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Adaptive resonance neural classifier for identification of gases/odours using an integrated sensor array

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Abstract

A new approach to intelligent gas sensor (IGS) design using a classifier based on adaptive resonance theory (ART) artificial neural network (ANN) is presented. Using published data of sensor arrays fabricated and characterised at our laboratory, we demonstrate excellent gas/odour identification performance of our classifier for a 4-gas, 4-sensor system to identify individual gas/odour. Since the ART neural network is a self-organising classifier trained in the unsupervised mode, it avoids the drawbacks associated with static feedforward neural networks trained with locally optimal backpropagation-type training algorithms applied by researchers in the recent past. The ART neural network offers easy implementability and real time performance in addition to giving excellent classification accuracy as demonstrated by our experiments. © 1998 Elsevier Science S.A. All rights reserved.

Keywords: Intelligent gas sensors; ART neural network; Gas/odour identification; Cluster discovery; Unsupervised learning

1. Introduction

There is a considerable interest in the recent literature in developing an intelligent gas sensor (IGS) using semiconductor sensor array and pattern recognition (PR) (or discrimination) technology [1-3]. Discrimination techniques are critical to the success of identification of gas/odour in an environment. In the past, partial model building (PMB) [4], fast fourier transform [5], principal component analysis (PCA) [6], cluster method [7], transform cluster analysis [8] and multiple regression method [9] etc. have been reported for the analysis of sensor array responses with different identification capabilities. In the cluster method reported by Shrumer [7] the scatter of data in a cluster was found to be large. The TCA method suggested by Nayak et al. [8], reduces the overlapping of clusters to some extent due to transformation of data using mean and variance of the training data set, but the problem of overlapping

of cluster still remains and linear discriminants could not be found in many cases.

Further, the conventional PR algorithms are sequential in nature while the human PR system is known to be massively parallel. This is one of the reasons for the wide performance gap between the man and machine in the area of PR (e.g., vision, speech recognition, smelling etc.). To bring machine performance closer to humans in gas/odour identification two distinct efforts are required, namely (i) parallel distributed processing and (ii) use of artificial intelligence (AI) techniques. AI is a computer science discipline that aims at utilising principles of biological information processing to develop intelligent software.

There is a need to synergise the sensor technology with AI techniques in PR to achieve high performance gas/odour identification. There are two main branches of the AI discipline namely (i) the knowledge based approach and (ii) the artificial neural network (ANN) approach [10]. While the former is more appropriate for symbolic reasoning systems, the later is appropriate to low-level perceptual tasks like seeing (machine vision), hearing (speech recognition) and smelling (odour iden-

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tification). Holmstrom et al. [11] have done an extensive study of relative performance of conventional versus neural classifiers. Based on their examination of 18 classical and neural classifiers on two data sets, they conclude that ANNs have many advantages over conventional PR algorithms. These include:

- 1. Higher discrimination power resulting in better classification accuracy.
- 2. ANNs are on-line learning systems.
- 3. They are parallel distributed computing systems offering real-time computation speeds.
- 4. ANNs are relatively easy to implement in hardware.
- 5. They are less sensitive to parameter variations.
- 6. ANNs are inherently fault tolerant.

Recently, several researchers have applied ANN techniques to gas/odour identification problem with varying degrees of success.

Gardner et al. [12] have applied ANN to identify alcohols using an array of Tin Oxide sensors. They used the backpropagation algorithm to train a 2-layer feedforward ANN in supervised mode. It is reported that the ANN outperformed principal components analysis (PCA) in this application.

Nakamoto et al. [13] have reported an application of neural network with quartz sensor array for perfume and flavour identification. The ANN model used had three layers and was trained with the Backpropagation algorithm. The authors report that the sample with 0.5 vol.% decanal could be identified with the ANN with a relatively high recognition probability, whereas the others could not be identified so well.

Barker et al. [14] have used data from organic thinfilm sensors to train an ANN. They used a feedforward ANN with 12 input-layer neurons, 4 output-layer neurons. They experimented with different configurations of hidden neurons and learning parameters. Experiments with two hidden layers proved inconclusive, but better results were obtained using three hidden layers. The learning algorithm used here was also backpropagation.

