


Figure 2. Electronic nose process diagram.

For data processing and classification, a machine learning algorithm is the best approach to classify the data from the electronic nose with greater accuracy as it is reliable and responds faster once the dataset has been previously trained.

With regard to missing values, while the authors considered ignoring them and continuing with the analysis, they do not recommend such approach as missing values can significantly impact the results of the analysis and may lead to inaccurate or misleading conclusions. Imputing the missing values is the second approach the authors applied in this study. This involves replacing the missing values with estimates based on the available data; the method applied for imputing missing values is mean imputation. The purpose of mean imputation, in this study, is to handle missing values in a dataset by replacing them with the mean or average value of the variable. This is used when the number of missing values is small, and the missing values are believed to be missing at random. Mean imputation is simple to implement and can be accomplished rapidly, making it a useful option when time is of the essence. It preserves the sample size and the distribution of the variable, which can be important for this research.

Outlier detection is a process of identifying data points in a dataset that are significantly different from the rest of the data. In this study, outlier detection is used to identify extreme data points that may be caused by errors in the data collection process or conditions of the surrounding environment that affect the sensor readings. Visual inspection is a simple way that was used to identify outliers in gas sensor data by plotting the data and visually inspecting it for points that are significantly different from the rest of the data. Statistical tests such as the Grubbs test were also used to identify outliers in a more formal way. The Grubbs test works by calculating a test statistic, which is based on the difference between the suspected outlier and the mean of the dataset. Lastly, machine learning algorithms were also applied. SVM, FFNN, and GPR algorithms work by training a model on a dataset and then using the model to identify data points that are significantly different from the rest of the data.

Before the data can be analyzed, preprocessing is performed to remove any noise or errors that have been introduced during the data collection process. Filtering and other operations are performed to cleanse and prepare the data prior to analysis. Since the analysis of gas sensor data entails its collection and storage in a way that is easily accessible for further processing, using a data acquisition system to collect it from the sensors and save it to a file or database facilitates the application of the ensuing statistical and analytical methods , such as calculating means and standard deviations, performing regression analysis to identify relationships between different variables, or using machine learning algorithms to build predictive models. Using graphs, as shown in the results and discussion, is an effective way to provide insight into the gas sensor data and help identify trends or patterns in it.

B. Electronic Nose Classification and Detection

Fig. 3 shows the process flow of the electronic nose for the classification of chemicals. Data is collected by using the different sensors that are being utilized. While the collected data cannot be used directly for performing the analysis process due to missing, noisy, or inconsistent data, as well as outlier values. Data preprocessing is thus important in electronic nose systems as this will lead to a more accurate model. Raw data must be converted into a clean data set by preprocessing it through one of the previously mentioned methods: ignoring missing values, filling in the missing values, converting the data, detecting outliers, and machine learning. The goal is to train the best-performing model possible based on the preprocessed data. Supervised training will be implemented where the data is tagged with the correct label, enabling classification and regression operations to be performed. Classification is used because the electronic nose will categorize the chemical once it is detected. On the other hand, regression is also utilized because it has the capability to handle data in the numeric output. In order to train an electronic nose model, it is necessary to divide it into three parts, namely, training data, validation data, and testing data. To fit the parameters of the classifier, a subset of the data is used for learning; this is undertaken through the training dataset. To fine-tune the parameters of the classifier, a subset of unseen training data is used, and to evaluate the adeptness of the model on unseen data, cross-validation is utilized. Finally, the test dataset is used to test the performance of the classifier. It should be noted that the training and validation sets are available during the training of the classifier, while the test set should be available during its testing. Basically, the training set is applied to construct a model and the validation set is used to validate the constructed model. When the model is trained, the same trained model will be used to predict using the testing data. A confusion matrix indicates how effective the model is through assessing the resulting true positive, true negative, false positive, and false negative parameters. The size of the matrix depends on the number of classes in the model. Evaluating the model is essential because it helps to identify the best model that represents the data and assess its effectiveness for future use. Since chemicals present in the environment need to be detected, each chemical is treated as a sample. The array of sensors is an important part of the electronic nose. If the sensors are not functional, it is not possible to collect raw data. Thus, an array of sensors serves as an interface for the electronic nose. Sensors can detect the chemicals present in the surrounding. An analog signal that is being recognized by the system will be converted to a digital form. The function of preprocessing is to collect data from the array of sensors. Verifying the input chemical is vital to classify if it is valid or not. Sampling of the data must be performed to represent the massive amount of raw data collected. Only the selected data can be fed into the model because due to limitations in memory size and speed capacity of the system. Ultimately, the function of data recognition in the electronic nose is to provide a

classification decision by an algorithm. The aim of machine learning is to classify data based on statistical information extracted from the model. The electronic nose system uses computational intelligence techniques to recognize chemical data, and the resulting output is an interface projecting the nature and numeric data of the chemical concentration that is being detected within the area.

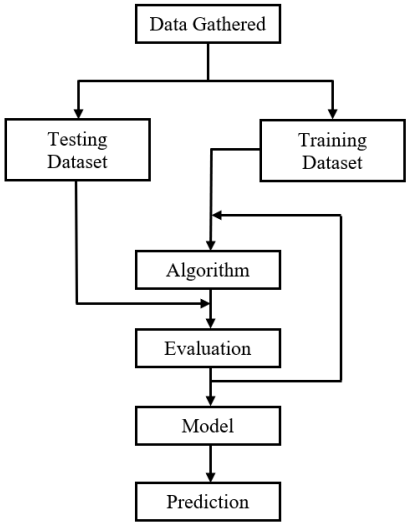


Figure 3. Process flow of electronic nose for classification of chemicals.

