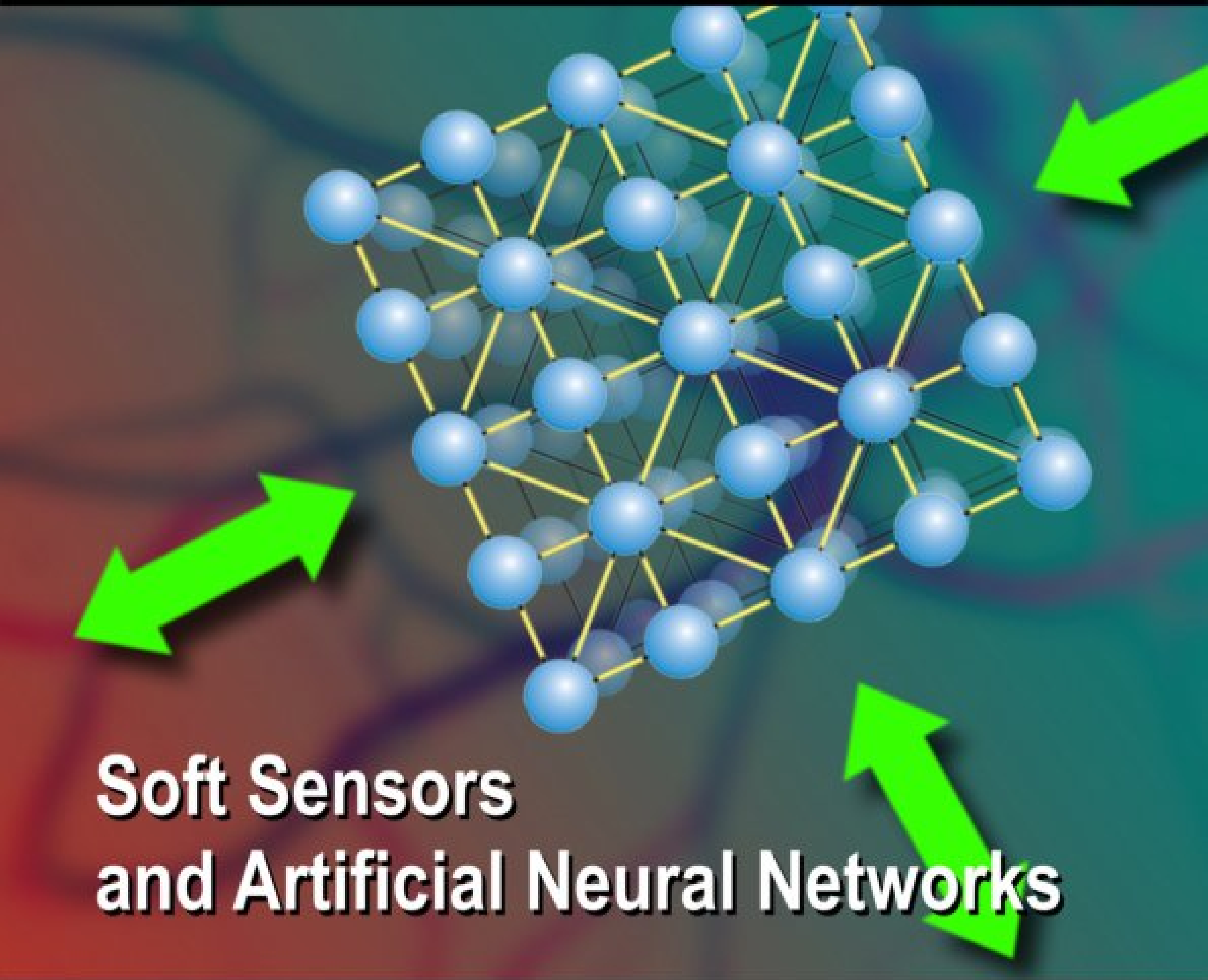
ISSN 1726-5479

# SENSORS & TRANSDUCERS

10/12 vol. 145



## Soft Sensors and Artificial Neural Networks

International Frequency Sensor Association Publishing

IFSA

Sensors & Transducers

Volume 145, Issue 10
October 2012

www.sensorsportal.com

ISSN 1726-5479

Sensors & Transducers Journal (ISSN 1726-5479) is a peer review international journal published monthly online by International Frequency Sensor Association (IFSA).
Available in electronic and on CD. 

**Sensors & Transducers Journal**

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**Volume 145**
**Issue 10**
**October 2012**

**www.sensorsportal.com**

**ISSN 1726-5479**

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*Sensors & Transducers Journal, Vol. 145, Issue 10, October 2012, pp. 191-202*

**Sensors & Transducers**

**ISSN 1726-5479**

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# Performance Comparison of PCA and ICA Pre-processors in Identification of Individual Gases Using Response of a Poorly Selective Solid-state Sensor Array

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*Received: 13 October 2012 /Accepted: 29 October 2012 /Published: 31 October 2012*

**Abstract:** Identification of odours/gases using an array of chemical sensors is a challenging task. The cross-sensitivity of individual sensors to different types of gases results in poor selectivity. This makes identification of individual gases a computationally demanding task. Unsupervised pattern recognition techniques like principal component analysis (PCA) have widely been used for odour identification. However, a more recent and highly popular pattern analysis technique viz. independent component analysis (ICA) has not been employed widely for odour identification applications. This paper presents performance comparison of PCA and ICA as pre-processing techniques in identification of four different types of gases/odours using published response of a chemical sensor array capable of sensing at room temperature. Raw data pre-processed with PCA and ICA were finally classified using a K-nearest neighbour (KNN) classifier. The efficacy of the techniques has been compared in both the cases. It was observed that performance of ICA as a pre-processing technique has been more consistent. Furthermore, the ICA-KNN classifier was found to give higher success rate and classification efficiency as compared to PCA-KNN classifier at different values of K.


