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IMPACT OF FEATURE REDUCTION AND OPERATING TEMPERATURE ON GAS IDENTIFICATION

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ABSTRACT

Tin-oxide based gas sensor requires an operating temperature typically in the range of 200 ˚C to 400 ˚C and its performance dependents on this temperature. In this paper a deep examination has been made to analyze the best operating temperature suitable for gas identification application in which an array of sensors is used along with an appropriate feature reduction algorithm. The two most common feature reduction algorithms for gas classification are principal component analysis (PCA) and linear discriminant analysis (LDA); both of them have been used in this analytical work. The feature reduction is followed by a binary decision tree (BDT) or K-nearest neighbor (KNN) based classifier. Results obtained with data from an array of sensors used for detecting C_6H_6, CH_2O, CO, NO_2 and SO_2 indicates that at 400 ˚C the BDT can classify 100% of gases after LDA based feature reduction, whereas KNN can classify 100% of gases at 200 ˚C and 300 ˚C using data before and after feature reduction. Furthermore, experimental results from the given sensor data suggest that with and without considering the operating temperature the BDT can classify 96% of gases using first four LDA components. While KNN can classify 98% to 99% of gases using first four LDA or first five PCA components of resulting data obtained after feature reduction. Thus, after LDA-based feature reduction both classifiers provide superior identification with minimum number of components.

Keywords: electronic nose, gas identification, feature reduction, sensor array.

INTRODUCTION

The concept of electronic nose has been introduced to identify gases based on the finger-prints obtained from gas sensors (Bedoui *et al*., 2013) (Das *et al*., 2013). However, in most cases the finger-prints of gases provide poor classification due to the problem of drift and non-selectivity (Shi *et al*., 2006). The problem of non-selectivity can be resolved by providing multiple readings for a given gas either by using single sensor in multiple times or multiple sensors in single time. In (Vergara *et al*., 2012) a temperature modulation approach to provide multiple reading for gas with a single sensor is used, whereas in (Guo *et al*., 2007) a 4x4 array of gas sensor is proposed in which each sensor provides a different response to the target gas thus providing 16 different signatures for a gas at a time. In both cases, multiple measurement values will be obtained to perform classification thereby increasing the feature vector size, which in turn will increase the complexity of the classifier (Gutierrez-Osuna 2002). Therefore an appropriate feature reduction algorithm is required to extract the most useful information from the data and rearrange the data for improved classification (Hastie *et al*. 2005). Different research approaches have already been presented for feature reduction like independent component analysis (Li *et al*. 2005), multidimensional scaling (Chandrasiri *et al*. 1999) etc. The two most commonly used feature reduction algorithms are principal component analysis (PCA) and linear discriminant analysis (LDA) (Ali *et al*. 2013).

In this research paper the performance of classifiers is analyzed after the application of PCA and LDA-based feature reduction approaches. In most cases the classifiers used for gas identification are taken from pattern recognition application (Brahim-Belhouari & Bermak, 2005). The most simplified classifiers for pattern recognition applications which can also easily be adopted on hardware are based on binary decision tree (BDT) and K-nearest neighbours (KNN). Therefore, both BDT and KNN are adopted individually to visualize the improvement in gas identification after PCA and LDA-based feature reduction for gas application. The presented work is part of an ongoing project in which a low-power multi-sensing gas identification platform is being developed for gas identification based on an array of tin-oxide gas sensors.

Furthermore, tin-oxide gas sensors require an operating temperature (OT) typically in the range of 200 ˚C to 400 ˚C. Therefore, the impact of OT on the performance of classifiers is analyzed and for this purpose the gas sensor is used to extract the data for five different gases at 200 ˚C, 300 ˚C and 400 ˚C. The obtained data are used for classification in three different ways. The first approach is to perform classification of gases at different temperatures. Whereas the other two approaches are used to check the impact of temperature modulation on the classifier's performance and for this purpose the data obtained at different temperatures are merged to form a single data set. Thereafter the classification is performed with and without the knowledge of the OT. For the given sensor data, it has been found that KNN classifier performs well after LDA-based feature reduction and detects 99% of gases with the condition that OT is known to the classifier.

