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PAPERS

A novel data-driven technique to produce multi- sensor virtual responses for gas sensor array-based electronic noses

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Accurate detection of gas/odor requires highly selective gas sensor. However, the high-performance classification of gases/odors can be achieved using partial-selective gas sensors. Since 1980s, an array of broadly tuned (partial-selective) gas sensors have been used in several fields of science and engineering, and the resulting gas sensing systems (GSS) are popularly known as electronic noses (e-Noses). The combination of similar or different sensors in the array indirectly compensates for the requirement of high selectivity in GSS. Further, e-Nose's performance inevitably depends on the salient features drawn from the initial responses of the gas sensor array (GSA). So obtained features are referred to as the responses of virtual sensors (VS). In this paper, we have proposed the three-input and three-output (TITO) technique to derive efficient virtual sensor responses (VSRs) which outperform its well-published peer technique. A GSA consisting of four elements is used to demonstrate the proposed technique. Our proposed technique augments the VSRs by four times compared to its peer. The efficacy of our proposed technique has been tested using nine fundamental classifiers, viz., linear support vector machine (100%), decision tree (97.5%), multi-layer perceptron neural network (100%), K-nearest neighbor (85%), logistic regression (100%), Gaussian process with radial basis function (95%), linear discriminant analysis (97.5%), random forest (100%), and AdaBoost (95%). Ten-fold cross-validation has been used to minimize the biasing impact of the intra- and inter-class variance. With the result, four classifiers successfully provide an accuracy of 100 percent. Hence, we have proposed and vindicated an efficient technique.

K e y w o r d s: electronic nose, gas classification, gas sensor array, virtual sensor response

1 Introduction

The previous three decades have evidenced the proliferation of designing electronic noses (e-Noses) to mimic the mammalian olfactory system (MOS) [1]-[3]. A variety of real- life paradigms saw the spike in applications of e-Nose for areas such as environment [4], healthcare [5], automobile [6], agriculture [7], foods & beverages [8], [9], beauty & cosmetics [10], robotics [11], safety & security [12], forensics [13], textiles [14], coal mines [15], *etc.* A brief introduction to e-Nose could be beneficial to the readers to understand the hypothesis behind virtual gas sensors (VGSs) and virtual gas sensor responses (VGSRs). Accurate detection of gas/odor requires a susceptible and specific gas sensor. The fabrication of such a gas sensor highly depends on the selection of sensing material leading the researchers to an endless loop of searching for the ideal material. Moreover, thus designed gas sensors respond to multiple gases/odors apart from the perfect condition of responding to the particular gas/odor. This cross- selectivity for multiple gases/odors or non-selectivity for the target gas/odor is the crucial issue while fabricating the gas sensors. This issue of selectivity while detecting/classifying gases/odors was overcome using an array of partially selective gas sensors [16].

This breakthrough introduced a surge in utilization of gas sensor array (GSA). Although, to the best of our information, no rule fixes the use of the optimal number of gas sensors in a GSA. This unconstrained use of gas sensors ensures hardware redundancy in the GSA. Also, using more gas sensors leads to considerable power consumption, occupies more area on the chip or mounting platform, makes circuitry complex, and increases the failure possibility of the gas sensor system (GSS). Thereby the concept of virtual gas sensors (VGSs) was proposed to use as few as possible physical gas sensors. In the recent literature, there are two popular ways to derive virtual sensors (VSs) or virtual sensor responses (VSRs). In one way, a single gas sensor was used, but their dynamic responses were captured by varying physical entities such as affinity [17], temperature [18], and resonant frequency [19], *etc.* In another way, the responses of a few physical gas sensors are used to derive the VGSRs using some transformation techniques [20].

