

# An Intelligent E-Nose System For Discrimination Of Alcoholic Odorants

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## Abstract:

This paper presents a neural network classifier for classification of individual wine odors. The data set used for classification was obtained from already reported responses of thick-film tin oxide sensor array exposed to five different alcoholic beverages. The proposed classifier was trained with back-propagation algorithm and fuzzy memberships were used as target vectors in the output feature space. Transformed Cluster Analysis (TCA) was used as a data pre-processing technique and it was observed that pre-processing the sensor output data with TCA significantly enhances the classification capability and the error performance of the proposed neuro-fuzzy classifier.

**Keywords:** Electronic nose, Intelligent Systems, Transformed Cluster Analysis, Fuzzy Logic, Artificial Neural Network, Back-propagation Algorithm, Thick-Film Micro sensor, Artificial Intelligence.

## 1 INTRODUCTION

The emergence of Artificial Neural Network (ANN) has added newer dimensions to traditional computing. Owing to their massively parallel architecture and fast computational capability, ANNs have virtually started ruling the scenario of Artificial Intelligence (AI) research. The massive effort put in by the researchers has resulted in a vast pool of algorithms to choose from when an ANN is to be trained. On the other hand, the advent of fuzzy-set theory has revolutionized our understanding of the universe [1]. This development could not have come at a better time. With super fast computers at our disposal and a pool of learning algorithms to choose from, fuzzy logic has been applied successfully with ANNs for many kinds of pattern recognition problems [2]. The last few years have witnessed the emergence of biologically inspired computational algorithms like genetic algorithm and swarm algorithms. ANNs have been found to be quite compatible with these newer algorithms [3]. Due to these developments, various pattern recognition techniques of yesteryears have been replaced by ANNs in the last few years. Partial Model Building [4], Fourier Transform Technique (FTT) [5], Multiple Regression Method, Discriminant Function Analysis and various Cluster Analysis methods are being used less frequently nowadays. The limitation of the abovementioned techniques lies in the fact that they are not very useful in handling highly non-linear data. But, ANNs are renowned for their non linear approximation properties. Still, ample scope exists for enhancement of the performance of ANNs both in terms of simplicity of architecture and the convergence time. The abovementioned techniques of yesteryears can prove to be a handy tool in enhancing the performance of ANNs as is done in this work. We have used Transformed Cluster Analysis (TCA) [6], as a pre-processing tool to enhance the performance of a neuro-fuzzy classifier applied for the identification of five different types of alcoholic beverages. TCA is primarily a simple centering and scaling technique for obtaining better cluster separation. In this work we have fed data pre-processed by TCA to a neuro-fuzzy classifier and found that the performance of the classifier had enhanced substantially.

## 2 PROBLEM FORMULATION

Fuzzy-sets are generalization of conventional set theory introduced by Zadeh to represent vagueness in everyday life. The human processing of sensory information including olfaction is based on fuzzy reasoning. Accordingly, computational models of sensory system must also use the principle of fuzziness to model uncertainty or vagueness associated with real world sensory concepts like smell. There is a plethora of research on the theme of combining the approximate modelling features of fuzzy sets with the learning and parallel and distributed processing capabilities of neural networks. The same has been attempted here by us as we have trained an ANN classifier with backpropagation algorithm with the target vector consisting of the fuzzy membership values of the training data. Also, the effect of a data pre-processing strategy called TCA is studied over the overall classification performance of the ANN classifier.

### 2.1 Experimental Setup

Responses of tin-oxide sensor array fabricated at our laboratory were used in this present work to evaluate the effectiveness of the proposed neuro-fuzzy network in odor/gas classification. Sensor array used in the experiment consists of four thick-film tin oxide gas sensors. Three dopants ZnO, Sb<sub>2</sub>O<sub>3</sub> and NiO 10% by weight were used to obtain four sensors with different characteristics. One of the sensors was fabricated without using any dopant. The array was fabricated on a single substrate to ensure uniform and identical heating of all the four sensors under thermal equilibrium conditions. The structural diagram of the sensor array is shown in Figure1 and fabrication details are available in Nayak et al. [6].