**Keywords:** Gas Sensor, E-nose, PCA, ICA, K nearest neighbour.

## 1. Introduction

Human olfactory system is unarguably the most complex and unexplored of all the sensory mechanisms. Though with the help of modern day technology we have been able to devise an Electronic Nose, its capabilities lag far behind as compared to the human olfactory system. The need for an E-nose system arises due to the inherent deficiencies in the traditional methods of gas/odour identification viz. gas chromatography and mass spectroscopy. These methods involve heavy apparatus and larger investment, putting constraints on their employability.

E-nose systems have emerged as a viable and cost effective alternative for gas chromatography and mass spectroscopy based odour classifiers. Being appreciably sensitive to a large number of odour/gases, e-noses are a versatile genre of solid-state sensing devices. Metal oxide based sensor arrays form an integral part of a typical electronic-nose system, reason being cost effectiveness and broad sensitivity of sensors [1-3].

Generally, the output from an E-nose is of high dimensionality. The samples thus obtained can be considered as "electronic markers or identifiers" of a particular gas. Metal oxide films are promising materials for implementation of solid-state gas sensors [4]. However, they suffer from some inherent limitations like cross-sensitivity leading to poor selectivity, saturating tendency at higher concentrations and high drift. Overcoming poor selectivity of the sensor array remains the most challenging task if an E-nose system is to be realized. Thus, there arises a strong need for an efficient computational model which could take into picture the high correlation in data due to the cross sensitivities of sensors while performing classification task. Thus drawing sharp decision boundaries between odour classes requires a highly efficient and problem independent computational paradigm.

Some of the conventional pattern recognition techniques like partial model building [5], Fourier transform [6], multiple regression method [7], discriminant function analysis [8] and transformed cluster analysis [9] lack the ability to handle the nonlinear transduction properties of the sensors [10]. Thus, design of an efficient odour classifier fall into the category of problems, exact solution of which cannot be found by any of the traditional pattern analysis technique.

Emergence of the field of soft computing has paved the way for appropriate modelling and optimization of these complex systems. Soft computing techniques primarily consist of artificial neural networks (ANN), fuzzy logic and evolutionary computing.

With their ability to adapt, learn, massive parallelism and their conceptual resemblance to biological neural networks, ANNs are the optimal choice in our attempt to electronically model the human sensory perceptions.

The input data vector in an odour classification system is the response of a sensor array. Being high dimensional in nature, this data cannot be fed directly to the classifier. With an increase in the dimensionality of the training data, there is an exponential increase in the number of training vectors required by the classifier to learn [11]. As the training data available to us is limited, to avoid performance degradation dimensionality reduction with least information loss is of utmost importance. This task of dimensionality reduction is generally performed using second order statistical tools. These tools are not applicable in certain cases. As a result higher order statistical tools are often required. The problem of redundancy becomes significant due to the cross-selectivity of the chemical gas sensors used. Co linearity of dimensions makes covariance matrix singular and noninvertible [11]. Some other small pre-processing steps are also required in order to make mathematical analysis simpler and to discard insignificant input data.

Many of the feature extraction techniques for E-nose data have been based upon PCA. As a classification technique PCA has shown its efficacy both on its own and as a pre-processing stage to a subsequent classifier [12-15]. On the other hand ICA too has shown promising results in the classification of multivariate data [16-17]. Due to the higher order statistics involved in it, ICA handles sensor drift more efficiently as compared to PCA [17].With the integration of K-nearest neighbour algorithm with PCA and ICA even better and steady results are possible. However it is evident from the literature survey that comprehensive performance comparison of PCA and ICA in identification of odour/gases has not been done so far. This paper is the first attempt towards classification based performance comparison of ICA and PCA to the best of author's knowledge.

## 2. Materials and Methods

An array of sensors was prepared and exposed to four different gases/odours. The sensors were fabricated by thick film screen printing technique at [Centre for Research in Microelectronics (CRME) IIT-BHU, Varanasi India]. A gas sensitive tin oxide paste was prepared and printed on to an alumina substrate. The paste was doped with 1 % Pd, Pt, Cuo, Zno and Cd. Thus, five of six sensors were doped with the above mentioned material, while the sixth sensor was left undoped. Gold electrodes (ESL 8080) were also printed along with gas sensitive layer of tin oxide and were subsequently fired onto alumina substrate. SAMCO plasma deposition system (model no. 10) was employed to generate oxygen plasma at low pressure by applying r.f. power at 13.56 MHz. The test gases (LPG, $CCL_4$, CO and $C_3H_7OH$ ) were injected into a test chamber of volume 2894.7 ml which contained the array. The resistance variations of all the sensors of array were measured simultaneously with time through a counter decoder circuit. Different concentrations (viz. 25 ppm, 50 ppm, 75 ppm, 100 ppm) of the test gases were injected into the chamber.