In [17], a virtual sensor array was derived by modulating the virtues of affinity of a single sensor realized based

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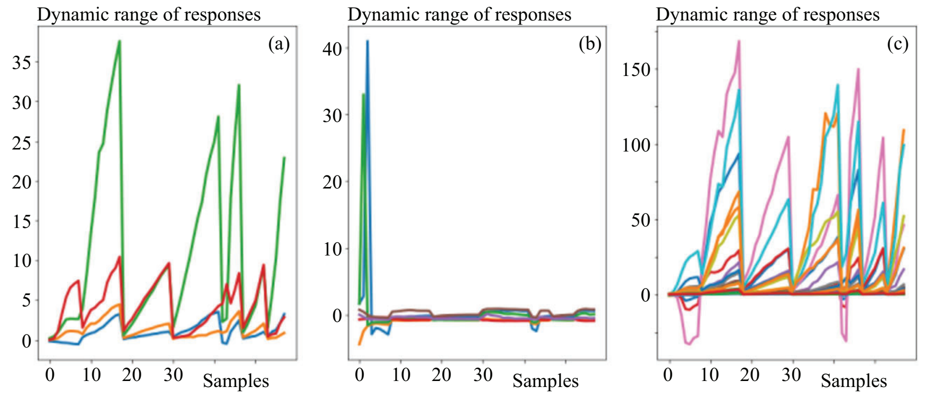

Fig. 1. Sensor responses with dynamic ranges: (a) – initial sensor responses of physical gas sensors, (b) – virtual sensor responses derived using the NDSRT technique, and (c) – virtual sensor responses derived using the proposed TITO technique with enhanced patterns

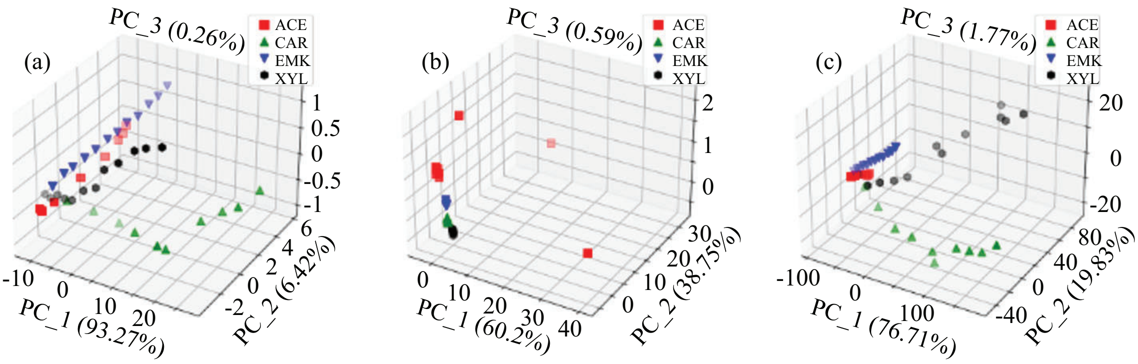

Fig. 2. 3D scatter plots for first three principal components corresponding to: (a) – initial sensor responses of physical gas sensors, (b) – virtual sensor responses derived using the NDSRT technique, and (c) – virtual sensor responses derived using the proposed TITO technique with enhanced patterns

on the principle of electrochemical chemo-transistor. The related modulation was achieved by converting the sensor's chemo- sensitive material between the varying affinity of redox states, controlled by the electrical process. The hypothesis of the virtual sensor array was applied to fish freshness analysis. Far *et al*, (2009) applied the concept of temperature modulation to virtually increase the number of sensors. In their work, the metal oxide (MOX)-based gas sensor was used to design a biological olfactory system (BOS). Here, the temperature modulation was carried out with the help of a micro-hotplate. Their approach improved the resulting performance and achieved a score of 96 percent [18]. Moreover, by modulating the frequency of several resonant modes, a virtual sensor array was performed by Li *et al* (2022) for the identification of volatile organic compounds (VOCs). They achieved the experimental results using machine learning algorithms with identification scores of 95.8 and 87.5 percent, respectively, for VOCs and mixtures [19].