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The remaining sections of this paper are organized as follows. Section 2 covers the experimental setup. The dimensionally reduction and classification algorithms are described in Section 3. Section 4 is concerned with the achieved results and their discussion. Section 5 concludes the paper.

EXPERIMENTAL SETUP

Gas sensor

Tin-oxide based microelectronics gas sensors are widely adopted in gas identification (Shi *et al.* 2006). These sensors require an OT in the range of 200 ˚C to 400 ˚C in order to become sensitive to the target gas (Shi *et al.* 2006)(Guo *et al.* 2007). The concept of convex Micro-hotplate (MHP) is used in (Guo *et al*., 2007) to reduce the power required to obtain desired OT. Thus, with 2.8V driving voltage the sensor can attain 300 ˚C in 5ms using MHP (Guo *et al*., 2007). Furthermore in order to resolve the problem of selectivity the gas sensors were arranged in an array of 4x4 gas sensor such that each sensor provides unique response for the target gas. In order to insure the unique responses for the target gas B. Guo (Guo *et al*., 2007) uses the post treatment schemes of metal catalyst (like Pt, Pd and Au) and ion implantation (like B, P and H). The micrograph of the 4x4 array sensor is shown in Figure-1.

In this research the 4x4 array of gas sensor shown in Figure-1 is used for data acquisition. The reason of selecting this gas sensor is because of low power consumption and to check the behavior of tin-oxide based gas sensor on different OT.

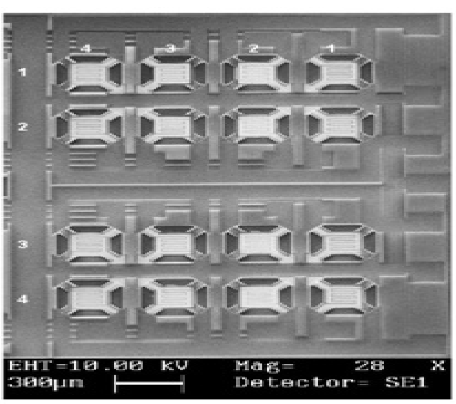

Figure-1. Micrograph for 4x4 gas array sensor (Guo, 2007).

Data acquisition

The experiment is conducted in a controlled lab environment where the 4x4 array gas sensor is kept in a gas chamber as shown in Figure-2. The gas sensor is exposed to different concentrations of a gas in such a way that the chamber is first flushed with air for 750 s and then the new concentration of gas is established in the chamber for the next 750 s. Therefore, each measurement cycle takes 1500 s to provide a single pattern. The aim of this research is to analyze the optimal OT for gas sensor along with the suitable feature reduction approach. Therefore, in order to examine the behaviour of the gas sensor for different operating temperatures, the data acquisition for five most hazardous gases (C_6H_6, CH_2O, CO, NO_2 and SO_2) is performed at three different temperatures (200℃ , 300℃ and 400℃). The general properties along with the health risks caused by these five gases are summarized in Table-1.

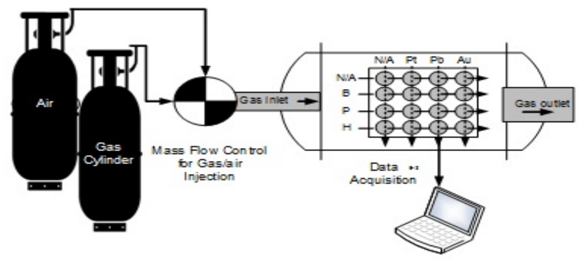

Figure-2. The process of data acquisition.