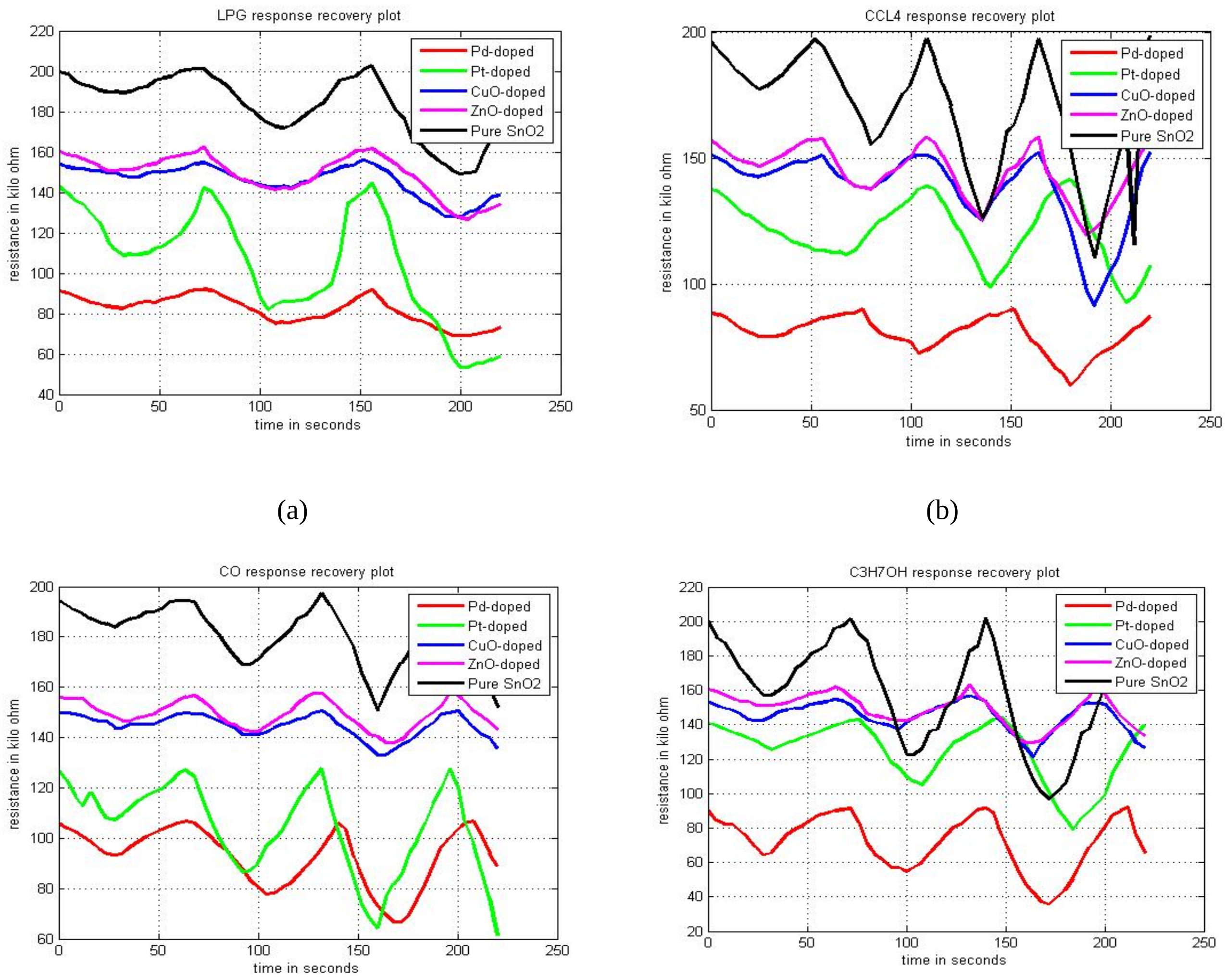
Figs. 1 (a)-(d) depict the dynamic response of the sensor array to four test gases at different values of concentration .It was observed after experimentation that Cd doped sensor did not show any significant sensitivity towards any of the test gases. Therefore, the dynamic response curves have been sampled only for the response of other five sensors.

The dynamic response curves of Fig. 1(a)-(d) are actually response recovery plots. When the test gas is adsorbed on the sensor surface, the conductivity of the sensor first increase and then reduces back to its original value. The time required for the test gas to reduce the conductivity of the sensor to its background conductance is known as recovery time. It has been observed that as the concentration of the test gas is increased, the recovery time increases. The experimental results thus obtained have already been reported [18] and in this work the same response has been used to extract data for gas/odour identification task. Due to their room temperature operation, oxygen plasma treated thick film sensors have a clear edge over conventional thick film sensors. However, this advantage is negated by their poor selectivity. Application of an appropriate computational technique can overcome the limitation of poor selectivity. This has served as a motivation for the author's to employ PCA and ICA as described in the subsequent section.

## 3. PCA and ICA for Unsupervised Clustering/learning

### 3.1. PCA as an Unsupervised Learning Technique

PCA is considered as one of the most important tool in the study of unsupervised neural networks. It can easily extract important and meaningful information from a high dimensional data with low class separability by reducing to a low dimensional one in order to reveal relevant underlying features.




(a) (b) (c) (d)

**Fig. 1.** Response-recovery plot of the array for different concentrations of the four gases: (a) LPG, (b) $CCL_4$, (c) CO, and (d) $C_3H_7OH$.

The goal of PCA is to re-express the given data in terms of a new basis so as to maximize the variances along the principal directions so computed.