Furthermore, data-driven VSs or VSRs are also popular in the context of e-Noses. As quoted earlier, in this way, the VSRs have been derived from a few physical gas sensor responses applying some transformation techniques. In [20], a Normalized Difference Sensor Response Transformation (NDSRT) technique was used to obtain VSRs. For the considered dataset, they have successfully increased the number of VSRs by $(n-1)/2!$ times of initial physical gas sensor responses, where n is the number of gas sensors in the related GSA. Moreover, they assessed their technique qualitatively, producing well-discriminable responses to classify the gases/odors. They did not demonstrate the classification of gases/odors experimentally for comparing the results quantitatively. Furthermore, zero padding and principal component analysis (PCA)-based VSRs have been used in [21].

However, the PCA-based approach does not increase the number of VSRs but provides the facility of VSR selection as per requirement. In this paper, we have proposed the three-input and three-output (TITO) technique for data-driven VSRs. The virtue of our proposed technique is that it increases the number of VSRs by $6(n-1)(n-2)/3!$ times. Moreover, it produces the up-scaled and down-scaled VSRs that scale-up the dynamic range of responses. In this regard, the enhanced dynamic range facilitates subsequent enhancement in the patterns of responses as shown in Fig. 1. Thus, the obtained VSRs using the proposed technique TITO bring the saliency for classification of gases/odors with higher accuracy. The efficacy of proposed technique has been verified using nine machine learning algorithms, *viz*, linear support vector machine (L- SVM), decision tree (DT), multi-layer perceptron neural network (MLPNN), K-nearest neighbor (KNN), logistic regression (LR), Gaussian process with radial basis function (GP- RBF), linear discriminant analysis (LDA), random forest (RF), and AdaBoost (AB). Experimental results show that our proposed technique outperforms the well-published data- driven VSRs technique "NDSRT". Furthermore, four of nine machine learning algorithms achieve a perfect classification score by using our proposed technique.

2 Materials and methods

In this section, details of our proposed approach have been presented under specific headings.

Physical gas sensor response

An e-Nose system basically possesses an array of partially selective gas sensors. And the resulting systems are widely popular and attracts researchers even today. The diversity of e-Nose applications makes it one of the best multidisciplinary streams in the domain of gas sensing. Current paradigms in this domain pile up the applied artificial intelligence (AI) to make the advanced GSSs or e-Noses robust and reliable using intelligent data-driven (pre-) processing. The considered dataset is the outcome of an integrated four-sensing elements (*eg*, tin oxide, molybdenum oxide, cadmium sulfide, and zinc oxide)-based GSA fabricated by thick-film technology. The complete detail can be seen through the references [20], [22]. Including a GSA, an e-Nose consists of three schematic building blocks, as shown in Fig. 3. The related metal-oxide-based GSA works on the principle of change in resistance of the sensing elements. Furthermore, exposing it to the considered gases/odors, four physical sensor responses are captured for four considered gases/odors, *viz*, acetone, carbon tetrachloride, ethyl-methyl ketone, and xylene. The performance of the GSA can be improved using VSRs, which have more capacity to discriminate the data [20].

Contextual outline of data-driven VSRs

It would be better to brief the NDSRT technique first that has been chosen to compare with the proposed data-driven TITO techniques for multi-sensor virtual responses. The initial responses of physical gas sensors are inadequate to distinguish among the considered gases/odors. Therefore, feature extraction and selection are the two paradigms used to enhance the discriminability. Thus, the curated datasets are obtained that consist of salient extracted/selected responses capable of providing high performance. The data-driven VSRs falls in the arena of feature extraction. NDSRT is a well-published data driven VSR technique that generates $(n-1)/2!$ times VSRs for n physical sensor responses. A mathematical algorithm for NDSRT can be understood as:

Consider a GSA with n physical gas sensors responsible for producing n initial sensor responses. Let X stand for an initial physical sensor response then it can be represented as $X = \{x_1, x_2, \dots, x_i, \dots, x_j, \dots x_n\}$, where x_i and x_j are the responses of i-th and j-th physical gas sensors. In this way, NDSRT-based virtual sensor response can be derived as,

$$r = \frac{x_i - x_j}{x_i + x_j}, \quad i < j. \tag{1}$$

Since it takes two physical sensor responses at a time, producing $\binom{n}{2} = n(n-1)/2!$ VSRs. For the considered dataset, NDSRT produces $\binom{4}{2} = 6$ VSRs for four physical gas sensor responses.