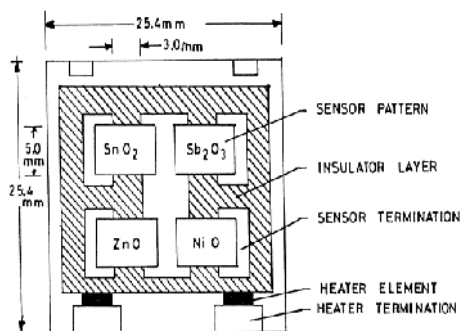


Figure1. The fabricated sensor array pattern.

The sensor array was kept in closed air ambient at room temperature and 10W power was used to energize the sensor heater. Sensors were allowed to stabilize in ambient condition with heater power on for more than 30 min. The change in resistance of each sensor was observed for different concentrations of various

alcohols and alcoholic beverages as reported by Nayak et al. The sensor characteristics for two types of Whiskeys, two types of Rums and Ethanol are reproduced here for ready reference as Figures 2(a)-2(e).

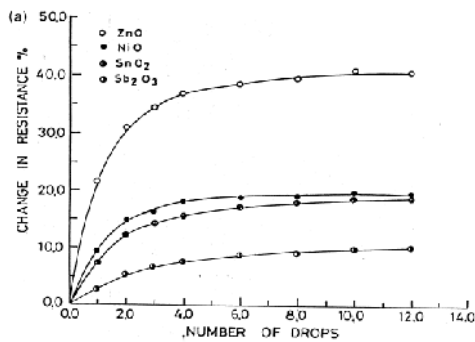


Figure 2(a). Steady-state response of the sensor array upon exposure to Whisky-1.

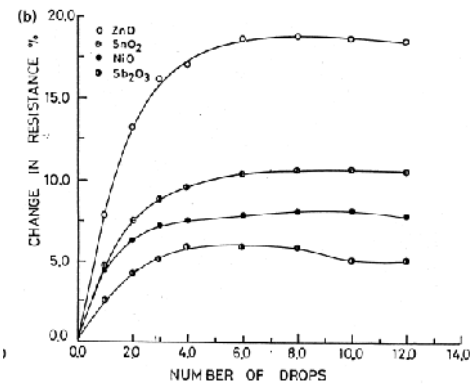


Figure 2(b). Steady-state response of the sensor array upon exposure to Whisky-2.

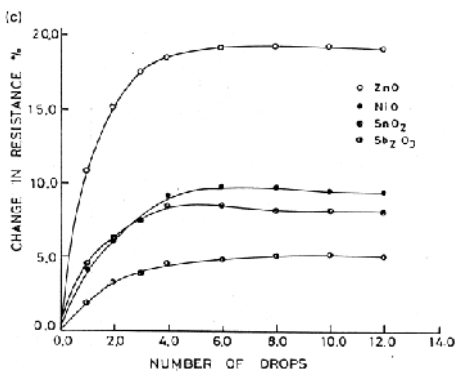


Figure 2(c). Steady-state response of the sensor array upon exposure to Rum-1.

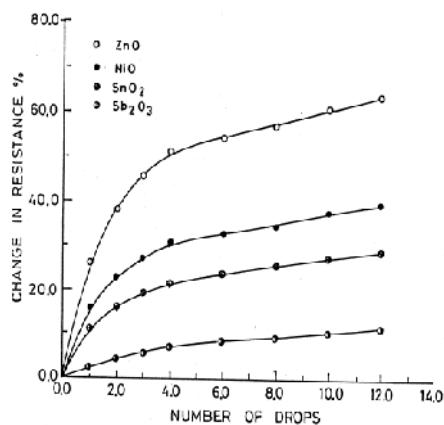


Figure 2(d). Steady-state response of the sensor array upon exposure to Rum-2.

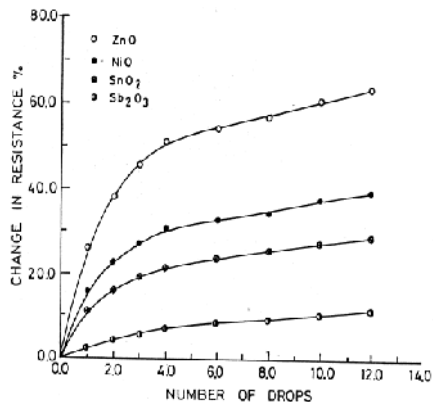


Figure 2(e). Steady-state response of the sensor array upon exposure to Ethanol.