A high-performance computer must be use for neural network training. Matlab is the software tool used in machine learning to build and train neural networks. Matlab takes fewer lines of code and builds a machine-learning model, and it provides the ideal development environment, through model training and deployment. An overall functional electronic nose software development application is used to process and monitor all the information in the system: from connecting wirelessly, through utilizing a classifying algorithm to detect sensor data, to the processing as well as storage of data for later analysis.

C. Harmful Gas Prediction Modelling

MATLAB is an effective tool in machine learning for predictive modeling and, in this study, it is an essential tool to achieve the main objective. An integrative statistical method with machine learning can forecast or predict upcoming outcomes. Predictive modeling is used in this study to create predictions for Ammonia, Ethanol, and Isobutylene. Three machine learning models were used to ensure the prediction models are accurate and show the same results: Support Vector Machine (SVM), Gaussian Process Regression (GPR), and Feed Forward Neural Network (FFNN). SVM is one of the deep learning algorithms that can undertake supervised learning for regression, as well as classification of datasets; it builds models that assign new samples to another group. GPR is one of the notable machine learning algorithms due to its accurate prediction capability. It can solve a wide range of supervised machine learning problems, even in the absence of sufficient data. FFNN is one of the simplest forms of artificial neural networks. The connections at each node do not form a cycle, and the data or information passes through multiple hidden nodes and is processed in one direction. It can also run independently with a small transition to guarantee moderation.

The GPR optimizable parameters for Ammonia are as follows: nonisotropic rational quadratic kernel function, constant basis function, kernel scale = 14.9017, sigma = 80.2488, prediction speed = ~7400 obs/sec, training time = 3564.5 secs, signal standard deviation = 80.2488, true standardized size, and Bayesian optimization for the optimizer. The GPR optimizable parameters for Ethanol are as follows: nonisotropic rational quadratic kernel function, constant basis function, kernel scale = 15.0599, sigma = 11.0124, prediction speed = ~35000 obs/sec, training time = 3618.3 sec, signal standard deviation = 11.0124, true standardized size, and Bayesian optimization for the optimizer. The GPR optimizable parameters for Isobutylene are as follows: nonisotropic rational quadratic kernel function, constant basis function, kernel scale = 15.1605, sigma = 13.7283, prediction speed = ~26000 obs/sec, training time = 3326.4 sec, signal standard deviation = 13.7283, true standardized size, and Bayesian optimization for the optimizer.

The SVM optimizable parameters for Ammonia are as follows: gaussian kernel function, box constraint = 1, kernel scale = 1, epsilon = 0.00378, true standardized data, prediction speed = ~17000 obs/sec, training time = 148.13 sec, and Bayesian optimizer. The SVM optimizable parameters for Ethanol are as follows: gaussian kernel function is, box constraint = 1, kernel scale = 1, epsilon = 0.00389, true standardized data, prediction speed = ~31000 obs/sec, training time = 237.6 sec, and Bayesian optimizer. The SVM optimizable parameters for Isobutylene are as follows: gaussian kernel function, box constraint = 1, kernel scale = 1, epsilon = 0.39444, true standardized data, prediction speed = ~26000 obs/sec, training time = 108.48 sec, and Bayesian optimizer.

The FFNN optimizable parameters for Ammonia are as follows: number of neurons per layer: 100, 50, and 20, respectively, the Bayesian optimizer, activation function: ReLU, iteration limit = 1000, number of fully connected layer = 3, sigmoid activation function, lambda value = 7.75074, and first layer size = 47. The FFNN optimizable parameters for Ethanol are as follows: number of neurons per layer: 100, 50, and 20, respectively, Bayesian optimizer, activation function: ReLU, iteration limit = 1000, number of fully connected layer = 3, sigmoid activation function, lambda value = $6.8907e^{-5}$, and sizes of the first, second and third layers are 1, 3, and 16, respectively. The FFNN optimizable parameters for Isobutylene are as follows: number of neurons per layer: 100, 50, and 20, respectively, Bayesian optimizer, activation function: ReLU, iteration limit = 1000, number of fully connected layer = 3, sigmoid activation function, lambda value = $4.3714e^{-7}$, and sizes of the first, second and third layers are 2, 53, and 220, respectively.

D. Model Evaluation Metrics

Artificial Neural Network (ANN), Support Vector Machine (SVM), and Gaussian Process Regression (GPR) models were used in this study. The Root Mean Square error (RMSE) is the standard deviation of the prediction errors. The prediction errors are the measure and the extent of spread from the regression line. They show how contiguous the data is to the best-fit line. The Mean Absolute Error (MAE) measures errors between the predicted and actual values. It provides information about the average error from the prediction, and it is the simplest measure of prediction accuracy. The coefficient of determination (R^2) measures the linear correlation of the data, and it is the goodness of fit. A value of 1.00 indicates a perfect fit and the model used is highly reliable. RMSE, MAE and R^2 are the significant parameters that require consideration to assess the accuracy of the system.

III. Results and Discussions

A. SVM, FFNN, GPR Optimization Results

Sensors have the capability to detect the present state of the surroundings and send it back to the system. Communication between the e-nose and the outside world is through a sensor. A typical gas sensor consumes 500-800mW of power. Furthermore, multiple sensors, and, notably, the ones used in this research, can consume a significant amount of power that can affect the performance of the system. Therefore, this study makes use of an optimization technique that can render the best possible and most effective operation of the system. This is achieved through the use of the SVM, FFNN, and GPR approaches, which can optimize system performance. The results of the different models demonstrate that a reduction in the number of sensors can be achieved, which will, in turn, lead to a lower energy consumption in the system.