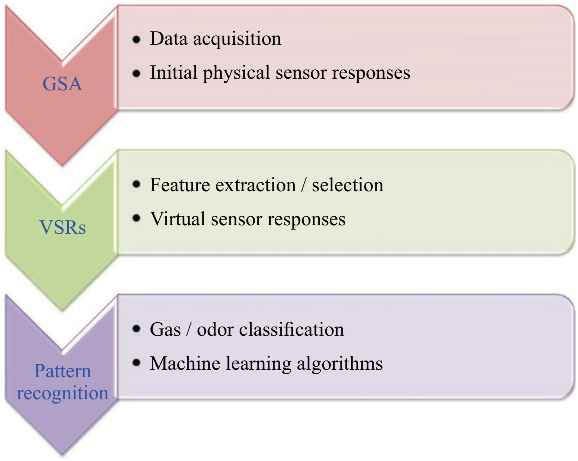

Fig. 3. Schematic building blocks of an electronic nose GSA: gas sensor array, VSRs: virtual sensor responses, and pattern recognition: machine learning algorithms

In contrast, we have proposed the TITO technique for generating VGSRs. It is capable of generating more VSRs than the NDSRT technique. For n physical gas sensor responses, the TITO technique produces $(n-1)(n-2)$ times VSRs for n physical sensor responses. Half of them, have up-scaled values, and the rest half have down-scaled values compared to the initial responses. The synergy of up-scaled and down-scaled responses scale-up the dynamic range of responses. In this regard, the enhanced dynamic range facilitates subsequent enhancement in the patterns of responses as shown in Fig. 1. Thus, the obtained VSRs using the proposed technique TITO bring the saliency for classification of gases/odors with higher accuracy. While compared to the NDSRT technique, the TITO technique produces $(2!)(n-2)$ times more VSRs, proving the proposed technique's adequate capacity. The mathematical formulations to derive TITO technique-based VSRs can be understood as:

Considera GSA with n physical gas sensors responsible for producing n initial sensor responses. Let X stand for an initial physical sensor response then it can be represented as $X = \{x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_k, \dots, x_n\}$, where x_i and x_j and x_k are the responses of i-th, j-th and k-th physical gas sensors. In this way, TITO-based virtual sensor response for $i < j < k$ can be derived as,

$$t_1 = x_i + x_j + \frac{x_i x_j}{x_k}, \quad t_2 = x_i + x_k + \frac{x_i x_k}{x_j}, \qquad (2)$$

$$t_3 = x_j + x_k + \frac{x_j x_k}{x_i}, \quad t_4 = \frac{x_i x_j}{x_i + x_j + x_k}, \qquad (3)$$

$$t_5 = \frac{x_i x_k}{x_i + x_j + x_k}, \quad t_6 = \frac{x_j x_k}{x_i + x_j + x_k}, \qquad (4)$$

Since it takes three physical sensor responses at a time, for the considered dataset, TITO produces $6\binom{4}{3} = 24$ VSRs for four physical gas sensor responses.

Machine Learning Algorithms

In this work, we have used nine machine-learning algorithms for the classification of the considered gases/odors. These are as follows:

The linear SVM classifier has been implemented based on the SVM library LibSVM [23]. For the multi-class classification objective, it uses one-vs-one (OVO) policy. Usually, the gas sensor responses (GSRs) may be affected by sensor drift, therefore, a stronger L2 regularization has been used. The decision tree algorithm has also been used for the aforesaid purpose. Fully grown trees without pruning have been used since GSRs are limited while using steady-state values. In contrast, while using transients (larger dataset) the memory consumption can be reduced using pruning which also results in less complexity and reduced size of the trees. A neural network-based single-layer MLP has been used with 100 neurons. It uses the Relu activation function, a learning rate of 0.001, and stochastic gradient descent (SGD) optimizer for 100 iterations to converge. The k-nearest neighbors (KNN) classifier has been used with 5 neighbors using uniform weights. For distance metric, the standard Euclidean space has been used. A logistic regression-based classifier has also been used that uses Newton's algorithm of the conjugate gradient. We have used 100 iterations to converge the algorithm. The gaussian process (GP) is a classification algorithm that works on Laplace approximation. A radial basis function (RBF) is used as the kernel for this classifier 1.0 RBF (1.0). The prediction approximates posterior using Newton's method in 100 iterations. It combines the binary predictors to achieve multiclass predictions using the one-vs-rest (OVR) policy. Linear Discriminant Analysis (LDA) classifier utilizes Bayes' rule to obtain the class conditional densities for generating a linear decision boundary. A random forest (RF) is an ensemble classifier that uses multiple decision trees (DTs) for classification on several subsets of the considered dataset. It uses the mean of such DTs to enhance the predictive score and reduce the adversity caused by overfitting. The split process considers ten DTs up to the five levels in the forest. The AdaBoost algorithm is also an ensemble classifier that aggregates predictions from multiple variants. We have used its 50 variants with a unit learning rate. Also, the SAMME.R' (Stagewise Additive Modelling using a Multi-class Exponential loss function, where R stands for Real) algorithm [24] has been used for boosting that terminates at the 50th iteration. It works faster than its predecessor SAMME' and achieves a lower error rate even using a few iterations.

3 Experimental results and discussion

Results

This paper proposes a novel TITO technique for multi-sensor virtual responses. In this technique, combinations of three physical sensor responses are chosen out of n using $\binom{n}{3}$. Thus, the obtained group of three physical responses produces six virtual sensor responses using equations (2)-(7). Three of six are up-scaled, and the rest three are down-scaled versions of initial physical sensor responses. Hence, we have six VSRs for each combination resulting in total VSRs $6\binom{n}{3}$. The simultaneous use of up-scaled and down-scaled responses scale-up the dynamic range of responses. In this regard, the enhanced dynamic range facilitates subsequent enhancement in the patterns of responses as shown in Fig. 1. The proposed technique has been verified by demonstrating VSRs on an authentic dataset recorded in our departmental laboratory. The proposed technique was successfully compared with the well-published data-driven virtual sensor response technique NDSRT'. The classification performance of the gases/odors using the considered dataset has been compared in the context of the initial physical sensor responses, NDSRT and TITO techniques-based virtual sensor responses. While using the mentioned machine learning algorithms we have applied ten- fold cross validation to suppress the impact of intra- and inter-class variance. Table 1, to Tab. 3 have shown the performance of classifiers on initial physical sensor responses, NDSRT and TITO techniques-based virtual sensor responses. Moreover, the performance comparison has been shown in Tab. 4. As depicted depicts, four machine learning algorithms can classify the considered gases/odors with an accuracy of 100%.

Conventionally, initial physical gas sensor responses are inadequate in satisfactorily classifying the gases/odors due to suffering from various aspects, viz., drift, noise, outliers, etc. Therefore, several strategies are applied to overcome the mentioned issues using drift correction or drift removal algorithms, noise suppression methods, and outliers' elimination techniques. In addition to such efforts, feature selection and feature extraction methods are also used to enhance the discriminability of the data. The VSRs belong to the paradigm of feature extraction that enhance the performance of e-Noses. As of now, it

Table 1. Performance of the considered machine learning algorithms (classifiers) for gases/odors' classification using the intial physical gas sensor responses