Let $x$ be a realization of a zero mean random variable $X$ such that $X \in R^m$

$$\mathbb{E}[X] \tag{1}$$

And **C** be an m-by-m correlation matrix given by

$$C = \mathbb{E}[XX^T] \tag{2}$$

The $i^{th}$ principal component of any input vector $x$

$$a_i = x^T q_i \quad i = 1,2 \ldots\ldots\ldots\ldots m \tag{3}$$

such that $q_i$ is a vector satisfying two conditions

$$\|q_i\| = 1 \tag{4}$$

$$Cq_i = \lambda_i q_i \qquad i = 1,2 \dots \dots \dots m \tag{5}$$

Here $\lambda_i$ is called the $i^{th}$ eigenvalue corresponding to the $i^{th}$ eigenvector $q_i$ subject to the constraint $\lambda_i > \lambda_{i+1}$ where each eigenvalue gives a measure of the variance along the principal direction been computed given by the corresponding eigenvector. Thus the data vector $x$ can be truncated knowing the percentage variance along each principal direction or the relative importance of each principal direction so computed in terms of the amount of information it contains is given by

$$r_k = \lambda_k / \sum_{j=1}^{m} \lambda_j \qquad k = 1,2 \dots \dots \dots m \tag{6}$$

### 3.2. ICA as an Unsupervised Learning Technique

#### 3.2.1. Blind Source Separation

The essence of ICA algorithm lies in its ability to project any non-Gaussian data vector linearly onto new but not necessarily orthogonal directions so that the resulting components are as statistically independent as possible. Absence of a covariance structure in higher order statistical tool like ICA limits the application of Gaussian data as input.

Let there be a data vector $X$ such that

$$X = [X_1, X_2, X_3, \dots \dots X_m] \tag{7}$$

such that each individual component $X_i$ is correlated with each other. The aim of the ICA algorithm is to estimate the mixing matrix $A$ such that

$$X = AS \tag{8}$$

gives the previously unknown statistically independent unmixed source vector $S$ where

$$S = [S_1, S_2, S_3, \dots \dots \dots S_m] \tag{9}$$

Multiplying both sides of equation by $A^{-1}$ we get

$$A^{-1} X = S \tag{10}$$

Writing $A^{-1} = W$ and calling it as the un-mixing matrix we can obtain the original source vectors back

$$S = WX \tag{11}$$

The above theory gives the essence of Blind Source Separation problem

#### 3.2.2 ICA Algorithms Classification

The ICA algorithm can be broadly classified into two families i.e. ICA algorithms based upon minimization of mutual information and the second being rooted upon the maximization of non-Gaussianity. The first family includes algorithm developed by Amari et al. which is based upon Kullback-Leibler divergence, the algorithm given by Phan which works on the maximum-likelihood estimation and the third being the information maximization algorithm given by Bell and Sejnowski which tries to maximize the entropy of the system.

Second family includes the Fast ICA algorithm which uses negentropy as the measure of non-Gaussianity. In our present work we have used the Fast ICA algorithm to solve the BSS problem. The actual algorithm proceeds as

Let $x$ be a realization of a zero mean, whitened random variable $X$ where

$$\mathbb{E}[X] \tag{12}$$

$$\mathbb{E}[XX^T] = I \tag{13}$$

If Condition (12) is not satisfied then subtract mean from $X$ before proceeding further and for the fulfilment of (13) condition, $X$ should be replaced by

$$X = ED^{-1/2}\, E^T\ X \tag{14}$$

where $E$ is the orthogonal matrix of eigenvector of $\mathbb{E}[XX^T]$ and $D$ is the diagonal matrix of the corresponding eigenvalues i.e.

$$D\ = diag(d_1\,, d_2\,, d_3 \dots\dots\dots d_m) \tag{15}$$

$$D^{-1/2} = diag\left(d_1^{-1/2}, d_2^{-1/2}, d_3^{-1/2} \dots\dots d_m^{-1/2}\right) \tag{16}$$

After the estimation of independent components the task of addition of mean back to the data can be performed by adding back to the estimated independent component matrix in case if first condition was not satisfied, where $u$ is the mean of $X$ that was subtracted initially.

### 3.3 ICA algorithm

Let there be any random value of weight vector $w_i$ such that

$$\|w_i\| = 1 \text{ and } w_0 = 0 \qquad i = 1, 2 \dots\dots\dots\dots m \tag{17}$$

$$w_i^+ = \mathbb{E}[\varphi'\,(w^T x)]w - \mathbb{E}[x\varphi(w^T x)] \tag{18}$$

$$w_i^+ = w_i^+ - \sum_{j=0}^{i-1} w_i^T w_j w_j \tag{19}$$

$$w_i^+ - w_i^+ / \|w_i^+\| \tag{20}$$

repeat until not converged. Here $\mathbb{E}$ is the expectation operator, $\varphi$ is a special function normally a $\tanh(u)\ or\ \exp\left(-u^2/2\right)$ and $\varphi'$ is the differential of it.

## 4. Problem Formulation

The response recovery curves shown in Fig. 1 have been sampled at regular intervals of time to yield a raw data vector. Figs. 2(a) and 2(b) show the three dimensional scattered plots for the raw data taking different combinations of sensors at a time. In total ten such plots can be drawn for the five sensors used but for the sake of convenience only two such plots have been shown. These plots reveal the poor class separability of the raw data. Hence, it is necessary to apply some suitable pre-processing technique before the data is fed to the final classifier. In order to gain more insight into the nature of the raw data, we have plotted correlation plots between samples of any two gases. Out of six such plots possible, two are being shown here for the sake of convenience as Figs. 3 (a) and 3 (b).