1) MSE plot

The Mean Squared Error is essential to prediction modeling because it measures the extent of error in the system. Getting the average squared difference between the observed and predicted value is a way of assessing it. An MSE value of 0, implies that the model is void of errors.

Fig. 4 show the MSE plots for Ammonia using the SVM, GPR, and FFNN models, respectively. The SVM model attains a value of 1.00 for R^2, RMSE = 0.83738, and MAE = 0.53805. The GPR model attains a value of 1.00 for R^2, RMSE = 0.14295, and MAE = 0.038904. The FFNN model attains a value of 1.00 for R^2, RMSE = 0.59746, and MAE = 0.089269.

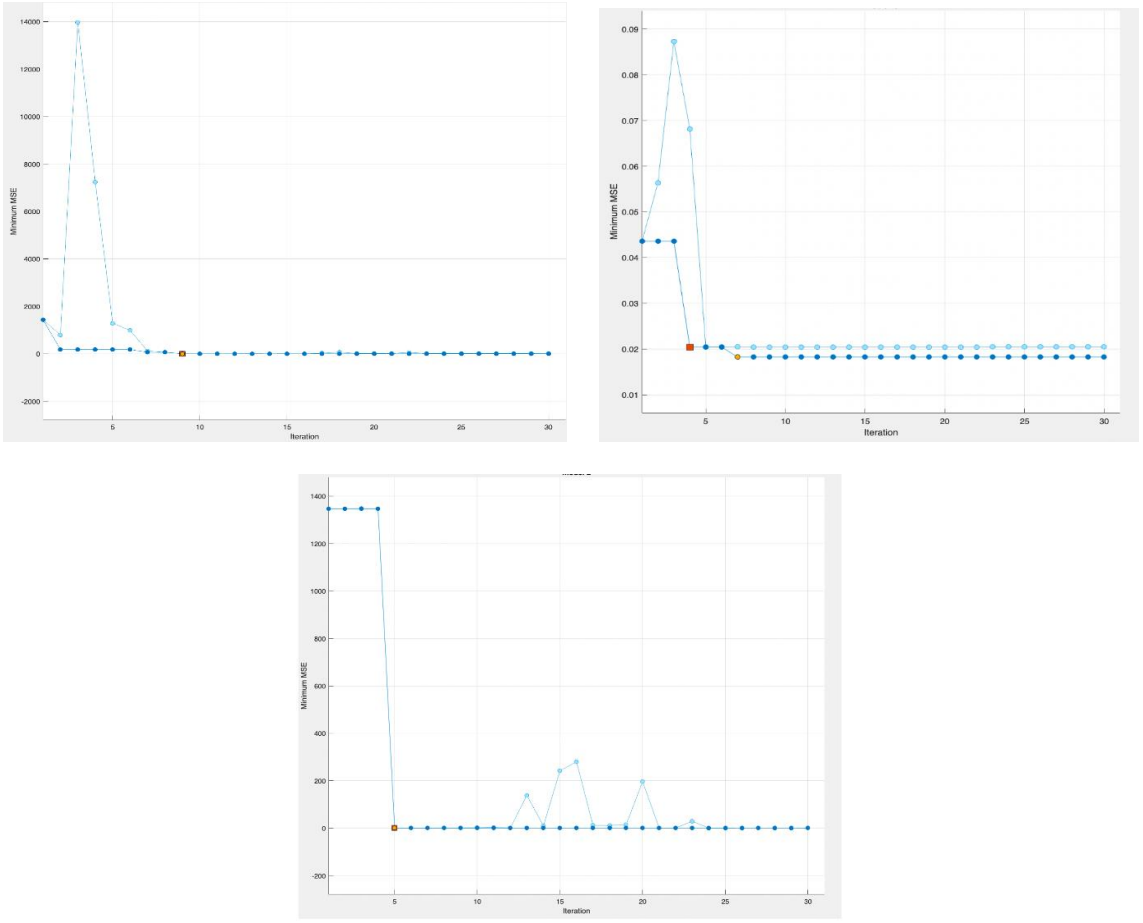


Figure 4. SVM, GPR and FFNN Ammonia MSE plot.