Learning algorithm	Test accuracy for ten-folds of cross validation										Average accuracy $\pm\sigma$
L-SVM	0.75	0.75	0.75	1.00	0.75	0.75	0.50	0.75	1.00	0.50	0.75 $\pm$0.158
DT	1.00	0.75	1.00	1.00	0.75	1.00	0.75	1.00	1.00	1.00	0.925 $\pm$0.114
MLPNN	1.00	1.00	1.00	1.00	1.00	0.75	0.75	1.00	1.00	1.00	0.950 $\pm$0.100
KNN	0.50	0.75	1.00	1.00	0.75	0.75	0.50	0.75	0.75	0.75	0.75 $\pm$0.158
LR	1.00	1.00	1.00	1.00	1.00	1.00	0.50	1.00	1.00	1.00	0.950 $\pm$0.150
GP-RBF	1.00	0.75	1.00	1.00	0.75	1.00	0.75	1.00	1.00	1.00	0.925 $\pm$0.114
LDA	0.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.75	1.00	0.950 $\pm$0.100
RF	0.75	1.00	1.00	1.00	0.75	0.75	0.75	1.00	1.00	1.00	0.900 $\pm$0.122
AB	0.50	0.75	1.00	0.50	0.75	0.50	0.75	1.00	0.50	0.75	0.700 $\pm$0.187

Table 2. Performance of the considered machine learning algorithms (classifiers) for gases/odors' classification using the NDSRT technique-based virtual gas sensor responses

Learning algorithm	Test accuracy for ten-folds of cross validation										Average accuracy $\pm\sigma$
L-SVM	0.75	0.75	0.75	1.00	0.75	0.75	0.50	0.75	1.00	0.50	0.75 $\pm$ 0.158
DT	1.00	0.75	1.00	1.00	0.75	1.00	0.75	1.00	1.00	1.00	0.925 $\pm$ 0.114
MLPNN	1.00	1.00	1.00	1.00	1.00	0.75	0.75	1.00	1.00	1.00	0.950 $\pm$ 0.100
KNN	0.50	0.75	1.00	1.00	0.75	0.75	0.50	0.75	0.75	0.75	0.75 $\pm$ 0.158
LR	1.00	1.00	1.00	1.00	1.00	1.00	0.50	1.00	1.00	1.00	0.950 $\pm$ 0.150
GP-RBF	1.00	0.75	1.00	1.00	0.75	1.00	0.75	1.00	1.00	1.00	0.925 $\pm$ 0.114
LDA	0.75	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.75	1.00	0.950 $\pm$ 0.100
RF	1.00	1.00	1.00	1.00	0.50	1.00	1.00	1.00	0.75	1.00	0.925 $\pm$ 0.160
AB	0.50	0.75	1.00	0.50	0.75	0.50	0.75	1.00	0.50	0.75	0.700 $\pm$ 0.187

Table 3. Performance of the considered machine learning algorithms (classifiers) for gases/odors' classification using the TITO technique-based virtual gas sensor responses

Learning algorithm	Test accuracy for ten-folds of cross validation										Average accuracy $\pm\sigma$
L-SVM	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00 $\pm$0.000
DT	1.00	1.00	1.00	0.75	1.00	1.00	1.00	1.00	1.00	1.00	0.975 $\pm$0.075
MLPNN	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00 $\pm$0.000
KNN	0.50	1.00	0.75	1.00	0.75	1.00	0.75	1.00	0.75	1.00	0.850 $\pm$0.165
LR	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00 $\pm$0.000
GP-RBF	1.00	1.00	1.00	0.50	1.00	1.00	1.00	1.00	1.00	1.00	0.950 $\pm$0.150
LDA	1.00	1.00	1.00	0.75	1.00	1.00	1.00	1.00	1.00	1.00	0.975 $\pm$0.075
RF	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00 $\pm$0.000
AB	1.00	1.00	1.00	1.00	0.75	0.75	1.00	1.00	1.00	1.00	0.950 $\pm$0.100

is obvious that we have four initial physical responses for the considered dataset.

In this case, NDSRT technique produces only six VSRs that are merely 1.1/2 times of the number of initial physical responses. In contrast, our proposed TITO technique produces more virtual sensors than NDSRT. It produces 6 times VSRs to the initial responses and 4 times to the NDSRT-based VSRs. Thus, the produced VSRs can be considered as (pre-)proposed or curated samples of dataset that have more capability to discriminate among the considered gases/odors. The patterns enhancement through our proposed TITO technique is clearly visible in Fig. 1.

