인공 후각 시스템을 이용한 휘발성 화학물질의 분류

변형기*, 백승화**, 김현기***
*명지대학교 산업기술연구소, **명지대학교 제어계측공학과
***수원대학교 전기공학과

Classification of Volatile Chemicals using Artificial Odour Sensing System

H. G. Byun*, S. H. Beack, and H. K. Kim*****
***Industry Technology Research Centre, MyongJi Univ.**
****Dept. of Control and Instrumentation Eng., MyongJi Univ.**
*****Dept. of Electrical Eng. Suwon Univ.**

Abstract

Neural networks are increasingly being used to enhance the classification and recognition powers of data collected from sensor array. This papers reports the effectiveness of multilayer perceptron network based on back-propagation algorithm combined with the outputs from "Electronic Nose" using electrically conducting polymers as sensor materials. Robust performance and classification results are produced with pre-processing method.

1. Introduction

There is currently much interest in the development of instrument that emulate the human sense of smell. An artificial sensing system is applicable to a large area of industry, which includes food, fermentation and brewing, beverage, cosmetics, environmental monitoring, and some chemical fields. Many of these systems have been given the name "Electronic Nose" because they are capable of or intended to sense some of the gases or odours that the human nose can discriminate, and they are based on broad specificity sensors.

Over the last decade Persaud and coworkers[1] have developed an electronic nose which uses organic electrically conducting polymers. The strategies involved are a radical departure from conventional thinking of chemical sensors since they utilise broadly selective sensors. The signals produced by an array of sensors consist of measurements of responses to odours producing different patterns. These patterns involve the application of an artificial neural networks These patterns involve the application of an artificial neural networks for discrimination between odours, because it possesses several advantages over conventional pattern recognition techniques in terms of adaptability, noise tolerance, fault tolerance, distributed associated memory, and an inherent parallelism generating a high speed of operation after training[2].

A variety of pattern recognition technique based on artificial neural networks may be applied to the classification of different odours, but the back-propagation [3], a model of multilayer perceptron network, is probably the most widely used artificial neural network paradigm and has been shown to be applicable to odour recognition.

This papers reports results obtained from back-propagation algorithm to patterns generated by odour sensing system for volatile chemicals. Of particular interest of us is not only just usage of back-propagation algorithm for odour recognition, but also the reduction of iteration times and improvement of the recognition performances. It can be solvable to use of pre-processing techniques. The techniques that have been developed allow an fast learning times and excellent recognition results for volatile chemicals classification problems. It may applicable to identification of highly complex mixtures of chemicals. This is an important problem in environmental pollution monitoring and in the cosmetics, food and defence industries.

2. Electronic Nose system based on an array of conducting polymer

There has been a trend away from the concept of designing sensors that are highly specific to one chemical species, because there is always some cross-sensitivity to other analytes. This cross-sensitivity can be utilised effectively if sensors with broad but overlapping specificities are combined into arrays.

One of useful set of materials that be utilised as sensors in a form of an "Electronic Nose" is

that of electrically conducting organic polymers. Persaud and Pelosi [4] have investigated the gas sensing properties of a large number of conducting polymers. These display reversible changes in conductivity when exposed to polar volatile chemicals. Unlike many commercially available gas sensors, rapid adsorption and desorption kinetics are observed at ambient temperatures.

Different polymers made from modified monomer units show broad overlapping response profiles to different volatile compounds. Miniature arrays consisting of up to twenty different conducting polymer materials have now been realised and commercially available.

A microprocessor driven circuit, measuring changes in resistance of individual sensor elements, interrogates the sensor array at user defined time intervals, and the data is stored in memory. Each sensor element changes in resistance when exposed to a volatile compound. However, the degree of response to a given substance depends on the type of polymer element; consequently, a pattern of resistance changes can be recorded and processed to produce a set of descriptors for that particular substance.

The array response is normalised to represent relative changes in resistance and thus concentration-independent patterns can be produced. These patterns show the relative response of individual sensor elements to specific gases and odours, and are used as inputs to discriminate between gases and odours based on artificial neural networks.

3. Description of the multilayer perceptron network

(3-1) Multilayer perceptron network

An artificial neural network is a processor of information, which can be represented in its simplest form by a set of connected and layered processing elements. The multilayer perceptron network was chosen as a typical artificial neural network. The usual number of layers found in such networks is three, as a three-layer network has sufficient computational degrees of freedom to solve most problems.

In a three-layer network, the processing elements are organised into distinct layers, namely the input layer, the hidden layer, and the output layer. The input layer receives inputs from the external source, and the hidden layer(s) introduces additional information processing. The output layer delivers the presentation of the input after processing has occurred. Each layer is usually fully connected to the succeeding layer. The system architecture for such a network is illustrated schematically in Figure 1.

