1st International Conference on Sensing Technology
November 21-23, 2005 Palmerston North, New Zealand

Analysis of gas mixtures using a single tin oxide sensor and fast pattern recognition

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Abstract

A modified fuzzy ART (*m*-fuzzy ART) based on a simple and fast learning method is proposed to estimate the concentration of the gas mixtures. Using a single tin oxide sensor operated in a temperature modulated mode, the features are extracted. The extracted features of which their dimensions are reduced by the principal components analysis (PCA) are used to identify single or mixture gases and estimate their concentration using several methods based on neural networks. The proposed *m*-fuzzy ART network is compared with the other methods. From computer simulations, the *m*-fuzzy ART networks are shown to learn training data faster than neuro-fuzzy networks with similar mean square error.

Keywords: gas mixture, tin oxide sensor, modified fuzzy ART, estimation of concentration

1 Introduction

There is an increasing need for a compact air pollution monitoring device based on an electronic nose [1]. This is a promising research area because a gas detector based on the electronic nose can be designed as a low cost, small size, and easy handling device having fast response time in compared with traditional methods, gas chromatography or mass spectrometry. These characteristics make this device applicable to many areas such as foods, environmental monitoring, and medical fields, together with the embedded technology.

However, semiconductor gas sensor arrays of the tin oxide type widely used as detecting elements in electronic nose system have chronic weak points. Their responses can be often influenced by drifts such as nonlinearities of sensors, humidity rate and temperature [2]. Also, they have lack of selectivity. To solve these problems, many researches have been conducted on identification and quantification of gas mixtures as well as single gases. Appropriate measurement techniques were presented to enhance metal-oxide sensor selectivity for gas mixture classification [3]. A new feature extraction method based on the discrete wavelet transform was proposed in gas mixture analysis [4]. The effect of humidity on the discriminating ability of gas mixtures was also considered [5]. A new drift counteraction method based on the on-line learning ability of the fuzzy ARTMAP neural network was introduced [6].

As far as a fuzzy neural network is concerned, both the complexity of the network size and the leaning time of algorithms in identification and quantification of gases are important factors to be applied to device platforms of sensor networks as well as portable electronic noses based on embedded techniques. Multilayer perceptron (MLP) neural networks have been the most widely used in classifying single or mixture gases and estimating their concentration [7]. This method can calibrate the measured data off-line by learning the data. After some time, drift impairs the pattern recognition ability of the system, which requires retraining. The neuro-fuzzy networks (NFNs) [8] show better performance than MLP neural networks in estimating concentration of gases but the networks of the NFNs are more complex than those of MLP neural networks. Both of them have problems of learning on-line and complexity of networks in applying to small electronic nose devices.

A simple and fast learning method, called modified fuzzy ART, is proposed to estimate the concentration of gases. This scheme is composed of two parts. A training phase is for designing fuzzy membership function automatically by partitioning training patterns. The other one is for estimating the desired output with test patterns. This *m*-fuzzy ART network is compared with the previous methods and discussed. From computer simulations, the *m*- fuzzy ART networks are shown to learn training data faster than NFNs with similar mean square error.

2 Experiment

The mixture gases of ammonia and hydrogen sulphide were chosen as target gases in the experiment. To test these gases, our experimental system is composed of three parts: the gas lines, a humidity generator, and a

test chamber. As shown in figure 1, the gas lines are composed of gas bottles containing dry synthetic air and mass flow controllers (MFC's). The measurement procedure is as follows. First, the synthetic air is brought into the humidity generator and then mixed with the test target gas via gas lines controlled by MFC's. Then the mixture is introduced in the test chamber. Finally, a microcontroller with gas sensors mounted in the gas chamber measures periodically the sensor output signals.

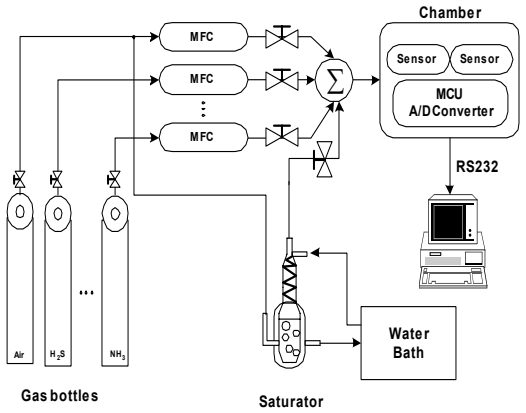

Figure 1: Experimental set-up.