Disscussion

Results have shown the outperformance of the proposed data-driven technique to produce multi-sensor vir-

Table 4. Comparison of the performances of the considered machine learning algorithms (classifiers) for gases/odors' classification using intial physical gas sensor responses, NDSRT technique-based virtual gas sensor responses, and TITO technique-based virtual gas sensor responses

Machine learning algorithm	Average accuracy $\pm\sigma$		
	Initial response	NDSRT-based VSRs	TITO-based VSRs
L-SVM	0.750 $\pm$0.158	0.750 $\pm$0.158	1.000 $\pm$0.000
DT	0.925 $\pm$0.114	0.925 $\pm$0.114	0.975 $\pm$0.075
MLPNN	0.950 $\pm$0.100	0.950 $\pm$0.100	1.000 $\pm$0.000
KNN	0.750 $\pm$0.158	0.750 $\pm$0.158	0.850 $\pm$0.165
LR	0.950 $\pm$0.150	0.950 $\pm$0.150	1.000 $\pm$0.000
GP-RBF	0.925 $\pm$0.114	0.925 $\pm$0.114	0.950 $\pm$0.150
LDA	0.950 $\pm$0.100	0.950 $\pm$0.100	0.975 $\pm$0.075
RF	0.900 $\pm$0.122	0.925 $\pm$0.160	1.000 $\pm$0.000
AB	0.700 $\pm$0.187	0.700 $\pm$0.187	0.950 $\pm$0.100

tual responses (e.g., TITO). Now the discussion about the outcomes of all the techniques is being presented. As shown Tab. 1, MLPNN, LR, and LDA produces the same average accuracy but the first and third of them are more efficient due to the low standard deviation. Six out of nine machine learning algorithms are capable of providing 90 or more 90 percent average accuracy using initial physical gas sensor responses. Evidently, virtual sensor responses are derived to obtain more salient responses that must have enhanced capability to discriminate among the considered gases/odors. From Fig. 1, it is neatly shown that the NDSRT-based VSRs coincides and do not enhance the patterns confined in the responses. Also, according to the Tab. 2, NDSRT-based VSRs do not show the performance enhancement. Except for RF machine learning algorithm each one show similar performance. Moreover, the performance while using RF merely enhanced by 2.5%. Although, NDSRT upscales the dynamic range of VSRs (as shown in Fig. 1) but not up to the mark so that a significant performance enhancement can be produced. In contrast, As shown in Tab. 3, TITO-based VSRs are capable of delivering 100% average accuracy while using four machine learning algorithms, *viz,* L-SVM, MLPNN, LR, and RF. Except for KNN, each classifier delivers average accuracy of 95 or more than 95 percent using our proposed technique. From the Tab. 4, the least performing classifier (*eg*, KNN) using our technique is capable of enhancing the classification performance by 10% compared to its peers. All these comparisons show the efficacy of our proposed TITO technique for generating efficient multi-sensor virtual responses that enhance the classification performance.

4 Conclusion

The efficient virtual sensor response technique proves the potential for performance enhancement of electronic noses. Conventionally, the gas sensor array consists of multiple sensors regardless of the optimal number of sensors. This practice evidently consumes more power and occupies more space on chips. Also, more sensor elements lead to frequent recalibration, which is tedious and time-consuming. A large number of sensor elements is also responsible for the extensive drift in the captured datasets. Thus, instead of using multiple sensor elements, the concept of virtual sensor responses would be beneficial. The potential of VSRs has been proved by the outperformance of the TITO technique (as shown in Tab. 4). Its efficacy has also been proven by producing efficient virtual sensor responses whose derivation follows a straightforward manner feasible to test in laboratory conditions. The potential use of such techniques allows the development of more efficient electronic noses. Consequently, the virtual multi-sensor responses deliver outstanding performance and save cost and power.

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