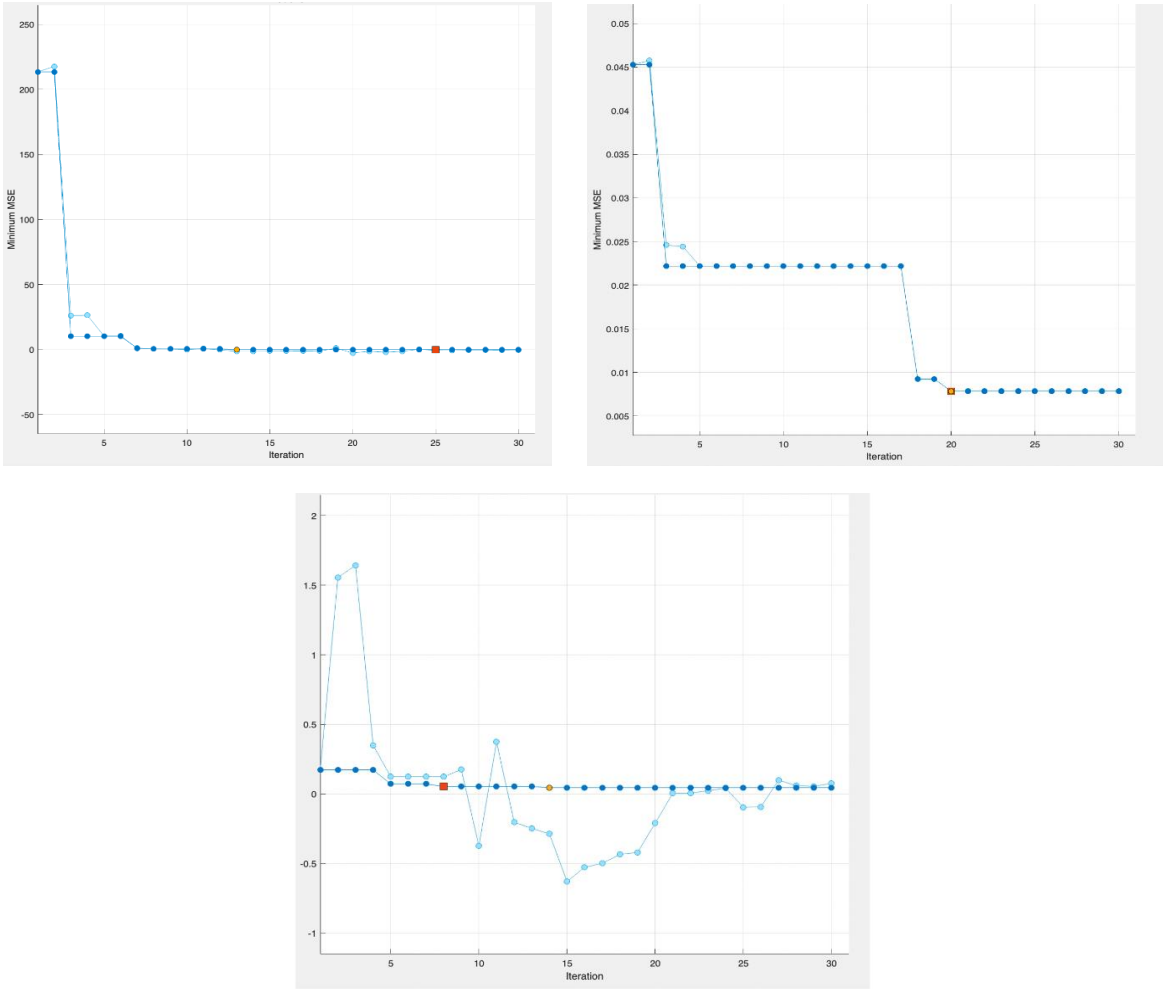
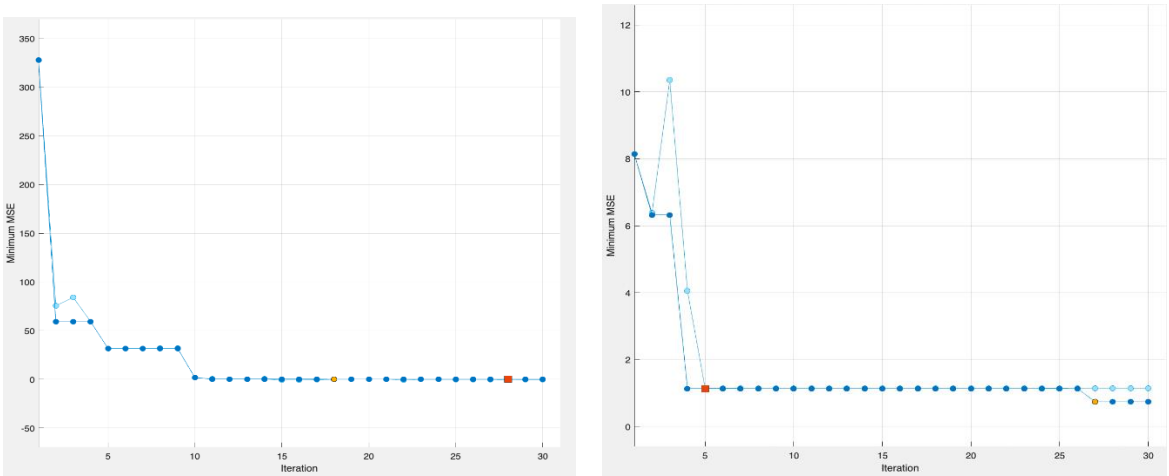


Figure 5. SVM, GPR and FFNN Ethanol MSE plot.

Fig. 5 shows the MSE plots for Ethanol using the SVM, GPR, and FFNN models, respectively. The SVM model attains a value of 1.00 for R^2, RMSE = 0.22692, and MAE = 0.053117. The GPR model attains a value of 1.00 for R^2, RMSE = 0.E, and MAE = 0.011398. The FFNN model attains a value of 1.00 for R^2, RMSE = 0.23021, and MAE = 0.07897.

Finally, Fig. 6 show the MSE plots for Isobutylene using the SVM, GPR, and FFNN models, respectively. The SVM model attains a value of 1.00 for R^2, RMSE = 0.808, and MAE = 0.1403. The GPR model attains a value of 1.00 for R^2, RMSE = 0.010648, and MAE = 0.0073113. The FFNN model attains a value of 1.00 for R^2, RMSE = 0.047909, and MAE = 0.027774.