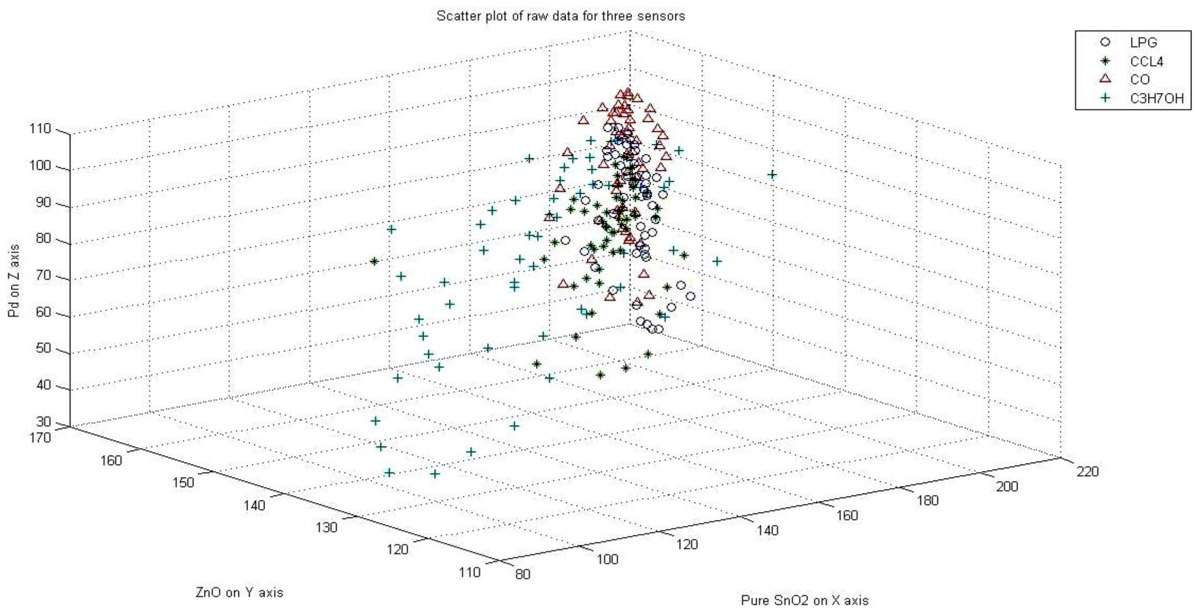



**Fig. 2(a).** Three dimensional raw data scattered plot with three sensors chosen at a time namely: $SnO_2$, ZnO and Pd.

We believe that the present problem can be viewed as a blind source separation (BSS) problem, the motivation for which arises due to the following facts:

1) The raw data is highly correlated as evident from the correlation plots depicted in Fig. 3.

2) The Non-Gaussianity of the data, making the present problem a suitable one for higher order statistical analysis as evident from the histogram plots in Fig. 4.

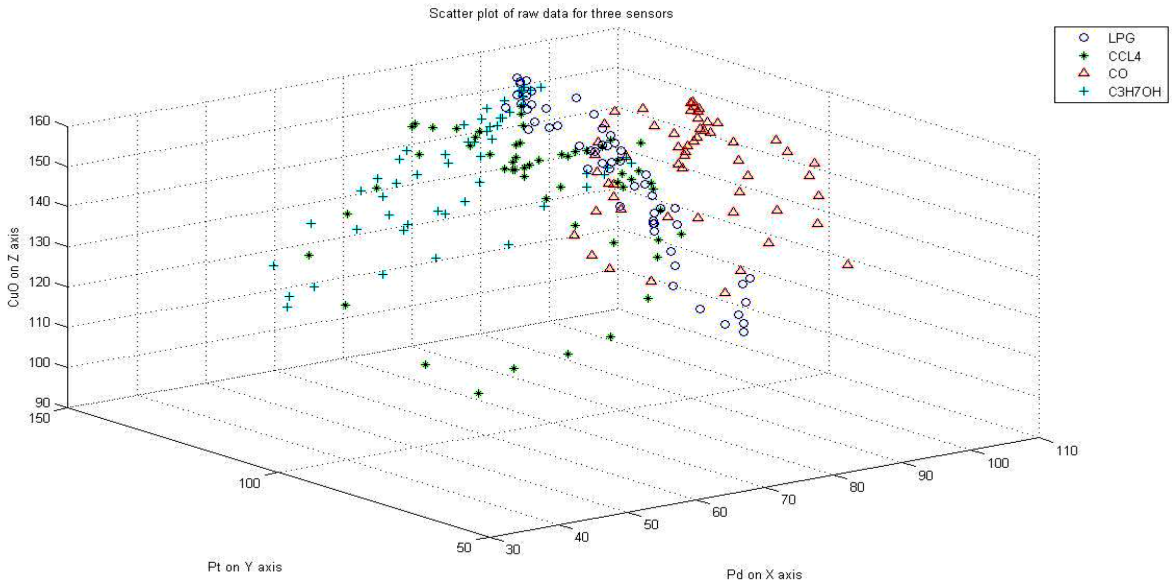
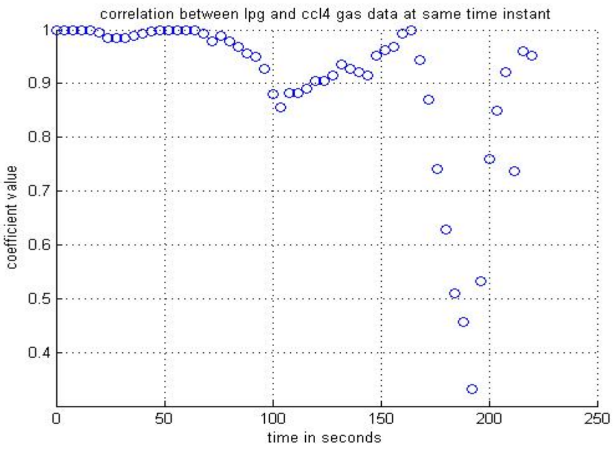
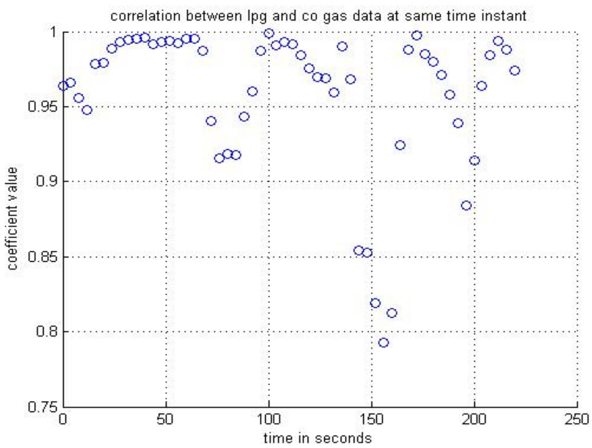