Furthermore, a concentrations range of 0 to 5 ppm is used for C_6H_6 and CH_2O. This is because the international agency for research on cancer (IARC) identifies them as human carcinogen (Baan *et al*., 2009), (Hauptmann *et al*., 2003). Whereas for CO, NO_2 and SO_2 the range of concentrations are from 0 to 250ppm, 0 to 10ppm and 0 to 15 ppm respectively. The data extraction is carried out for four concentrations of each gas, however the four concentrations are selected from the concentration range of each gas. Thus, the selected concentrations for C_6H_6 and CH_2O are 0.25, 0.5, 2.5 and 5 ppm, while for CO the concentrations are 5, 25, 150 and 200 ppm. Similarly, for NO_2 they are 1, 3, 5, 10 ppm and for SO_2 they are1, 2, 5 and 25 ppm are selected. The process of data acquisition for each gas is repeated three times for each concentration such that each gas sensor has 12 patterns/temperature and a total of 36 patterns for three temperatures.

The sample training and testing patterns obtained from single sensor of gas array for NO_2 at three different OT is shown in Figure-3. The y-axis of the graph is representing the sensor voltages while the x-axis is representing the number of observations. It is observed from the extracted data that the rate of voltage change with respect to concentration decreases with the increase in OT and therefore the response of the sensor is more appropriate at 200℃, as shown in Figure-3.

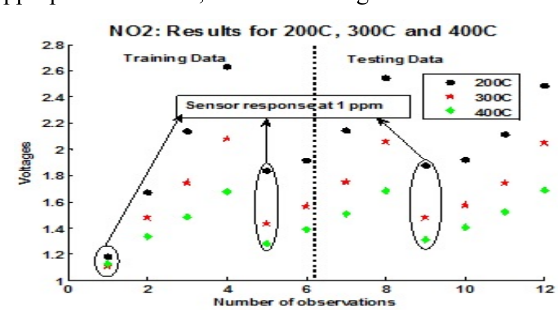

Figure-3. Steady states for NO_2 at 200℃, 300℃ & 400℃.

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Table-1. Physical properties and hazards of gases used in the experiment.

Gases	Physical Properties	Hazards
C_6H_6	Colorless Sweet odor	Acute myeloid leukemia in human (Baan et al., 2009)
CH_2O	Colorless Strong smell	Leukemia and nasopharynx cancer in human (Hauptmann et al., 2003)
CO	Colorless Odorless	Headache, disorientation, dizziness
NO_2	Reddish brown color Pungent odor	Eyes, nose and throat infection Acute and Chronic bronchitis (Garrett et al., 1998)
SO_2	Colorless Non-flammable	Respiratory problem (Spengler et al., 1979)

FEATURE REDUCTION AND CLASSIFICATION ALGORITHMS

The gas sensor array provides 16 different values for a single gas at a time. The values are treated as signatures of the gas and are used for identification. It is worth mentioning that 4 different concentrations have been considered in this research, whereas in practical scenarios the number of concentrations varies with the type of gas plant. Hence the sample training size will be much larger than the one adopted in this research and therefore feature reduction algorithm is required to reduce the data size for training and testing. Another reason for feature reduction is to arrange the data in order to improve the percentile of gas identification. Furthermore, increasing the feature size will increase the complexity of the classifier and thereby increase the processing time. The two most common feature reduction approaches are PCA and LDA and in this paper both of them are analyzed to check the performance of the BDT and KNN based classifiers.

Principal component analysis (PCA)

PCA is used to transform the sample data X from m-dimensional space to n-dimensional space such that m<n. Each component in n-dimensional space is known as principal component which contains most information about data X from lower to upper which means that the first principal component contains most useful information of the data (Honeine, 2012). Let, X be a vector of ixj, i is the number of patterns used for training purpose (where i=1…n), whereas j is the number of sensors in array (where j = 1…m). In this research a 16 array gas sensor is used therefore m=16. In order to perform PCA-based feature reduction, the mean value of each sample will be computed as shown in Equation. 1. Then normalization of the training data is performed using Equation. 2. Thereafter covariance matrix is computed for the obtained normalized data using Equation. 3. After having the covariance matrix, Eigen vector and values are computed. The sample data is then transformed to a new reduced space after multiplication with the Eigen vector. For testing purpose the test data after normalization will be directly multiplied by the Eigen vector using Equation. 4.