## 2.2 Data Set Extraction and Pre-Processing

Output of four gas sensors for each alcohol and alcoholic beverage was sampled to offer a set consisting of eight data samples representing sensor outputs at different concentration. Sensor responses represented in Figures 2(a)-2(e) were sampled to offer such five different sets corresponding to individual alcohol/alcoholic beverage.

### 2.2.1 Transformed Cluster Analysis (TCA)

2D scatter plots for sensor responses shown in Figures 2(a) to 2(e), obtained by taking the responses of two sensors at a time are given in Figure 3(a) for S-1 as SnO<sub>2</sub> and S-2 as SnO<sub>2</sub> doped with Sb<sub>2</sub>O<sub>3</sub>. The clusters are not well separated due to partially overlapping response. The pre-processing of data not only helps in separating clusters from each other but also reduces the scatter of data into a cluster. We have used TCA

method as a data pre-processing technique proposed by Nayak using mean and variance of data obtained from a sensor response.

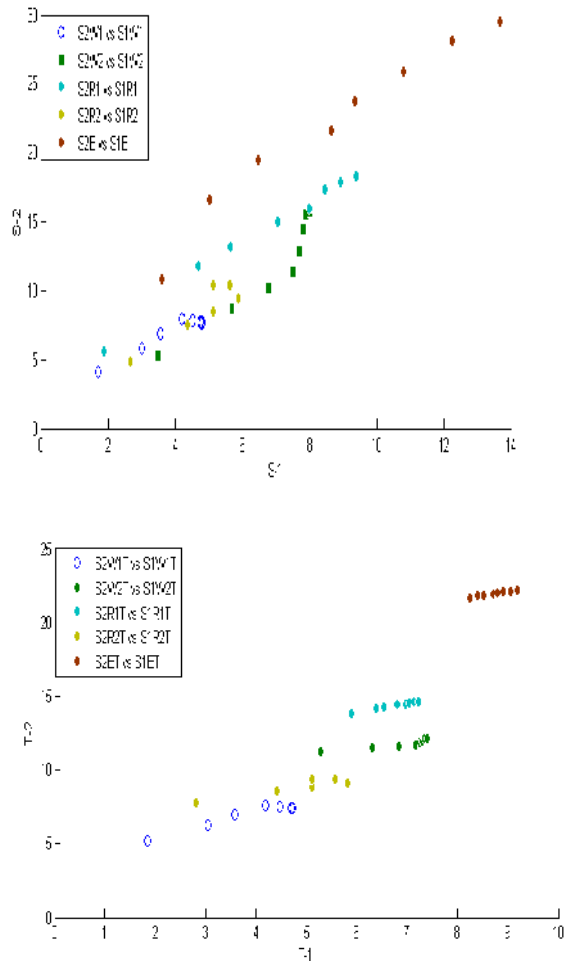


Figure 3(b). 2-D scatter plot for the transformed responses of sensors S-1 and S-2.

Figure 3(a). 2-D scatter plot for the responses of sensors S-1 and S-2

For a given test odor/gas, the mean of the individual sensor response is evaluated as

$$X_{ij} = 1/r \sum_{k=1}^r X_{ijk} \quad (1)$$

where,  $X_{ijk}$  is the  $i$ th sensor reading for the  $j$ th gas at  $k$ th concentration.  $X_{ij}$  is the mean value of the  $i$ th sensor for  $j$ th gas and  $r$  is the total no. of observations for  $j$ th gas.