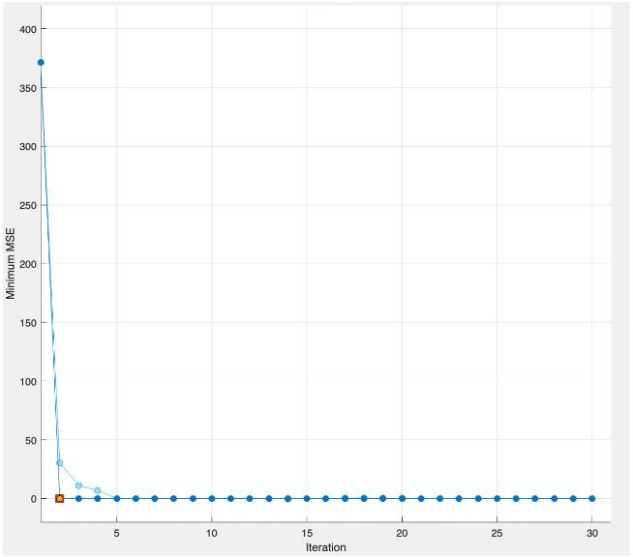


Figure 6. SVM, GPR and FFNN Isobutylene MSE plot.

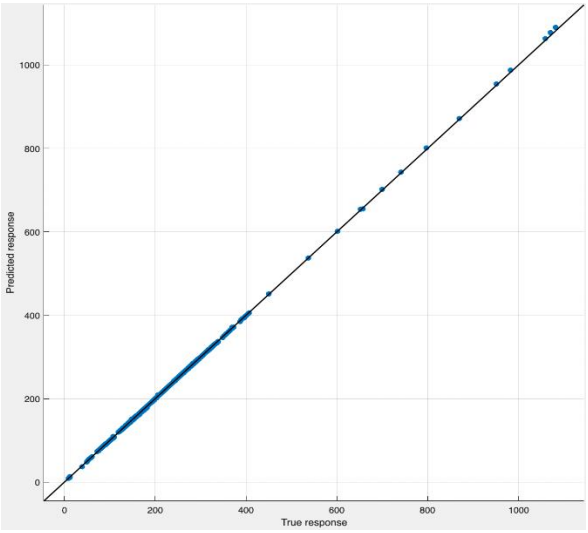
2) Validation predicted vs actual plot

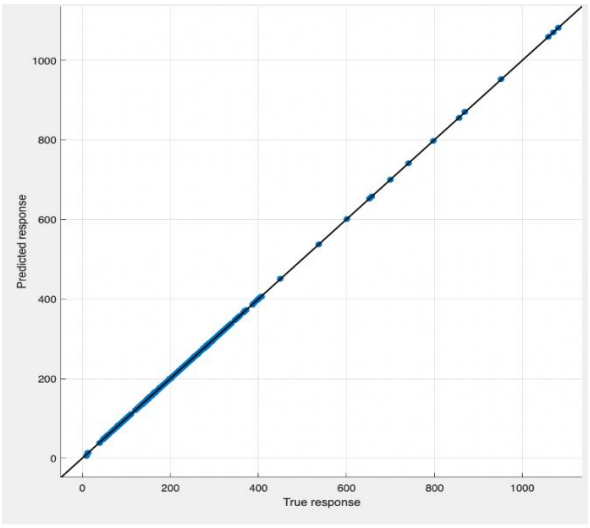
SVM models 1, 2, and 3, GPR models 4, 5, and 6, and FFNN models 7, 8, and 9 have three inputs such as Toluene, Methane, and Carbon Monoxide. The output of all models is Ammonia, Ethanol, and Isobutylene, respectively. Table II gives the summary of the results for all the models per gas. The values obtained for RMSE, R^2, and MAE are an indication that the prediction models are accurate.

The use of machine learning in this system, with the sensor substitution technique, provides an improvement to the current electronic nose technology. Prediction of gases with the use of the different models produces an accurate result. The sensor substitution technique reduces the use of sensors in the system due to its capability to predict gases. The energy consumption of the e-nose is beyond efficient and effective due to the reduction in the number of sensors in the system. As shown in Figs. 7–9, a notable accuracy and good fit is demonstrated throughout all the models.

TABLE II. SUMMARY OF RESULTS FOR SVM, GRP, AND FFNN MODEL

Chemical	SVM	GPR	FFNN
	RMSE		
Ammonia	0.83738	0.14295	0.59746
Ethanol	0.22692	0.08856	0.23021
Isobutylene	0.808	0.010648	0.047909
	R^2		
Ammonia	1.00	1.00	1.00
Ethanol	1.00	1.00	1.00
Isobutylene	1.00	1.00	1.00
	MAE		
Ammonia	0.53805	0.038904	0.089269
Ethanol	0.053117	0.011398	0.07897
Isobutylene	0.1403	0.0073113	0.027774