Helene Debeda et al. [15] have used ANN for posttreatment of thick film pellistor array data for recognition of three combustible gases: Methane; Propane; and Ethanol. The backpropagation learning algorithm had to run for 300000 iterations to train a 3-layer feedforward neural network. Even then at certain concentrations the gases were misclassified.

Markus Schweizer-Berberich et al. [16] have applied neural network systems to dynamic response of polymer-based sensor arrays for a binary mixture of n-octane and toluene. The authors use structured neural network model consisting of recurrent, linear and nonlinear neurons. Training is performed by a modification of backpropagation known as Quickpropagation. The authors experienced difficulties in training when the training and testing data are taken from different time periods. It is clear from the above, that almost all authors have used supervised learning of neural networks with backpropagation algorithm or its modifications. According to our experience with application of ANN in a large number of PR tasks, the backpropagation has following disadvantages as a training algorithm for real data sets like gas sensor data:

- 1. The algorithm uses a gradient based search strategy which gets stuck in the nearest local minimum with no guarantee on global convergence.
- 2. Convergence is very slow and highly sensitive to the weight initialisation and learning parameter choice. In practice, on real data sets the algorithm requires sever trials with weight initialisations and parameter choices before converging with acceptable error tolerance.
- 3. The algorithm is very sensitive to the precision of the activation function and its derivative and hence not cost effective in hardware implementations for on-line training in the field.
- 4. The algorithm requires the user to choose a learning parameter and a momentum term. These choices remain fixed during training session. This causes a number of problems in convergence since the topology of the error surface in the weight space is multimodal and quite complex, a choice of parameters that seems adequate in one region of the search space becomes totally unsuitable in another region. This effect leads to slow convergence or even instability in many cases.

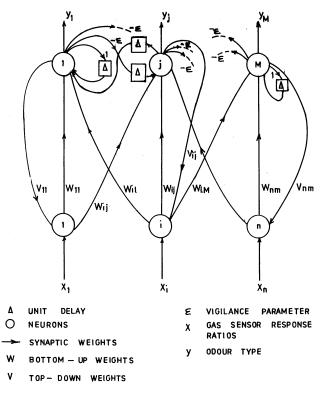


Fig. 1. Structure of the ART neural network model.

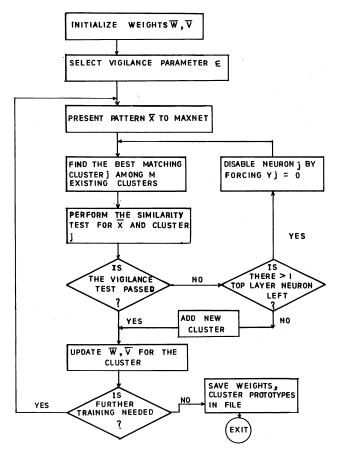


Fig. 2. Flowchart showing the operation of the ART neural classifier.

Further, so far the emphasis of the IGS researchers has been on the use of the feedforward ANN, which is a static system with no self organisation property. It cannot adapt its structure or parameters to the topological features of the pattern space created by the output from an array of sensors with partially selective characteristics to different gases.

In this paper we present a novel IGS approach for identification of individual gas/odour using doped tin oxide sensor array and adaptive resonance theory (ART) self-organising neural network. We obtained excellent classification performance for four-gas foursensor system using the ART neural network as the parallel distributed computing platform for unsupervised cluster discovery in the training mode, followed by classification of unknown gas/odours in the sniffing mode. The sensor data used in the present work are based on the sensor responses reported by Nayak et al. [23] and applied in their TCA method [8], however, the classification accuracy with the ART neural network reported here is much superior to that obtained by Nayak et al.

2. Traditional clustering

Scientists believe that evolutionary learning by humans must have originated thousands of years ago in an unsupervised mode, since there were no teachers, instructions, templates, or books at that time. The basic PR for sensory skills like gas/odour identification is therefore acquired by brain using unsupervised self-organisation in neural networks. This serves as a motivation for using unsupervised training in ANNs for IGSs.