The variance can be calculated as

$$V_{ij} = 1/r \sum_{k=1}^r (X_{ijk} - X_{ij})^2 \quad (2)$$

Where,  $V_{ij}$  is the variance of the  $i$ th sensor for  $j$ th gas. Now, the equation of the transformation can be written as

$$T_{ijk} = (X_{ijk} - X_{ij}/V_{ij}) + X_{ij} \quad (\text{For, } V_{ij} \geq 1) \quad (3)$$

and

$$T_{ijk} = (X_{ijk} - X_{ij})V_{ij} + X_{ij} \quad (\text{For, } V_{ij} < 1) \quad (4)$$

The data were processed using (3) and (4) and the scatter plot for the transformed responses of sensors S-1 and S-2 were drawn. As is evident from Figure 3(b), the scatter in the data clusters has been clearly reduced and the separation between the clusters has also improved to some extent. T-1 and T-2 are transformed responses of S-1 and S-2 in Figure 3(b)

### 2.2.2 Fuzzification of Sensor Response

The training of the neural network classifier was done by representing the sensor response data with their fuzzy membership values in the output feature space. All sensor response values belonged to any of the five fuzzy sets representing five wine classes. A method to assign membership in the output feature space has been developed by us and is explained for one such set. Centroid  $S_i$  was computed for each set  $i$ . Here,  $S_i = \{S_{i1}, S_{i2}, S_{i3}, S_{i4}\}$  where,  $S_{i1}, S_{i2}, S_{i3}, S_{i4}$  are the centroids for sensors S-1, S-2, S-3 and S-4 respectively for  $i$ th gas at varying concentrations.

The distance of the sensor response vector at concentration  $j$  can be obtained in the sensor response ratio vector space as given in the following equation:

$$d_{ij} = \{(S_{ij1} - S_{i1})^2 + (S_{ij2} - S_{i2})^2 + (S_{ij3} - S_{i3})^2 + (S_{ij4} - S_{i4})^2\}^{1/2} \quad (5)$$

Here,  $d_{ij}$  = distance of sensor responses from centroid  $S_i$  for  $i$ th gas, at concentration  $j$ , and  $S_{ij1}, S_{ij2}, S_{ij3}$  and  $S_{ij4}$  are the sensor responses for  $i$ th gas at concentration  $j$  corresponding to responses of sensors S-1, S-2, S-3 and S-4 respectively.

Thus, the membership  $m_{ij}$  in the output feature space, in the fuzzy set for  $i$ th gas at  $j$ th concentration can be represented using triangular membership function as:

$$m_{ij} = |d_{ij}|_{\max} - d_{ij} / |d_{ij}|_{\max} - |d_{ij}|_{\min} \quad (6)$$

Two different sets consisting of 40 data samples were obtained by sampling the sensor characteristics of Figures 2(a)-2(e). One set was raw data directly obtained from sampling and another set was data preprocessed by TCA. Eqs. (5) and (6) were used with both these sets to assign degree of memberships. A neural network classifier trained with backpropagation algorithm was used for the classification and was fed with both sets of data. The system error and convergence performance were noted and compared in both the cases.

### 3 SIMULATION EXPERIMENTS

The simulation was carried out on the MATLAB platform and TRAINGDM version of the backpropagation algorithm was used. The architecture of the neural classifier was optimized experimentally by varying the no. of neurons in the hidden layer. For the sake of simplicity only a single hidden layer architecture was chosen. The no. of neurons in the hidden layer were varied from two to nine and classification performance was noted. Both raw and TCA preprocessed training data were fed to the classifier. Respective fuzzy membership values of the raw and transformed sensor responses were used as target vectors of the neural classifiers.

Both raw and transformed data sets were randomized beforehand to neutralize any effect of bias on data selection. 75% of the samples from both sets were used as training data whereas, 25% were designated as test data to test the classifier performance. Learning rate (l.r) and momentum constant (m.c.) were optimized by repeated experimentations and results were compared. Both l.r. and m.c. were varied from a value of 0.1 to 0.9 during experimentations to arrive at an optimum combination. The error function used has been mean square error (MSE). The Trained neural network was then used in test mode. For the optimization of architecture the network was trained with a fixed 30,000 epochs. For assessing the convergence performance, network was trained by varying no. of epochs from 5,000 to 30,000.