As shown in Figure 1, each of these is multiplied by a connection weight, and the products are summed. This summation of products is termed Net and must be calculated for each processing element in the network. The network input to a processing element in layer j is

$$Net_{pj} = \sum_i w_{ji} o_{pi} \qquad (1)$$

where p denotes the pattern number, w_{ji} is the weight between processing elements layer j and i , and o_{pi} is the output from a processing element in layer i.

The output of processing element j is

$$o_{pj} = F(Net_{pj}) \qquad (2)$$

where F is an activation function.

The output o_{pj} in eq.(2) is further processed by a non-linear activation function F that squashes the data.

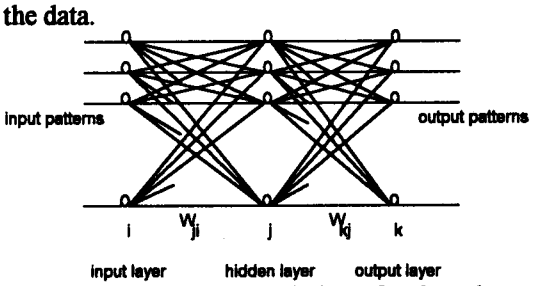

Figure 1. A schematic depiction of a three-layer network architecture

The sigmoid activation function, which is continuous and non-linear, is usually used for a three-layer network application. This activation function compresses the range of Net so that output o_{pj} lies between zero and one. Thus, the output o_{pj} is given by

$$o_{pj} = 1/[1+\exp[-Net_{pj} + \theta_j] \qquad (3)$$

In the above equation, the parameter θ_j serves as a threshold or bias. The computational process for the processing element in layer k from Figure 1 is finally carried out such that:

$$Net_{pk} = \sum_j w_{kj} o_{pj} \qquad (4)$$

and the corresponding outputs

$$o_{pk} = F(Net_{pk}) \qquad (5)$$

The supervised artificial neural network functions by accepting the inputs, processing them, producing an output, compares this output with the desired output, and adjusts the weights to produce a better output. Therefore, the actual output o_{pk} in eq.(5) is compared with the desired output t_{pk} using error measurement. The average network error is

$$E = \frac{1}{2p}(\sum_{p}\sum_{k}(t_{pk} - o_{pk})^2) \quad (6)$$

where p is the number of patterns.

(3-2) Back-propagation algorithm

The back-propagation algorithm based on the generalised delta rule is the most popular learning rule in use. This learning algorithm was popularised by Rumelhart *et al* [3] in the late 1980s. The learning algorithm, which is described in this section, was based on the work of them. According to their suggestions for the back-propagation learning rule, the weightings of the processing elements in each layer are changed by an amount proportional to the product of the error signals δ which are propagated back through the network from output layer to input layer, such that:

$$\Delta_p w_{kj} = \eta \delta_{pk} o_{pj} \quad (7)$$

and

$$\Delta_p w_{ji} = \eta \delta_{pj} o_{pi} \quad (8)$$

where η is the rate of learning, δ_{pk} is the error signal of the output layer, and δ_{pj} is the error signal of the hidden layer.

Eq.(7) presents the weight changes between output and hidden layers, and the changes of weights between hidden and input layers are shown in eq.(8). The error signals, δ_{pk} and δ_{pj}, can be described using the chain rules respectively as follows:

$$\delta_{pk} = (t_{pk} - o_{pk}) o_{pk}(1 - o_{pk}) \quad (9)$$

and

$$\delta_{pj} = o_{pj}(1 - o_{pj}) \sum_{k} \delta_{pk} w_{kj} \quad (10)$$

Selection of a value for the learning rate η in eqs.(7) and (8) has a significant effect on the network performance. Usually, η must be a small number to ensure that the network will settle to a solution; however, a small value of η means that the network will have to perform long iterations. It is often possible to increase the value of η as the learning proceeds.

After the learning process, involving a set of gases and odours, the recognition procedure for each pattern is easily carried out using the adjusted weights between the layers within short period.

(3-3) Pre-processing techniques for input patterns

Before the input patterns are fed into the three-layer fully connected neural network using a back-propagation of errors learning regime, it is quite common in pattern recognition to use a pre-processing technique to transform the original data into their most expedient form. This technique may be reduced iteration time and improved the learning performance. A technique of pre-processing is called autoscaling. All sensor responses, which include the normalised responses of individual sensors, are autoscaled using mean-centreing with the standard deviation. The autoscaled responses g_{ij}', where i is the number of input patterns and j is the number of features in the sensor array, is calculated by dividing the mean-centre value g_{ij} - $\bar{g}_j$, where $\bar{g}_j$ is the mean value of the features in the sensor array of each pattern, by the standard deviation σ_j:

$$g_{ij}' = g_{ij} - \bar{g}_j / \sigma_j \quad (13)$$

and

$$\sigma_i^2 = (\sum (g_{ij} - \bar{g}_j)^2)(N-1)^{-1} \quad (14)$$

where i is the number of input patterns, j is the number of features in the sensor array, and N is the number of entire input patterns.