Table 1: Measured gas mixtures and their concentrations

NH_3 (ppm)	H_2S (ppm)					
	0	1	2	3	5	7
0		*v*	*v*	*v*	*v*	*v*
10	*v*	*v*				
20	*v*		*v*			
30	*v*			*v*		
40	*v*				*v*	
50	*v*					*v*

For our application, a single TGS2602 gas sensor was used for detecting air contaminants instead of consisting sensor arrays. This simple method was available by using the change of sensitivity about operating temperature. This sensor was connected to the microcontroller board to read the sensor resistance change in presence of the target gas. The output voltage of the sensor was read by a 12bit-ADC module of an MSP430 ultra-low power microcontroller from Texas Instruments.

The measurements were recorded for five different concentration levels of pure H_2S, NH_3, and their mixtures, respectively (Table 1). Each measurement was replicated five times so that there were 75 measurements by the following procedure. First, the sensor was preheated for 30 seconds and with turning off the sensor heater, the output voltages of the sensor were read at every 100 milliseconds for 1.5 seconds. Therefore, 15-dimensional data set was extracted from the experiment for pattern recognition.

3 Modified Fuzzy ART as fast pattern recognition

The proposed *m*-fuzzy ART architecture, as shown in figure 2, consists of two phases. A training phase is for designing fuzzy membership functions automatically by partitioning training input patterns. The other one is for estimating the desired output with the test pattern.

3.1 Fuzzy ART architecture

The training phase of figure 2 describes the fuzzy ART network architecture. The learning step of the network is as follows. An *m*-dimensional input pattern, $\mathbf{a}= \{a_1, a_2, \ldots, a_m\}$ where $I_i \in [0, 1]$ and $i= 1, 2, \ldots, m$, is presented to F_0 layer. The complement-coded input pattern is compared with the prototypes $\boldsymbol{W}_j \in \boldsymbol{R}^{2m}$ in the F_1 layer by using a choice function as shown in (1). The prototype that has the highest degree of fuzzy subset is selected by (2). Note that $|\mathbf{x}| \equiv \sum_i x_i$, $x \wedge y \equiv min(x_i, y_i)$ and the choice parameter is a small positive number

$$T_j = \frac{|I \wedge W_j|}{\alpha + |W_j|} \tag{1}$$

$$T_J = \max\{T_j : j = 1 \cdots n\} \tag{2}$$

Resonance occurs if the prototype chosen by the choice function satisfies (3) where the vigilance parameter ρ is a threshold by users.

$$\frac{|I \wedge W_J|}{|I|} \geq \rho \tag{3}$$

A prototype satisfying (2) is chosen as a winner prototype. If this prototype satisfies (3), it will be updated according to (4) where β is the learning rate parameter. In case the winner prototype does not satisfy (3), search process continues until the chosen ***J***

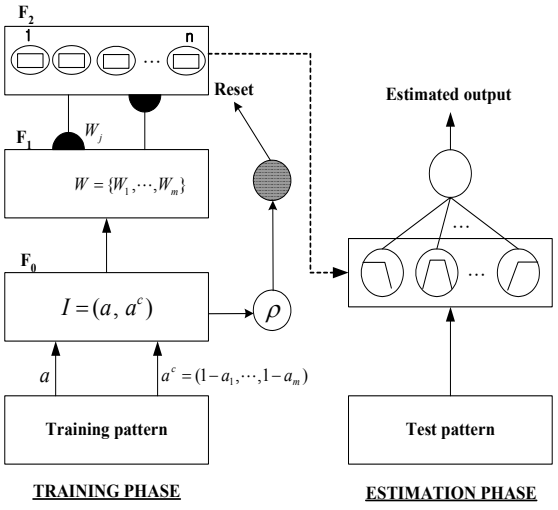

Figure 2: Architecture of *m*-fuzzy ART model.

satisfies (3). Otherwise, a new prototype is created to describe the current input pattern.

$$W_J^{new} = \beta(I \wedge W_J^{old}) + (1-\beta)\, W_J^{old} \qquad (4)$$

It is called fast learning when β =1. The maximum size of prototype $\boldsymbol{J}$ is adjusted by the vigilance parameter.