### 4 RESULTS AND DISCUSSIONS

The results obtained from simulation experiments show that the classifier trained with TCA preprocessed data has far better classification performance, lower system error, faster convergence and simpler architecture than that trained with raw data. Figures 4(a) and 4(b) show the variation in system error with learning rate for different values of momentum constants when the classifier was trained with raw data. Figures 4(c) and 4(d) show the same when the classifier was trained with TCA preprocessed data. The system error was reduced to about one sixth of its value when the network was trained with TCA preprocessed data. From, Figures 4(e) and 4(f) it is clear that the network gives lower error at lesser no. of neurons in the hidden layer and in lesser no. of epochs when trained with TCA preprocessed data. The network gave a minimum system error of 0.02 at an l.r. of 0.3 and m.c. 0.6 with only 3 neurons in the hidden layer when trained with TCA preprocessed data for 30,000 epochs. At these optimized parameters and weights, the network gave 100% classification by sniffing all 10 test samples and putting them into appropriate category.

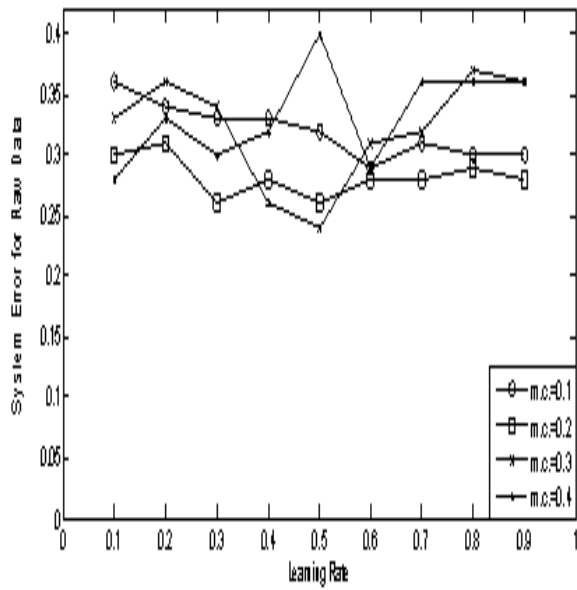


Figure 4(a). Variation in system error with learning rate for different values of momentum constant (m.c.) network trained with raw data

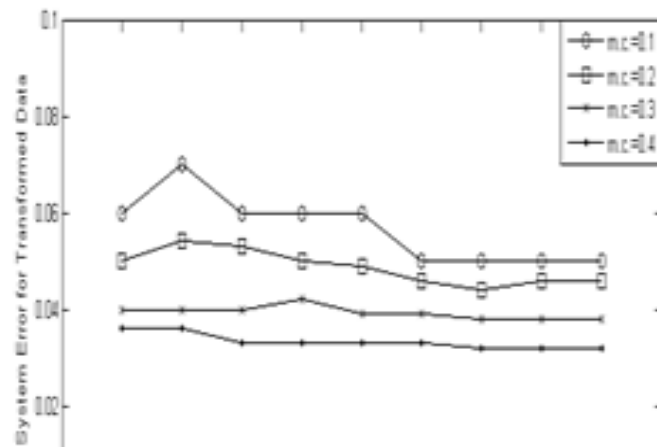
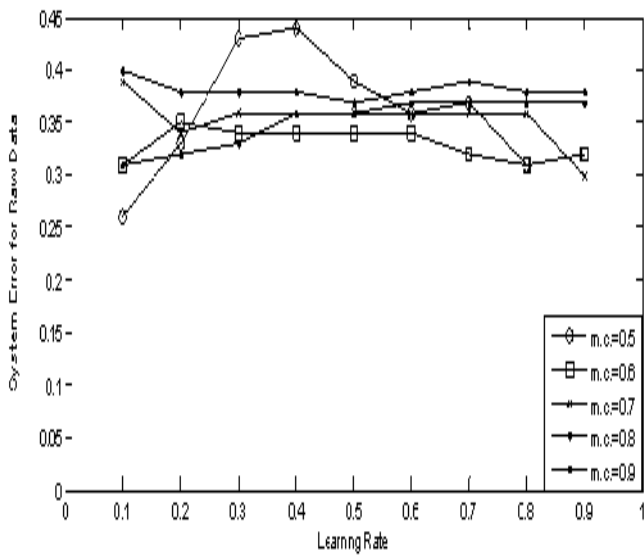