In unsupervised learning, the basic criteria used is the similarity of objects within a cluster. This results in labelled grouping of sensor data that can be subsequently used for classification. This grouping of similar objects and separating of dissimilar objects is known as clustering. The clustering problem is to identify the number of classes according to a similarity measure and of assigning membership of new patterns to these classes.

Traditionally, a discriminant is used as a function of patterns that gives an output which is an estimate of the class membership of that pattern. It is possible to start with statistical PR [17] and using Bayes decision rule to obtain discriminants which can be processed in a deterministic manner. The discriminant consists of a measure of distance and patterns are classified either according to the class membership of the nearest neighbours, or with the nearest prototype or cluster-centre. ISODATA [18] is the most popular traditional algorithm for exploring the structures of clusters in pattern based information processing. It is a modification of the K means technique with addition of some heuristics. Since it depends on heuristic knowledge, in general, it requires extensive experimentation before one can arrive at meaningful conclusions.

Real potential of the clustering approach is utilised when its inherent parallelism is exploited to implement it on the asynchronous distributed computing platform provided by ANN.

3. Neural networks for cluster discovery

The unsupervised learning technique for cluster discovery has been implemented on neural networks to take the advantages of fast asynchronous distributed processing and inherent learning capability of ANNs. Considerable research work has been done by Carpenter and Grossberg [19,20], Kohonen [21] and Amari [22] in implementing clustering procedure on neural platforms. The key mechanism used in self-organising clustering neural networks is lateral inhibition to select one node out of a set of nodes that has the greatest output.

Of all the neural network models that discover cluster ART model is the most versatile since it allows controlled cluster formation through the choice of a

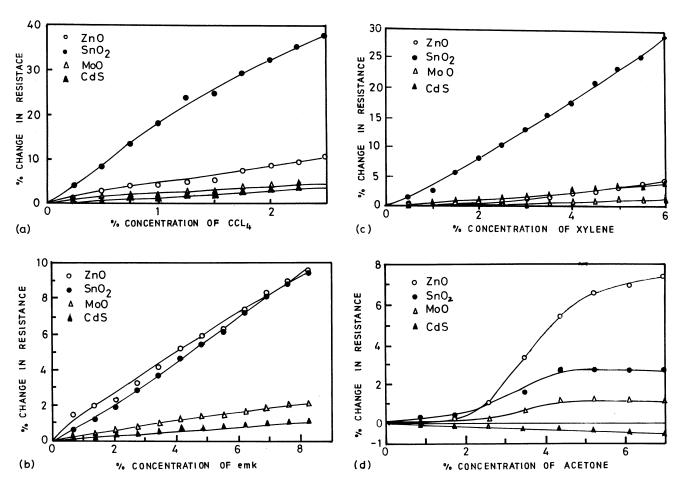


Fig. 3. (a) Sensor characteristics for acetone exposure in N_2 ambient under energised conditions (2 W supply). (b) Sensor characteristics for carbon tetra chloride exposure in N_2 ambient under energised conditions (2 W supply). (c) Sensor characteristics for ethyl methyl ketone exposure in N_2 ambient under energised conditions (2 W supply). (d) Sensor characteristics for xylene exposure in N_2 ambient under energised conditions (2 W supply).

vigilance parameter as described in the next section. We have got excellent results for gas/odour identification using sensor array data from our Micreoelectronics Centre using the ART neural network classifier.

4. The ANN

Fig. 1 gives a generic self-organising neural network based on ART proposed by Carpenter and Grossberg [20]. This network consists of a lateral inhibition layer at the top that augments the largest output and suppresses others and a bottom layer of neurons that receive the input. Essentially the network follows the classification principle of 'follow the leader' after it creates the first cluster with the first training data received. It creates a second cluster only if the second pattern is sufficiently dissimilar to the first one.