**Fig. 2 (b).** Three dimensional raw data scattered plot with three sensors chosen at a time namely: Pt, Pd, CuO.




(a)




(b)

**Fig. 3.** Correlation between two randomly chosen gases from the four individual gases: (a) LPG and $CCl_4$, (b) LPG and CO.

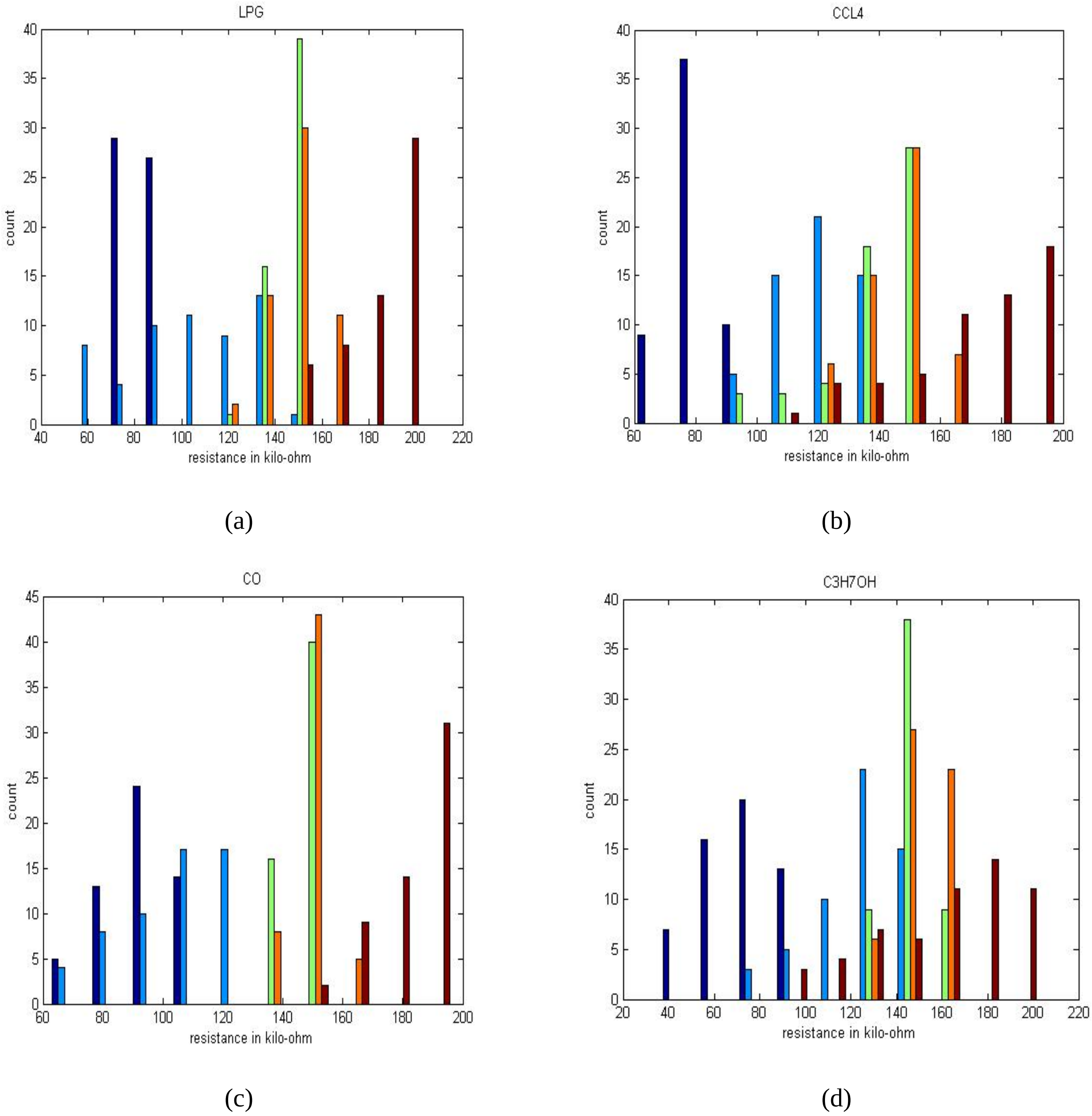
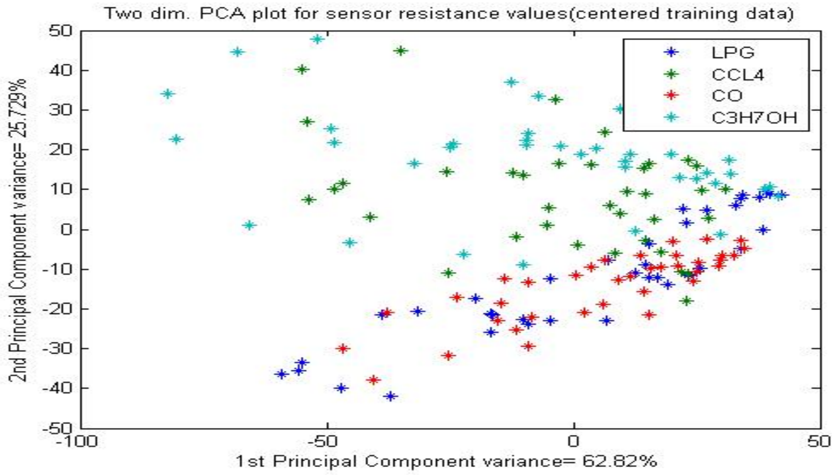