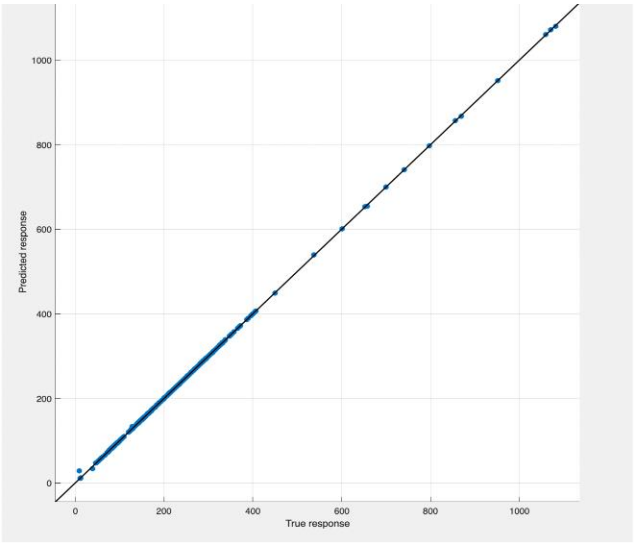
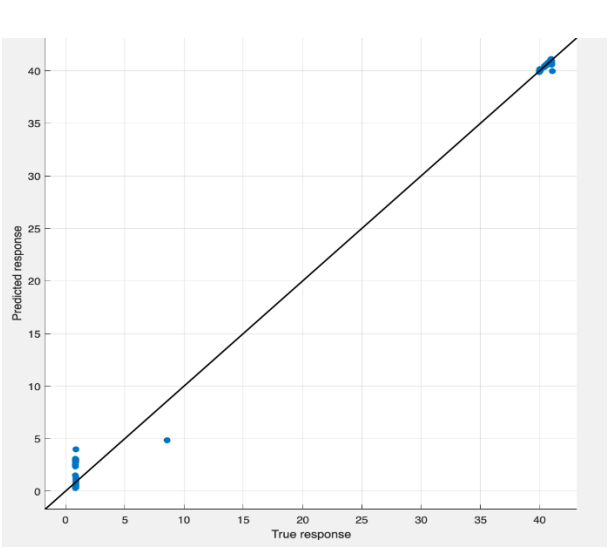
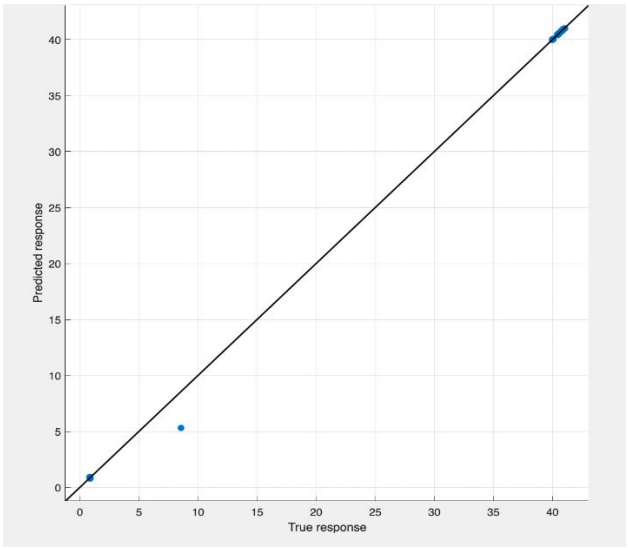


Figure 7. SVM, GPR and FFNN Ammonia validation predicted vs actual result.





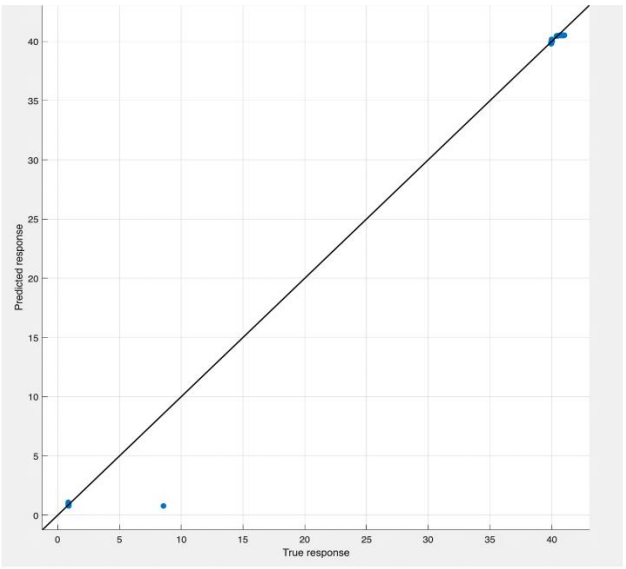


Figure 8. SVM, GPR and FFNN Ethanol validation predicted vs actual result.