4. Experimental results

Figure 2 shows the averaged concentration response curve obtained from methanol. The filled rectangles represented the actual response of sensors according to concentrations, and the line of least-squares fit plotted. The same procedure was repeated for the next four volatile chemicals including ethanol, n-butyl acetate, butanone, and a mixture of ethanol in methanol. The concentration-response profiles for the five volatile chemicals were approximately linear over the concentration range covered. This characteristic allows simple computation methods to be used for information processing.

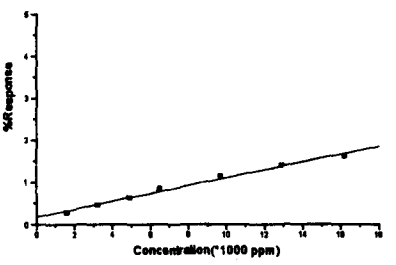

Figure2. Concentration curve for methanol

When we look at the relative responses of individual sensors to each other in an array, it is observed that unique patterns are generated for each volatile chemical(Figure 3). The multilayer perceptron network pattern recognition programme, based on the back-propagation algorithm, was applied to discriminate between response patterns of five volatile chemicals. Each volatile chemical that consisted of twenty data sets, which obtained during gas measurements, for training and recognition.

The first ten data sets were used for the training procedure; the next ten data sets for recognition.

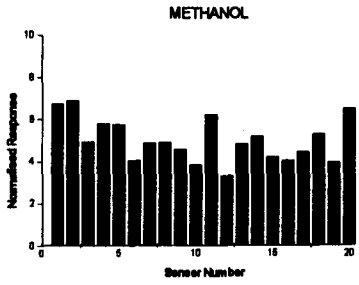

Figure 3. Pattern generated from methanol

Classification experiments were carried out to establish whether a back-propagation algorithm could be trained successfully to recognise each pattern of the volatile chemicals to determine the extent of which the output values converge to the desired (target) values, and the ability of the network to classify the volatile chemicals.

The input layer possesses twenty processing elements . This input layer is fully connected to the hidden layer. The number of hidden layers and processing elements could be selected to accelerate and improve the convergence performance in the training process. One hidden layer and five hidden processing elements, which were found to give good results experimentally, were used. During these experiments, the variations in the number of hidden layer and hidden processing elements did not have a significant effect on the network performance except for the increased iteration time requirements.

Table 1 shows the recognition results for the fifty volatile chemical samples for the five volatile chemical classes without any pre-processing technique.

Class	1	2	3	4	5
Methanol	10				
Ethanol	2	7			1
n-butyl acetate			10		
Butanone				10	
Mixture				1	9

Table 1 Recognition results of the fifty volatile chemical patterns into five classes.

Recognition results for the fifty volatile chemical samples and the average neural network outputs for each class are shown in table 2. This results agree when the pattern autoscaling method was used as the pre-processing technique for the input layer processing elements; this showed the fast convergence performance and excellent recognition results compared with sensor array without pre-processing method.

	1	2	3	4	5
Methanol	10				
Ethanol		10			
n-butyl acetate			10		
Butanone				10	
Mixture					10

Table 2 Recognition results of the fifty volatile chemical patterns into five classes. The patterns were pre-processed by pattern autoscaling

The values of the learning rate η and momentum rate α affect the performance of the multilayer perceptron network. It was recognised that η 0.9 and α 0.6 gave good results.

5 Conclusion

Using a three-layer network architecture and a back-propagation algorithm, it was found that sample patterns of five chemical species could be recognised in all cases.

The experimental results showed that the choice of a pre-processing method for input layer processing elements influenced the performance of the multilayer perceptron network.

It can be concluded that multilayer perceptron network based on back-propagation algorithm has the capability to classify volatile chemicals when used in conjunction with the conducting polymer based sensor array. It will be realised as Electronic Nose in near the future.

Reference

1. Persaud, Travers , "Multielement arrays for sensing volatile chemicals", Intelligent Instruments and Conmputers, Elsevier Press, pp147-154, July/August, 1991
2. Persaud, Pelosi, "Sensor arrays using conducting polymers for an artificial nose", NATO ASI Series E: Applied Science, Vol. 212, Springer-Verlag, pp 237-256, 1992.
3. Rumelhart, Hinton , Williams, "Learning representations by error propagation", Nature, Vol. 323, pp.533-536, 1986.
4. Pelosi , Persaud, "Gas sensors: Towards an artificial nose", NATO ASI Series F: Computer and System Science, Springer-Verlag , pp 361-382,1988