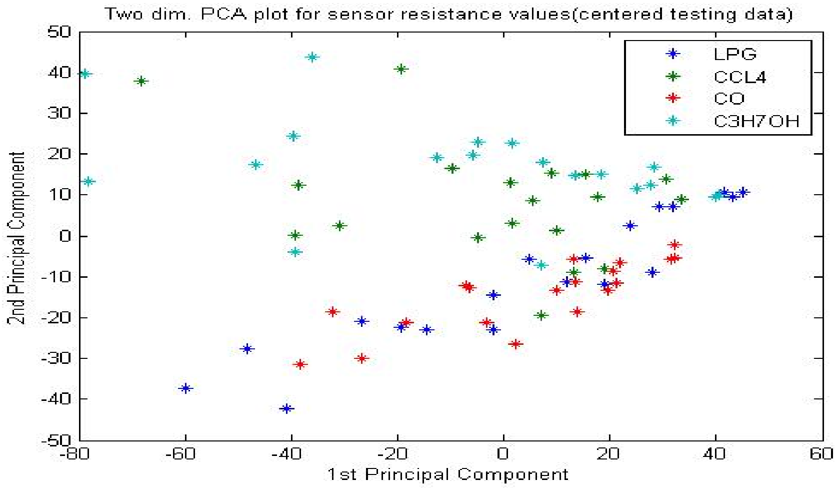

**Fig. 4.** Histogram plots for four individual gases (a) LPG, (b) $CCL_4$ , (c) CO and (d) $C_3H_7OH$.

## 5. Simulation Results and Discussions

In the course of action we proceeded first with the application of PCA on the raw data followed by ICA on the same. Fig. 5 shows the results of PCA pre-processing for both training and testing vectors. Similarly, Fig. 6 depicts two dimensional plots for individual independent components when ICA was applied. Though in the case of ICA ten two dimensional plots between five independent components can be plotted, we have chosen only one due to space limitations. Separate plots have been plotted for training as well as testing data. After this the KNN algorithm was applied on the data pre-processed by PCA and ICA respectively. The results of application of KNN algorithm can be seen in terms of classification efficiency plots for both the cases. It can be inferred from Fig. 7 (a) and 7 (b) that PCA pre-processed data gives higher classification efficiency only at higher values of K, making the classification process more computationally intensive. However, ICA pre-processed data gives a higher success rate even at lower values of K. Furthermore, the classification efficiency for the ICA-KNN classifier is never zero for any value of K for any gas unlike PCA-KNN classifier whose classification efficiency becomes zero for some gases at higher values of K. From the KNN plots it can be concluded that in general, KNN on ICA performs better in terms of classification efficiency as compared to KNN on PCA.




(a)

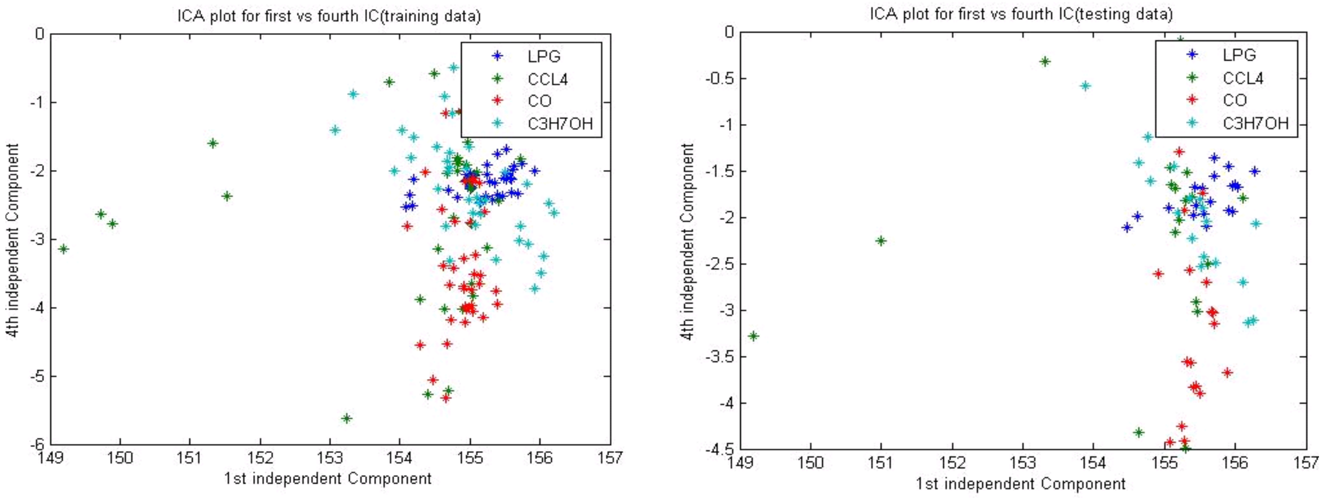



(b)