$$Mean\ (X) = \begin{bmatrix} \overline{u_1} \\ \vdots \\ \overline{u_n} \end{bmatrix} \qquad where\ \overline{u_i} = \frac{\sum_{j=1}^{m} X_{ij}}{m} \tag{1}$$

$$Normalized\ (X) = \alpha = \begin{pmatrix} X_{11} - \overline{u_1} & \cdots & X_{1m} - \overline{u_1} \\ \vdots & \ddots & \vdots \\ X_{n1} - \overline{u_n} & \cdots & X_{nm} - \overline{u_n} \end{pmatrix} \tag{2}$$

$$Covariance\ (X) = \beta = \frac{\alpha\alpha^T}{m-1} \tag{3}$$

$$PCA = Eigen_{vector}(\beta) \times \alpha \tag{4}$$

Linear discriminant analysis (LDA)

LDA based feature reduction is the most commonly adopted supervized learning approach. The basic function of LDA is to reduce the intra-class-differences and increase between-class differences simultaneously (Tang *et al*., 2005). PCA training can be achieved directly using sample data X while in contrary LDA works on class differences of sample data. Therefore, sample data X is divided into classes $C1_x$, $C2_x$,…,Cn_x to perform LDA as shown in Equation. 5. After dividing the data into classes the mean of each class will be computed and then the average mean (Avg_mean) is computed by summing means of individual classes and divide them by the total number of classes as shown in Equation. 6. In LDA each class will be normalized according to its corresponding mean and then compute the covariance matrix for the normalized class (CoM_{ND}). The boundary mean is computed by calculating the difference between the average mean of all classes from the mean of the individual classes using Equation. 7 and then the covariance of boundary mean is computed (CoM_B). The Eigen vector will be computed for the

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matrix representing the ratio between the average CoM_{ND} and average CoM_B. The final LDA will be obtained by multiplying the matrix of Eigen vector with the sample data X. For testing purpose, the test data will be directly multiplied by the Eigen vector to provide LDA for test patterns.

$$Sample_{data}(X) = \begin{bmatrix} \left.\begin{matrix} X_{11} & \cdots & X_{1m} \\ \vdots & \cdot & \vdots \\ X_{a1} & \cdots & X_{am} \end{matrix}\right\} Class1(C1_X) \\ \begin{matrix} \vdots & & \vdots \end{matrix} \qquad \vdots \\ \left.\begin{matrix} X_{b1} & \cdots & X_{bm} \\ \vdots & \cdot & \vdots \\ X_{n1} & \cdots & X_{nm} \end{matrix}\right\} Classn(Cn_X) \end{bmatrix} \tag{5}$$

$$Avg_{Mean}(\mu_A) = \frac{\sum_{k=1}^{n} Mean\,(Ck_X)}{n} = \frac{\sum_{k=1}^{n} \mu\,(Ck_X)}{n} \tag{6}$$

$$Boundary\ Mean\ (\mu_{Bk}) = \ \mu\ (Ck_X) - \mu_A \tag{7}$$

Binary decision tree (BDT)

The BDT is used to perform classification after the feature reduction. The purpose of selecting BDT-based classifier is because of its simplicity in terms of software and hardware implementation (Li & Bermak, 2011). The goal of this research is to analyze the effect of OT of gas sensor on classification along with the influence of the classifier on the analysis. Therefore a simplified classifier is required to provide the classification results in an adequate manner.

The BDT requires a number of predictors which is defined as the number of variables used for tree formation. Whereas, the designed BDT consists of three major parameters which include the decision node (DN), the tree leaves and the tree depth. The BDT formation starts from single root DN and expands to further DN in each step until a point is achieved after which no further DN is connected. The point after which no DN is connected and no expansion is possible is referred to as classification point. Thus, the maximum number of steps required to reach the final classification point is used to determine the tree depth. Moreover, the branches which have classification points are termed as tree leaves.