The central part of the ART neural network computes in parallel the matching scores reflecting the degree of similarity of the present input to the previously encoded clusters during the bottom-up phase of processing. The initialising input to the *m*th top-layer neuron is the scalar product between the input X and the bottom-up weight vector W_m , i.e.

$$Y_{\mathbf{m}}^{0} = \mathbf{W}_{\mathbf{m}}^{\mathsf{t}} \mathbf{X}, \text{ for } \mathbf{m} = 1, 2, \dots M$$

$$\tag{1}$$

where, M is the total number of neurons in the top layer and

$$\mathbf{W}_m = [w_{1m} \, w_{2m} \dots w_{nm}]^T \tag{2}$$

After this initialisation, the layer of neurons undergo recurrent updates according to the relation:

$$\mathbf{Y}^{\mathbf{k}+1} = \Gamma[\mathbf{W}_{\mathbf{M}}, \mathbf{Y}^{\mathbf{k}}] \tag{3}$$

where the weight matrix W_M is of the form:

$$\begin{bmatrix} 1 & -\varepsilon & -\varepsilon & -\varepsilon & \dots & -\varepsilon \\ -\varepsilon & 1 & -\varepsilon & -\varepsilon & \dots & -\varepsilon \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\varepsilon & -\varepsilon & -\varepsilon & -\varepsilon & \dots & 1 \end{bmatrix}$$
(4)

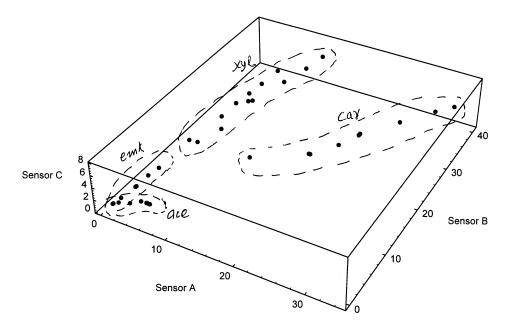


Fig. 4. 3D scatter diagram of three sensor responses for four gases at varying concentrations. All sensor responses are plotted as percent change in resistance. X-axis: Sensor A (ZnO), Y-axis: Sensor B (SnO₂), Z-axis: MoO.

where the lateral interaction coefficient ε is bounded by $0 < \varepsilon < 1/M$. All the neurons are exactly identical to each other and have the identity activation function, Fig. 2, given by:

$$f(net) = net \text{ for } net > 0$$

= 0, otherwise (5)

When the ANN has run for a sufficient time so that the recursion index k is large enough, only one of the neuron outputs remains nonzero and all other neuron outputs are forced to zero due to the effect known as lateral inhibition. Let the winning neuron with nonzero output be the *j*th neuron. Then for this neuron the initial conditions must have been:

$$y_j^0 = \sum_{i=1}^n w_{ij} x_i = \max_{m=1,2,\dots,M} \sum_{i=1}^n w_{im} x_i$$
(6)

After the recurrences in the top layer have subsidised the number of the node (i.e. j) is the cluster number.

This is followed by the top-down computation phase which checks the similarity of the candidate cluster with the cluster reference data stored in the ANN weights and performs a vigilance test on normalised $v_{ij}x_i$. The user can control the cluster discovery process by specifying a suitable value for a vigilance parameter ρ such that:

$$0 < \rho < 1 \tag{7}$$

 ρ decides the degree of similarity or 'match' between a cluster already stored in the ART NN and the current pattern. When such a match is found the network is said to be in a state of resonance. The complete operation of the ART NN is explained in the flowchart given in Fig. 2.

5. Simulating the ART NN

To study the effectiveness of the ART NN model in gas/odour identification we developed a simulation program in C language running on a Pentium based computer. The simulation consists of the following main steps:

5.1. Step 1

The vigilance parameter ρ is selected and for *n*-dimensional input vectors and *M* top-layer neurons, the ANN weights are initialised. The weight matrices *W*, *V* are both $(M \times n)$ and are initialised as follows:

$$\mathbf{W} = \begin{bmatrix} \frac{1}{1+n} \end{bmatrix}$$
(8a)

$$\mathbf{V} = \begin{bmatrix} 1 \end{bmatrix} \tag{8b}$$

5.2. Step 2

Input vector \mathbf{x} is presented at the input nodes.