3.2 Fuzzy rule extraction with fuzzy hyperbox regions

Through the process of training phase, hyperbox regions are learned by the fuzzy ART algorithm for a given training datum. Using this hyperbox, fuzzy rules (5) are extracted by associating the input hyperbox (*IH*) and the corresponding output hyperbox (*OH*). Thus, the number of rules is generated as many as those of hyperboxes.

$$\boldsymbol{R_j}: \text{IF } \boldsymbol{x} \text{ is } IH_j \text{ THEN } \boldsymbol{y} \text{ is } OH_j \qquad (5)$$

The degree of membership of fuzzy rules for given test patterns is determined by the membership function of the hyperboxes as follows,

$$d_A(\boldsymbol{x}, k) = \begin{cases} 1 & for\, u_k \le x_k \le U_k \\ 1-\max(0,\min(1,\gamma(u_k - x_k))) & for\ x_k < u_k \\ 1-\max(0,\min(1,\gamma(x_k - U_k))) & for\ x_k > U_k \end{cases} \qquad (6)$$

where A= IH_j , $x_k \in \boldsymbol{x}$, u_k is the minimum value, U_k is the maximum value of x_k in hyperbox region, and γ is a sensitivity parameter. Finally, a defuzzification process is performed for estimating the desired output with test input patterns. The center of gravity is used as follows:

$$\hat{y} = \frac{\sum_{j=1}^{n} d_j \times h_j}{\sum_{j=1}^{n} d_j} \qquad (7)$$

where, d_j is the degree of membership of input patterns as to fuzzy rules up to n, and h_j is the center value of the output membership.

4 Results and discussion

Figure 3 shows PCA results for whole data set of all measurements. It is observed that over 99% of the variance within the data is contained in the first two principal components. The PCA plot reveals a modest geometric structure of the data, which is characterized by the same concentration of hydrogen sulfide stretched along parallel directions. The data matrix in a new space of lower dimension is used as the inputs to several pattern recognition methods. Main tasks related to this work are to identify single or mixture gases and to estimate their concentration. So pattern recognition system is designed by two steps. First, a pattern classifier discriminating single and mixture gases is constructed. Second, the estimators of concentration

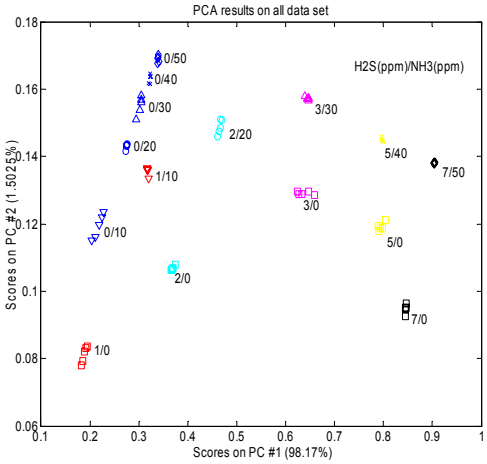

Figure 3: PCA results of the measurements.

are designed for single and mixtures gases, respectively.

4.1 Qualitative analysis

The MLP neural network was applied to classify the single or mixture gases. The network had two, six, and three neurons in the input, hidden, and output layers, respectively. The output neurons correspond to the three different classes, H_2S, NH_3, and H_2S+NH_3. This network was trained by 60 data sets, which were obtained from four repeated measurements in 15 combinations of single and mixture gases. When the left out data of 15 measurements were tested for validation of network, the success rate was 100%. The reason why this perfect recognition rate comes out is that it is easy to separate the single and mixture gases as shown in figure 3.

4.2 Quantitative analysis

The estimation models of three types were built for the quantification of H_2S, NH_3, and their binary mixtures. First, three MLP neural networks were constructed for two single gases and their mixture. The network consisted of two, six, and one neurons in the input, hidden, and output layers, respectively. The data of 20 were prepared for training the networks. A One-leave-out validation method was performed with five data sets

Second, three neuro-fuzzy networks for each gas to be detected were designed. A network had four layers, including an input layer, all of which are trained by an error-backpropagation learning scheme. The output of the neuro-fuzzy network was obtained using the conventional center of gravity method of the defuzzification process. The detailed procedures were described in [8]. Figure 4 shows that the actual concentration versus the estimated concentration of NH_3 by the neuro-fuzzy network method. Finally, the proposed *m*-fuzzy ART model was implemented in estimating concentration. At training phase, five fuzzy

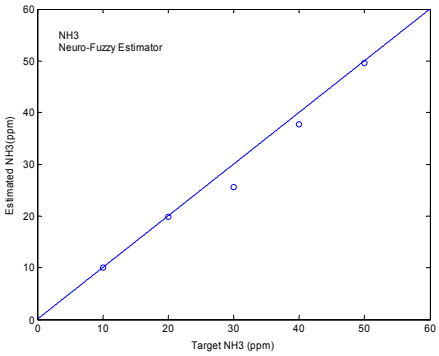

Figure 4: Target versus estimated concentration of NH_3 by neuro-fuzzy network method.