Figure 4(b). Variation in system error with learning rate for different values of momentum constant (m.c.) network trained with raw data



Figure 4(c). Variation in system error with learning rate for different values of momentum constant (m.c.) network trained with TCA preprocessed data

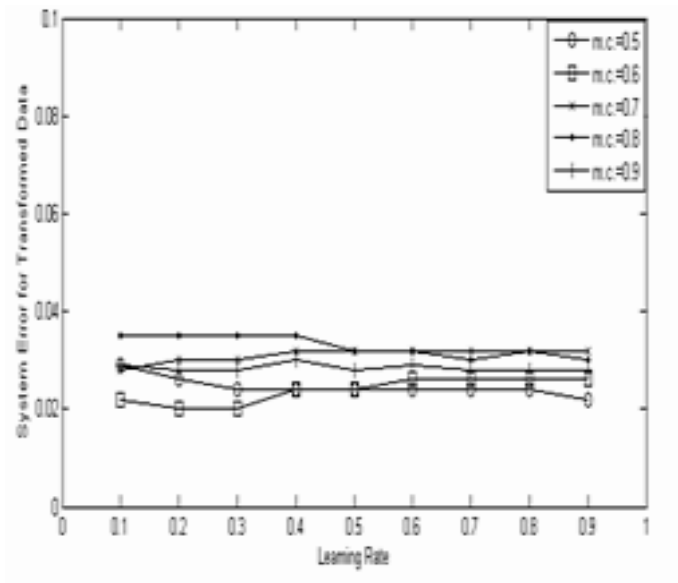
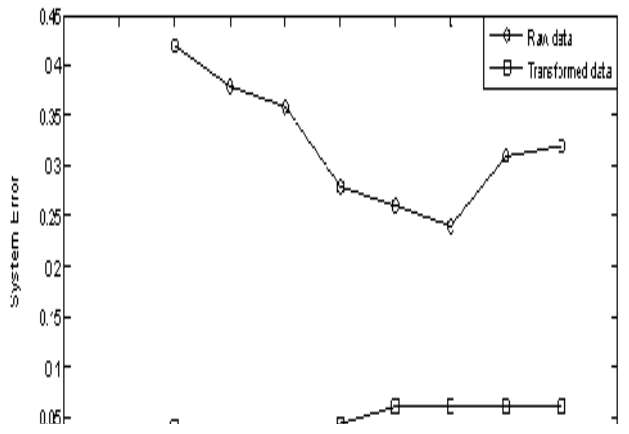


Figure 4(d). Variation in system error with learning rate for different values of momentum constant (m.c.) network trained with TCA preprocessed data



network trained with TCA preprocessed data

Figure 4(e). Variation in system error with no. of neurons.

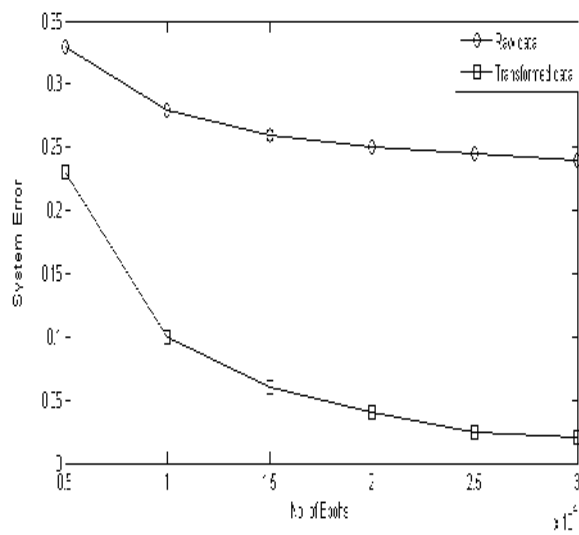


Figure 4(f). Variation in system error with no. of epochs.

## 5 CONCLUSIONS

The significant improvement in the performance of the ANN classifier obtained , proves the efficacy of TCA as a preprocessing tool. Its compatibility with fuzzified data makes it even more promising. Preprocessing with TCA can result in simpler VLSI hardware of neuro-fuzzy networks. This remains a separate research topic and can be dealt with in some future works

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