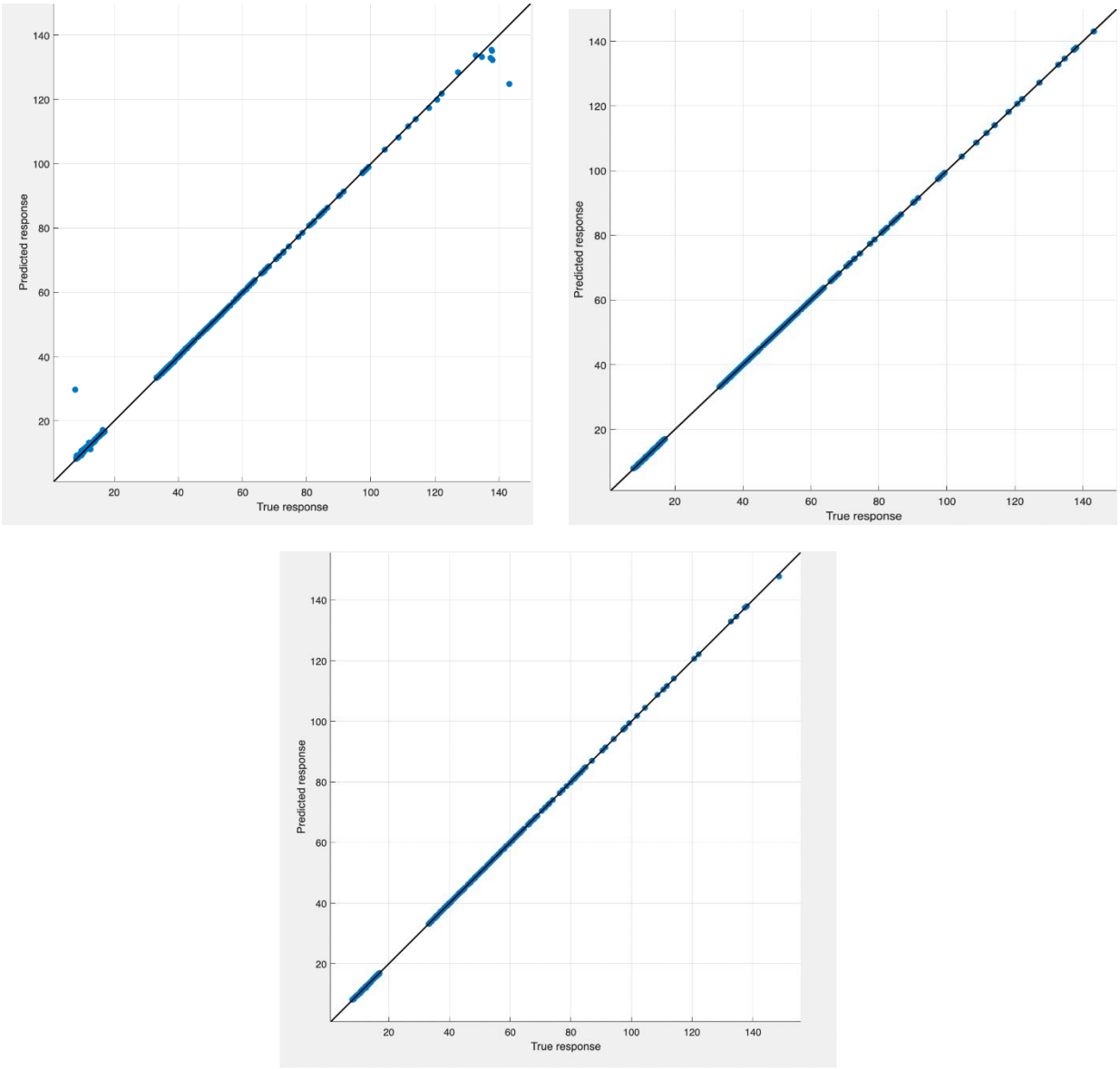


Figure 9. SVM, GPR and FFNN Isobutylene validation predicted vs actual result.

A cost-benefit analysis is a tool used to evaluate the potential costs and benefits of this study. The benefits of an electronic nose with prediction modeling using machine learning for detecting harmful gases are improved safety, increased efficiency, cost savings, and improved decision making. The electronic nose can detect harmful gases in the environment, helping to prevent accidents, and protect workers and the public. Prediction modeling using machine learning can assist in predicting the possible presence of harmful gases, allowing for proactive measures to be taken and reducing the need for unnecessary continuous monitoring. Thus, the electronic nose, in combination with prediction modeling, can help to reduce the cost of monitoring harmful gases, as it can be done more efficiently and accurately than traditional methods. Equally, the electronic nose and prediction modeling can provide more accurate and timely information, helping decision-makers to make informed decisions about the presence of harmful gases. Cost is an important factor in a cost-benefit analysis, especially in this study, because it projects the resources needed to achieve the benefits of the project. Initial purchase, maintenance, repair, training, and implementation costs are the types of cost that need to be considered for this study And, admittedly, this may present a high initial purchase cost and require regular maintenance and repair, which can incur additional costs. Users may need to be trained on how to use the electronic nose and prediction modeling system, which can increase such costs. Lastly, there may be additional costs associated with the implementation of the system and its integration into existing systems and processes. However, overall, the potential benefits of the electronic nose and prediction modeling system, such as improved safety and efficiency, would outweigh its initial costs, especially since the system is able to significantly reduce the risk of accidents and the cost of monitoring harmful gases. Nonetheless, it is important to carefully consider all potential costs and benefits associated with implementing the system prior to deciding on its adoption.

IV. Conclusions and Recommendations

The use of regression analysis in each model shows a good prediction pattern. Prediction models such as SVM, GPR, and ANN are important to electronic nose technology as they are able to predict and optimize the outcome. The study is able to predict Ethanol, Ammonia, and Isobutylene. The results of R^2, MAE, and RMSE prove that the prediction models with regression analysis are appropriate for the detection of harmful gases. Also, the use of multiple sensors in the e-nose can be avoided to minimize the energy consumption in the system. It is recommended that the use of the Internet of Things in this study be implemented to enable remote monitoring of the system. As a final thought, given the continuous advances in machine learning technology, future and perhaps more advanced algorithms may be alternatively considered for prediction.

Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

A. I. spearheaded this research, while E. D., A. B., E. S., R. V., L. G. L., and R. N. assisted during its conceptualization and formulation.

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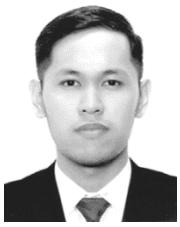
Ana Antoniette C. Illahi received her bachelor of science in computer engineering from Adamson University in 2004. She received her master of science in computer engineering from Mapua University in 2010 and currently taking a doctor of philosophy in electronics and communications engineering from De LaSalle University. She is currently an Assistant Professor at De La Salle University. Her research interests are artificial intelligence, algorithms, software engineering, and systems automation.

Elmer P. Dadios is presently a full professor at the De La Salle University, Manila, Philippines under the Manufacturing Engineering and Management Department, and the Graduate Program Coordinator of Gokongwei College of Engineering. He currently leads government-funded research on bomb removal robots, traffic surveillance, and smart aquaponics. He obtained his degree in Doctor of Philosophy (Ph.D.) at Loughborough University, United Kingdom. He accomplished his degree in Master of Science in Computer Science (MSCS) at De La Salle University (DLSU), Manila, and his Bachelor of Science in Electrical Engineering degree from Mindanao State University (MSU), Marawi City, Philippines. For his professional experiences, he became part of a Scholarship Committee and Administrative Staff working for the Department of Science and Technology (DOST) Philippine Council for Industry, Engineering Research, and Development. He was as well a Research Coordinator and a Director at the DLSU. He had experiences as Session Chair, Program Chair, Publicity Chair, and General Chair in various local and international conferences, and became an External Assessor at the University of Malaysia. He won numerous awards such as Top 100 Scientists Listed in Asian Scientist Magazine and Leaders in Innovation Fellowship "Fellow" given by the United Kingdom Royal Academy of Engineering. He had published numerous technical and scientific research papers regarding robotics, artificial intelligence, software engineering, automation, and intelligent systems. Dr. Dadios is presently the President of the Mechatronics and Robotics Society of the Philippines. Aside from being a Senior Member of the Institute of Electrical and Electronics Engineers (IEEE), he is also the Region 10 Executive Committee, the Section and Chapter Coordinator, and the