memberships were formed by adjusting vigilance parameter. Three *m*-fuzzy ART models were simulated with ρ=0.980 in single gas of H_2S and ρ=0.988 in the others. This fuzzy regions correspond to five levels of concentration, 1, 2, 3, 5, 7(ppm) of H_2S and 10, 20, 30, 40, 50(ppm) of NH_3, respectively. Then, five fuzzy rules are extracted in accordance with the number of fuzzy hyperboxes. Five validation data which were chosen in each level of concentration were prepared. Through fuzzy reasoning and defuzzification process, the concentration of the single and mixture gases is estimated as shown in figure 5 and 6. The estimated concentration is very close to the actual concentration.

The performance of three estimation models to quantify concentration of gases is compared in table 2. The neuro-fuzzy network method is superior to the MLP method on both training time and mean square error (MSE). But the neuro-fuzzy network is little more complex than the MLP neural networks.

Even though, the MSE indices of the proposed *m*-fuzzy ART model are similar to those of NFNs, training time of this method is faster than that of NFNs. Since *m*-fuzzy ART models save minimum and maximum of the trained data, network sizes are smaller than NFNs.

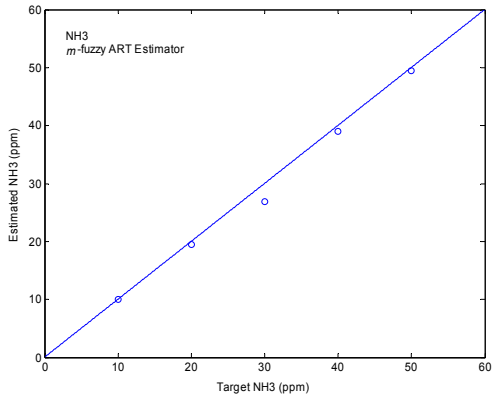

Figure 5: Target versus estimated concentration of NH_3 by *m*-fuzzy ART network method.

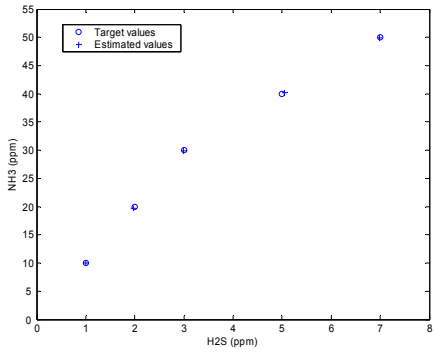

Figure 6: Target versus estimated concentration of NH_3 and H_2S mixtures by *m*-fuzzy ART network method.

The ART network is known to rapidly learn a rare event that predicts different consequences from a class of similar events. Thus, unlike MLP-based network, which takes a long time to retrain the rare event, the proposed model is useful for handling drift on line due to this property like fuzzy ARTMAP. In future work, it will be shown that the proposed method has ability to correct drift in real time.

5 Conclusions

The analysis of gas mixture for identification and quantification of ammonia and hydrogen sulphide is presented by using a single sensor operated in a temperature modulated mode and a fast pattern recognition method. The thermally modulated high-dimensional features of measurement data are reduced by the PCA method. An MLP neural network classifier results in perfect identification of single and mixture gases. The concentration of the identified single or mixture gases is estimated by three pattern re-

Table 2: Result of estimated concentration by MLP, NFN, and *m*-fuzzy ART

Method	Test Gas	MSE	Training time (epoch)
PCA+MLP	H_2S (single)	0.0440	50000
	NH_3 (single)	11.1005	60000
	H_2S (mixture)	0.0075	20000
	NH_3 (mixture)	0.2172	
PCA+NFN	H_2S (single)	0.0047	15000
	NH_3 (single)	5.0623	25000
	H_2S (mixture)	0.0003	15000
	NH_3 (mixture)	0.0268	
PCA+ *m*-fuzzy ART	H_2S (single)	0.0127	1
	NH_3 (single)	2.3587	1
	H_2S (mixture)	0.0006	1
	NH_3 (mixture)	0.0284	1

cognition methods; MLP neural networks, neuro-fuzzy networks, and the proposed methods. The neuro-fuzzy networks outperform MLP neural networks on MSE and training time. The proposed method, *m*-fuzzy ART networks are compared with the other methods. From computer simulations, the *m*-

fuzzy ART networks are shown to learn the training data faster than NFNs with similar MSE.

6 Acknowledgements

This work was supported by grant No. R01-2005-000-11047-0 from the Basic Research Program of the Korea Science & Engineering Foundation.

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