5.3. Step 3

The matching scores are computed using (1). The selection of best matching existing cluster is performed according to the criteria (6).

5.4. Step 4

The similarity test for the winning neuron j is performed as follows:

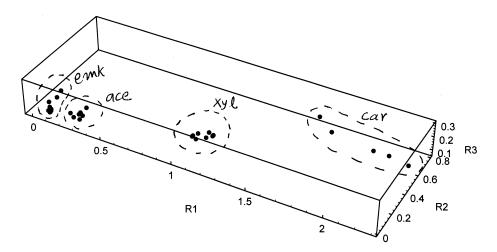


Fig. 5. 3D scatter diagram of sensor response ratios for four gases at varying concentrations. X-axis:R1 = (Sensor A)/(Sensor B), Y-axis: R2 = (Sensor C)/(Sensor B), Z-axis: R3 = (Sensor D)/(Sensor B).

$$\frac{1}{\|X\|} \sum_{i=1}^{n} v_{ij} x_j > \rho$$
(9)

where ρ is the vigilance parameter chosen by the user and we have used L₂ or Euclidean Norm since the gas sensor array responses are real valued.

If the test (9) is passed the algorithm goes to step 5. If the test has failed, the algorithm goes to step 6, if the top layer has more than a single active node. Otherwise the algorithm goes to step 5.

5.5. Step 5

Entries in the weight matrices W and V are updated only for the winning node index j as follows:

$$w_{ij}(t+1) = \frac{v_{ij}(t)x_i}{0.5 + \sum_{i=1}^{n} v_{ij}(t)x_i}$$
(10)

$$v_{ij}(t+1) = x_i v_{ij}(t)$$
(11)

This updates the weights of the *j*th cluster-newly created, or the existing one. The algorithm goes to Step 2.

Table 1 ART NN simulation results: choice of ρ

Experiment no.	Choice of vigilance ρ	% Classification error
1	0.05	12
2	0.08	8
3	0.11	5
4	0.14	0
5	0.15	0
6	0.16	0
7	0.18	7
8	0.21	11

5.6. Step 6

The node *j* is now deactivated, i.e. $y_j = 0$, so that this node does not participate in the current cluster search. The algorithm goes back to step 3 to establish a new cluster.

6. Experiments

To evaluate the effectiveness of the ART NN for identification of individual gases/odours, we have used the responses of sensor array reported by Nayak et al. [23]. The sensor used in these experiments consists of an array of four sensors with an integrated heater on a substrate. Four different sensors of the array were fabricated with SnO_2 as a base material and doped with different materials, namely, ZnO (sensor A), MoO (sensor C) and CdS (sensor D) and SnO_2 (sensor B) itself with no doping. The sensor array was fabricated using thick film technology. The fabrication process is described in detail in reference [23]. The test rig used to collect sensor array response data and experimental conditions in the laboratory are also described in the above reference.

The four gases/odours used in these experiments are Acetone (ace), Ethyl Methyl Ketone (emk), Carbon Tetrachloride (car) and Xylene (xyl). The outputs measured were percent change in resistance of different sensors when exposed to various concentrations of the above four gases. As mentioned earlier, data used in the present analysis are derived from the results of [23], therefore, the sensor characteristics from [23] are reproduced here for ready reference as Fig. 3(a-d).

6.1. Feature selection

It is well known that the success of PR is crucially

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Table 2
ART NN simulation results: optimum weights

Cluster 0	Cluster 1	Cluster 2	Cluster 3
1.060, 0.240, 0.123	0.130, 0.063, 0.200	0.280, 0.100, 0.077	0.777, 0.753, 0.570

Vigilance parameter $\rho = 0.15$.

Bottom-up weights obtained after simulation.

dependent upon the appropriate choice of features. The following reasoning enabled us to arrive at effective features for the gas/odour identification problem.