**Fig. 5.** PCA plot for (a) training data (b) testing data.

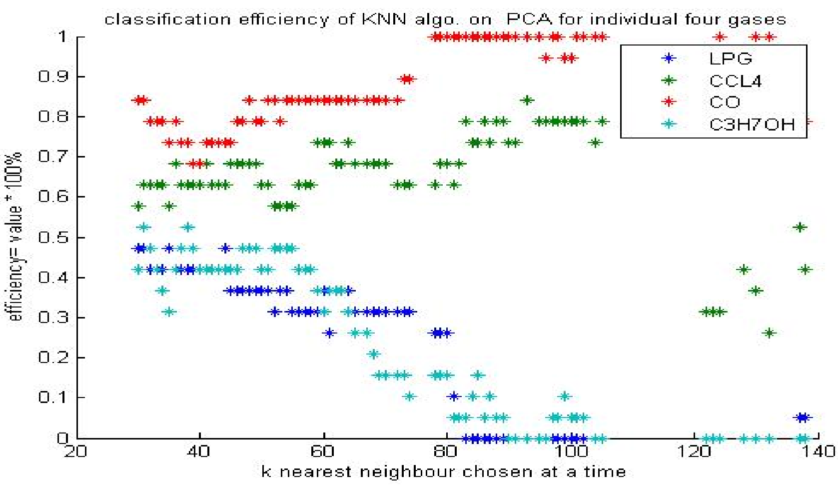
## 6. Conclusions

This paper describes the comparative performance of PCA and ICA as pre-processing techniques for identification of individual odours. After being fed to a K nearest neighbour classifier, it was observed that raw data subjected to ICA pre-processing was classified with a higher success rate than the data which was pre-processed using PCA. From Fig. 7, it can also be concluded that intra-class spread in case of ICA pre-processed data is much less as compared to the PCA pre-processed one. Though none of the above techniques i.e. ICA-KNN and PCA-KNN has been able to completely classify all the data into four classes, the results seem to be encouraging given highly jumbled and correlated nature of the raw data. It can safely be concluded that with some improvements, the ICA-KNN classifier can be used as a popular alternative to the more widely used PCA-KNN classifier.

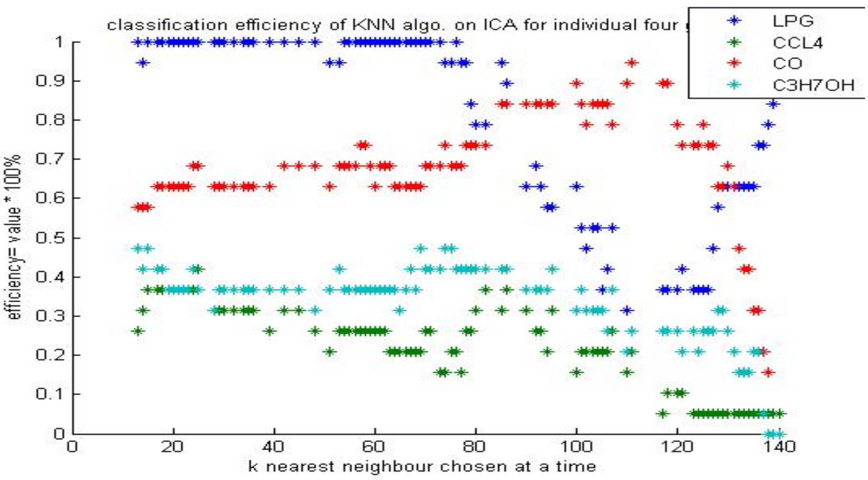



(a) (b)

**Fig. 6** ICA plots for various for 1st and 4th independent components: (a) Training data, (b) Testing data.




(a)




(b)

**Fig. 7.** Classification efficiency plot for KNN on (a) PCA, (b) ICA for various values of K.

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# Guide for Contributors

## Aims and Scope

*Sensors & Transducers Journal (ISSN 1726-5479)* provides an advanced forum for the science and technology of physical, chemical sensors and biosensors. It publishes state-of-the-art reviews, regular research and application specific papers, short notes, letters to Editor and sensors related books reviews as well as academic, practical and commercial information of interest to its readership. Because of it is a peer reviewed international journal, papers rapidly published in *Sensors & Transducers Journal* will receive a very high publicity. The journal is published monthly as twelve issues per year by International Frequency Sensor Association (IFSA). In additional, some special sponsored and conference issues published annually. *Sensors & Transducers Journal* is indexed and abstracted very quickly by Chemical Abstracts, IndexCopernicus Journals Master List, Open J-Gate, Google Scholar, etc. Since 2011 the journal is covered and indexed (including a Scopus, Embase, Engineering Village and Reaxys) in Elsevier products.

## Topics Covered

Contributions are invited on all aspects of research, development and application of the science and technology of sensors, transducers and sensor instrumentations. Topics include, but are not restricted to:

- Physical, chemical and biosensors;
- Digital, frequency, period, duty-cycle, time interval, PWM, pulse number output sensors and transducers;
- Theory, principles, effects, design, standardization and modeling;
- Smart sensors and systems;
- Sensor instrumentation;
- Virtual instruments;
- Sensors interfaces, buses and networks;
- Signal processing;
- Frequency (period, duty-cycle)-to-digital converters, ADC;
- Technologies and materials;
- Nanosensors;
- Microsystems;
- Applications.

## Submission of papers

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