K-nearest neighbors (KNN)

KNN is a non-parametric technique widely used in pattern recognition and statistical estimation to classify the unobserved data on the basis of similarity measures (Cocosco *et al*., 2003). KNN classifiers are based on learning from the corresponding neighbors by comparing a given test case with training samples that are similar to it. The new instance of coming class is compared with the already existing samples whose classes are known and then the incoming instance will be given a class whose samples are having closest distance with the incoming instance (Destercke, S. *et al*., 2012). Each training sample is depicted in n-attributes, whereas each sample demonstrates a point in a n-dimensional space so it has a notion of distance. In this research Euclidean distance has been used to recognize the closest neighbors. The Euclidean distance between sample x_m and x_n (n=1,2,…,j) is defined as

$$d(x_m, x_n) = \sqrt{\sum_{p=1}^{j} (x_{mp} - x_{np})^2} \tag{8}$$

SIMULATION RESULTS

The data extracted from gas sensor is for five different gases with three different OT. Therefore, in order to determine the best feature reduction approach along with the optimal operating temperature and classifier, MATLAB simulation was carried out in two phases. The first phase is to determine the optimal temperature and for this phase the data obtained at the same temperature are considered as a single data set. Thus, the whole data are divided into three sub-sets where each of them corresponds to a different OT of 200 ˚C, 300 ˚C and 400 ˚C respectively. Thereafter the simulation process is carried out on individual subsets to analyze the best suitable OT for the gas classification using BDT and KNN. In the second phase the whole dataset is considered as a single sample and simulation is performed to determine the best feature reduction approach.

Simulation results using data obtained at different OT

The data for five different gases obtained from the sensor array at 200 ˚C, 300 ˚C and 400 ˚C are used to analyze the impact of OT on the performance of BDT and KNN classifiers. Both classifiers were trained and tested using the raw data (obtained at individual OT) as well as the reduced data after PCA and LDA based feature reduction, the results for different OT is shown in Table-2. In case of BDT it can be observed that with the increasing OT the classification using raw data improves from 86% to 90%. Whereas LDA-based feature reduction also improves the classification for up to 97.22% at 200 ˚C and provides 100% at 400 ˚C. However, the PCA-based feature reduction shows declining effect on classification with the increase in temperature. Thus, it can be concluded that for the extracted data obtained from the gas sensor, BDT based classifier the optimum OT which suits for PCA and LDA based feature reduction is 200 ˚C.

While in case of KNN, 100% classification can be obtained at 200 ˚C and 300 ˚C from the raw data with 16 sensor values. The same results can also be obtained after reducing the 16 values up to the first three values obtained using PCA or LDA-based feature reduction. Similar to BDT, the results obtained from KNN for the extracted data also recommends 200 ˚C as an optimum temperature at which about 100% classification can be obtained using only the first two components of PCA and LDA. The fact that 200 ˚C is the suitable OT for the given conditions can also be visualized from Figure-3, in which the sample points at 200 ˚C offers a greater rate of change in voltages between two concentrations of particular gas.

Table-2. Classifier performance on different operating temperature before and after feature reduction.

Classifier	OT (˚C)	Raw-Data(%)	LDA (%)		PCA (%)		
			2-LDA	3-LDA	2-PCA	3-PCA	4-PCA
BDT	200	86	97.2	100	94	94	94
	300	87	93	93	80	93	93
	400	90	100	100	47	77	77
KNN	200	100	100	100	97	100	100
	300	100	97	100	70	100	100
	400	93	100	100	63	90	90

Simulation results for the combined data set

It is noted that for the extracted data BDT and KNN provide superior classification after LDA based feature reduction on different OT. However to further examine the performance of these classifiers after LDA and PCA-based feature reduction the data obtained at different OT of 200 ˚C, 300 ˚C and 400 ˚C is combined to generate an overall dataset. The combined data are then used to train the classifiers before and after feature reduction algorithms in two different ways. In the first approach training is done using the data obtained by 4x4 array of the gas sensor without considering the OT on which the data obtained. While in the second approach the OT is also included in the feature vector and thus the feature vector size increases to 17, in which 16 values are those obtained from a gas sensor while the last value is the OT. The results of the first and second approach are shown in Table-3 and Table-4 respectively. The simulation results in Figure-4 are only shown for the single case when OT is unknown.