The response of a tin oxide sensor is a non-linear function of the concentration of any gas to which it is sensitive and may be modelled as:

$$R = K[C]^{\gamma} \tag{12}$$

where, R is the sensor response-measured as percent change in resistance, C is the gas concentration (is a nonlinearity index and K is the constant of proportionality.

Due to cross-sensitivity, we expect the clusters formed by the sensor responses in the pattern space to be overlapping. Indeed, this is verified by the 3-d scatter plots obtained by taking the responses of three sensors at a time. One such plot is shown in (Fig. 4). Hence, simple percent resistance changes do not seem to constitute a good feature set for gas/odour identification.

Next, considering the responses R_1 and R_2 of two sensors to two different gases. Then, we have:

$$R_1 = K_1[C]^{\gamma 1} \tag{13}$$

 $R_2 = K_2[C]^{\gamma^2} \tag{14}$

Now, the ratio of the sensor responses can be written as:

$$\frac{R_1}{R_2} = \frac{K_1}{K_2} [C]^{\gamma 1 - \gamma 2}$$
(15)

Here, as $(\gamma_1 - \gamma_2)$ tends to zero, the ratio becomes independent of the gas concentration *C*.

In practice, the quantity $(\gamma_1 - \gamma_2)$ is much smaller than either γ_1 , or γ_2 alone, hence the ratios of sensor responses are less sensitive to concentration variations than individual responses. This is behaviour is also verified from the actual laboratory data as shown in the 3-d scatter diagram of sensor ratios as shown in (Fig. 5). Here, we have used the intrinsic SnO₂ sensor (i.e. sensor B) as the base sensor and divided the outputs of the other three sensors with the outputs from sensor B at corresponding concentration readings. Thus, we derive the three ratios from the four sensor outputs and use these ratios as the features of the training set for the ART neural network.

6.2. Experimental procedure and results

We sampled the four sensor characteristic curves Fig. 3(a-d) to obtain the outputs for the sensors A, B, C and D for the four gases emk, xyl, car and ace at various concentrations. From this the three ratios A/B, C/B and D/B were computed at various concentrations thus obtaining a training set. The reason for selecting sensor B (undoped SnO₂) response for normalising other sensor responses is that it has sufficient dynamic range with varying concentrations for all four gases/ dours used in this study. Thus, the three ratios A/B, C/B and D/B have less sensitivity to concentration variations and give good separation in the feature space. The ART neural network simulation was implemented in C language on a Pentium based computer and verified using synthetic data.

The ratio data was then partitioned into two parts one part to be used for training and the other part for testing the neural network after the training, i.e. in the sniffing mode. 50% data was used for training and the remaining data was used for testing in the sniffing mode. In the sniffing mode the performance of this ANN classifier was studied using the test data that are mutually exclusive from the training data. The simulation program stores the weight vectors in a disk file when the training algorithm satisfies the termination condition. This weight file is read in by the program in the sniffing mode to determine percent classification error using test data.

Several simulation runs for training the ART neural network were then carried out using the training data and various choices of the vigilance parameter ρ were tried. Some results are shown in Table 1. It was found that a choice of $\rho = 0.15$ gives the best results. The optimum classifier weights obtained are shown in Table 2.

For the optimum choice of the vigilance parameter ρ , the classifier gave 100% correct classification in the concentration ranges studied. With nonoptimal ρ choices the classifier performance degrades gradually. Also, at higher concentrations the sensors tend to saturate loosing their discrimination power.