Section Elevation Committee Chair. He is also a Vice Chair of the National Research Council of the Philippines and an active member of the Steering Committee, Asian Control Association (ACA), the Philippines American Academy of Science and Engineering (PAASE), and the Society of Manufacturing Engineers (SME).

Argel A. Bandala received his bachelor of science in electronics and communications engineering from the Polytechnic University of the Philippines in 2008. He received his master of science in electronics and communications engineering and doctor of philosophy in electronics and communications Engineering from De La Salle University in 2012 and 2015 respectively. He is currently an associate professor and researcher at De La Salle University. He is a full professor in the Electronics and Communications Engineering Department at De La Salle University and a researcher of the Intelligent Systems Laboratory. His research interests are artificial intelligence, algorithms, software engineering, automation, and swarm robotics. Dr. Bandala is very active in the IEEE Philippine Section where he served as the Section Secretary for the years 2012 to the present. He also serves as the secretary of the IEEE Computational Intelligence Society Philippine Section from 2012 to the present. He is also an active member of the IEEE Robotics and Automation Society from 2013 to the present.



Ronnie S. Concepcion II is mainly working on applied artificial intelligence for sustainable and precision agriculture in open and controlled environment engineering to have a clean food production system, integrated computer vision, and computational intelligence for crop phenomics as affected by biotic and abiotic stressors, nutrient absorption optimization, plant electrophysiology, unconventional computing, organic circuits, bioelectricity, biomedical engineering and underground imaging using capacitive resistivity.

Ryan Rhay P. Vicerra is an associate professor in the Department of Manufacturing Engineering and Management. He is a doctor of philosophy in electronics and communications engineering with a specialization in artificial intelligence, control systems, and swarm robotics. He is author of journal articles in the field of Swarm Intelligence for aerial and underwater robot systems; and computational intelligence-based systems like fuzzy logic systems, genetic algorithm, and neural networks.

Edwin Sybingco is a faculty of the DLSU ECE Department. He completed his doctoral of philosophy in electronics and communications engineering at De La Salle University area of Digital Signal Processing (DSP) focusing on big data and intelligent systems. He received his Master of Science (Electronics and Communications Engineering) from De La Salle University. He already published more than 30 scientific papers internationally in the field of DSP, Machine Vision, Computational Intelligence, and robotics.

Laurence A. Gan Lim is a full professor and former chair of the Mechanical Engineering Department of De La Salle University (DLSU) in Manila, Philippines. He obtained his doctor of philosophy from Coventry University in the U.K. where he developed algorithms to automatically classify colonic histopathological images using computational intelligence. Dr. Gan Lim earned both his bachelor's and master's degrees in mechanical engineering from DLSU where he developed and implemented fuzzy logic control in a micro-hydro power laboratory equipment. He served as Chair of the IEEE Philippine Section in 2014. His research interests include computational intelligence, image analysis, mechatronics, robotics, and fluid mechanics. He has published papers in reputable technical journals and conferences. Dr. Gan Lim authored the section about Mechatronics in the 2009 Philippine Science Compendium on Engineering and Industry Research. He is a lifetime member of the Philippine Society of Mechanical Engineers (PSME).

Raouf Naguib was awarded his BSc from Cairo University in 1979 and his MSc (with Distinction) and PhD from Imperial College of Science, Technology and Medicine, University of London, in 1983 and 1986, respectively. He is currently a Visiting Professor and Part-Time Senior Lecturer at Liverpool Hope University, UK. Prior to this he was Professor of Biomedical Computing and Head of the Biomedical Computing and Engineering Technologies Applied Research Group at Coventry University, UK, and subsequently the Director of BIOCORE Research & Consultancy International, UK. He has published over 400 journal and conference papers and reports in many aspects of health informatics, environmental health, social health, biomedical and digital signal processing, biomedical image processing and the applications of artificial intelligence and evolutionary computation in cancer research. He has also published a book on digital filtering, and co-edited two books on the applications of artificial neural networks in cancer diagnosis, prognosis and patient management: and artificial intelligence and environmental sustainability. He was awarded the Fulbright Cancer Fellowship in 1995-96 when he carried out research in the USA, at the University of Hawaii in Mānoa, on the applications of artificial neural networks in breast cancer patient management. Prof Naguib is a member of several national and international research committees and boards and has served on the Administrative Committee of the IEEE Engineering in Medicine and Biology Society (EMBS), representing Region 8, and the Society's Distinguished Lecturers Committee and Infostructure Committee, as well as the UK EPSRC Peer Review College. He also represented the IEEE-EMBS on the IEEE-USA Committee on Communications and Information Policy. He currently serves on several international review panels, including the European Commission, Qatar National Research Fund, UAE National Research Foundation and the Canadian Foundation for Innovation (CFI). In 2003, Prof Naguib was appointed as Adjunct Research Professor at the University of Carleton, Ottawa, Canada, and in 2005 he was appointed as Honorary Professor at De La Salle University, Manila, Philippines.