In case of BDT, it is observed that for the given data, classification obtained after LDA is almost equal to the classification obtained using the first four principal components. Whereas for the given data with and without the knowledge of OT, BDT provides up to 96% classification after LDA based feature reduction, which is 4% to 5% more better than the classification after PCA. Moreover, with only first two components of LDAs the BDT can classify up to 91% of the gases and the classification improves with the increase number of LDA components, while in case of PCA up to 80% of gas identification is achieved using data with and without the knowledge of temperature. Thus, for the given data, LDA with the least number of components provides significant improvement in the classification performance of BDT.

Whereas, KNN-based classifier provides 98% classification of the raw data for both cases where OT is known and unknown. However, similar classification results can also be obtained from the first three LDA or first five PCA components. Hence the above 95% classification is achieved by using only three values obtained from the reduced feature size after LDA. The obtained results also reveal that KNN-based classifier is more efficient than the BDT. Furthermore, in case of KNN the classifier performance improves significantly after LDA-based feature reduction than that of PCA. Thus, similar to BDT, KNN exhibits efficient classification with the least values of LDA than PCA.

Table-3. Gas identification using 4x4 array gas sensor without the knowledge of operating temperature.

Classifier	Properties	Raw-Data	LDA			PCA			
			2-LDA	3-LDA	4-LDA	2-PCA	3-PCA	4-PCA	5-PCA
BDT	Steady State	84%	91%	89%	96%	77 %	87%	91%	91%
KNN	Steady State	98%	92%	96%	97%	73%	84%	96%	96%

Table-4. Gas identification using 4x4 array gas sensor with the knowledge of operating temperature.

Classifier	Properties	Raw-Data	LDA			PCA			
			2-LDA	3-LDA	4-LDA	2-PCA	3-PCA	4-PCA	5-PCA
BDT	Steady State	84%	90%	92%	96%	80%	80%	90%	92%
KNN	Steady State	98%	92%	94%	99%	79%	79%	87%	98%