The vector diagram for ART neural network weights is shown in (Fig. 6), where only bottom-up weights Ware shown for clarity. The top-down weight matrix V is simply the transpose of W. Fig. 6(a) gives the weight

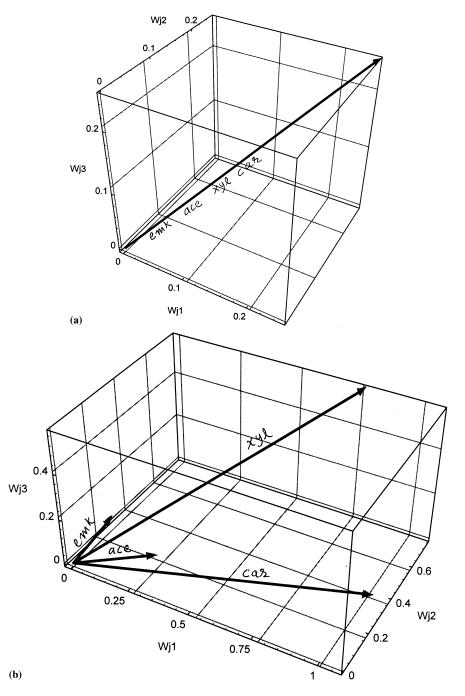


Fig. 6. The ART neural classifier weight vectors \mathbf{W} : (a) before training; (b) after unsupervised training on 4-gas classification problem. Only the bottom-up weights \mathbf{W} are shown for clarity. The top-down weights \mathbf{V} are $[\mathbf{W}]^{T}$.

vectors before training. Here, all the four vectors are collinear due to weight initialisations according to (Eq. (8a)). These vectors are adjusted by the unsupervised training algorithm using training mode data. The final weight vectors after successful training for the 4-gas problem are shown in Fig. 6(b). The weight triplets shown in Table 2 are the co-ordinates of the cluster centres in the sensor response ratios pattern space and the four clusters discovered correspond to the four gases/odours used in these experiments namely, emk, xyl, car and ace respectively.

Further, for comparison of our method against supervised NNs, we used the same data-set to train a feeedforward NN with sigmoid activation function. The NN architecture had four input neurons, six hidden-layer neurons and four output layer neurons (i.e. a topology of 4-6-4). Total weights used by this model was 58 (as against 12 weights used by the ART model). The standard error backpropagation learning algorithm was used with random weight initialisation. After a large number of trials the best result we got was with learning rate = 0.8 and momentum constant = 0.7. The best-case classification error in the sniffing mode was 10%. Thus it is evident that the unsupervised ART NN has following significant advantages over the supervised NN model:

- 1. ART NN does not use random weight initialisation hence gives repeatable performance.
- 2. It uses less number of weights.
- 3. It uses linear activation function and hence is easy to implement.
- 4. It achieves superior classification accuracy and exhibits graceful degradation against nonoptimal vigilance parameter choices.
- 5. It has faster convergence rate and does not exhibit the problem of local minima entrapment.

7. Conclusion

In this paper we report very encouraging gas/odour identification results for individual gases/odours using metal oxide gas sensor array and ART NN classifier trained in unsupervised mode. Also, the results obtained using ART NN have been compared against supervised feedforward NN showing significantly superior performance of the former on the same dataset. Majority of IGS researchers have used feedforward ANN which is a static model with no self-organisation property. It cannot adapt its structure to the topological features of the pattern space created by the outputs from a sensor array with partially selective characteristics to different gases/ odours. The ART NN model removes all the disadvantages of feedforward NN e.g. local minima, slow convergence, non-linear activation function, random weight initialisation etc.

The training of the ART ANN is done in an unsupervised mode using 50% of the sensor response samples where the network self organises to discover clusters in the training data. The trained ART NN is then tested in the sniffing mode using sniffing mode test data that is mutually exclusive from the training mode data. This approach avoids the problems associated with supervised training of the feedforward neural networks reported by other authors in the recent past.

The ART NN is also easily implementable in hardware using operational amplifier since it uses a linear activation function as against the non-linear sigmoid activation used by feedforward ANNs. Since the training is done in an unsupervised mode and does not require labelled training samples, the ART ANN can be easily trained in the field on-line. Recalibration is also simpler for new gas/odour types or change in operating environment.

The trained ART ANN can give real-time response because of the inherent parallel distributed computing for classification of gases/odours in the sniffing mode. It is thus clear, that the ART ANN is very suitable as a classifier in an IGS system.

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Biographies

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