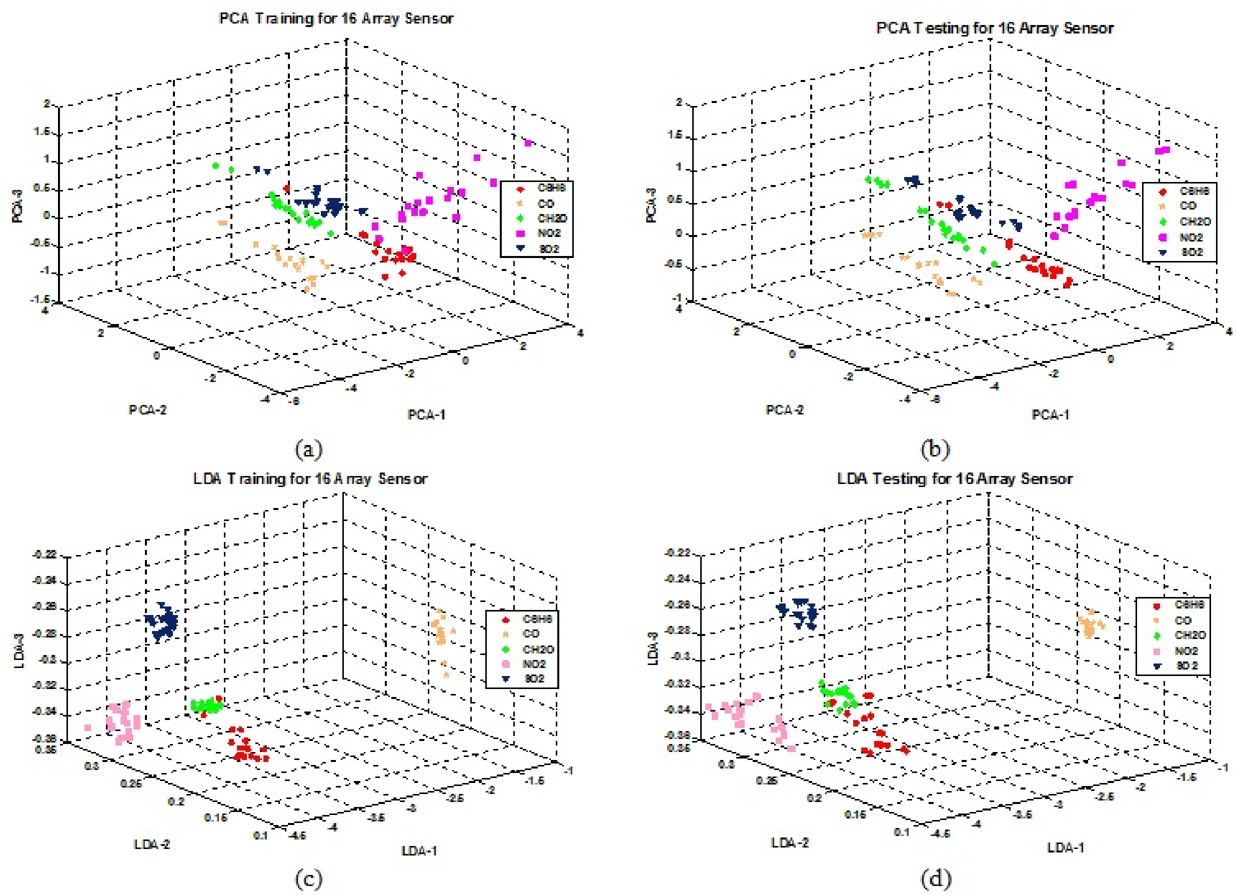

Figure-4. Simulation results for 4x4 array gas sensor without the knowledge of OT; (a) and (b) PCA training and testing, (c) and (d) LDA training and testing.

CONCLUSIONS

In this paper the performance of BDT and KNN-based classifiers is analyzed along with two most commonly used feature reduction approaches of PCA and LDA for the given gas application. Moreover, the gas sensor requires an OT range from 200 ˚C to 400 ˚C in order to become sensitive for the target gas and therefore the gas data for five different hazardous gases have been taken at different OT. This data has been used for performance evaluation of the classifiers in two different ways. The first one deals with the performance of the classifier under different OT using PCA and LDA feature reduction techniques. The obtained results show that after LDA, BDT can provide 100% classification rate at 400 ˚C. Whereas KNN provides 100% classification rate at 200 ˚C using raw data as well as with the first 2 LDA or 3 PCA components. KNN can also classify 100% of gases at 300 ˚C however, for the reduced data, this classification is achieved using three components of PCA and LDA. Therefore the optimum temperature for our designed application is 200 ˚C at which 100% classification is achieved using only two components.

Thereafter the data is used to examine the overall performance of the classifier after PCA and LDA based feature reduction. The whole data obtained at three different OT is merged to provide a complete sample space. The first evaluation is performed on classifier such that it does not have the knowledge of the corresponding

OT. Whereas the other evaluation of classifier is carried out with the knowledge of the OT. In case of BDT, it is observed that the classification obtained after LDA is almost equal to the classification obtained using the first four principal components. Furthermore up to 96% gas identification is obtained after LDA-based feature reduction on the given data with and without the knowledge of OT, respectively.

Whereas, KNN based classifier provides 98% classification of raw data in both cases where OT is known and unknown. However, similar classification results can also be obtained from the first three LDA or first five PCA components. Hence above 95% classification is achieved by using only 3 values obtained from the reduced feature size. The results also reveals that for our experiment KNN based classifier is more efficient than the BDT. While the classification obtained after LDA based feature reduction is more accurate than that obtained after PCA.

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