Olfactory Target/Background Odor Detection via Self-expression Model

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***Abstract*—Extreme Learning Machine (ELM) is a promising single hidden layer feed-forward neural network learning method, which achieves fast learning by randomly tuning the hidden layer. In this paper, we propose a self-expression ELM (SeELM) for olfactory target/background detection. Specially, it is known that metal oxide semiconductor (MOS) sensor in electronic nose (E-nose) can response to several target gases and interferences (background) simultaneously, which would seriously deteriorate the detection accuracy of target gases. Considering that there are numerous interferences in real-world application scenario, it is impossible for us to collect them. With a prior knowledge that the target gases samples can be easily collected, a novel SeELM method is proposed to address this issue. The idea is represented as two aspects. First, the target gases being detected by an E-nose can be fixed as invariant information, which is utilized to construct a self-expression model. Second, with the self-expression detector, the unknown backgrounds can be easily recognized in terms of the violation. Experimental results proved that the proposed SeELM method is significantly effective for Target/Background detection in E-nose.**

Keywords—Extreme learning machine, self-expression, background detection, electronic nose

I. INTRODUCTION

Recently, a new learning algorithm for solving a single-layer hidden feed-forward neural network (SLFN), known as extreme learning machine (ELM) proposed in [1], has turned out to be the remedy for neural network learning approaches. Inconceivably the speed of ELM can be thousands of times faster than the traditional network learning algorithms [2–7], while the structure of ELM is rather simple. Furthermore, ELM is efficient in hierarchal learning [8-9]. The magic of ELM is that the parameters of weight and bias can be assigned randomly independent of training data. Besides, the output weights can be solved with different constraints. ELM has been widely used in regression and classification problems [7-9] due to its wide variety of feature mapping functions (sigmoid, RBF, etc.).

Electronic nose (E-nose), as a gas sensor system with pattern recognition ability, is across multiple subjects, such as gas sensor, chemistry, electronics, artificial intelligence, etc. Gas sensor technology and artificial intelligence are the research foundation of artificial olfaction system. The performance of an E-nose depends on the selected gas sensors, which should have good cross-sensitivity, selectivity, reliability and robustness [10]. There are commonly two challenging problems in E-nose community. One is the time-varying sensor drifting, the other is the interferences independent of the targets. Researchers have proposed different methods for issuing the drift [11-17]. However, there is little work on the interferences (background outliers) in E-nose. The issue is closely related with the cross-sensitivity characteristic of gas sensors. Specifically, during the process of target gases sensing, the gas sensors also have sensitive response when exposed to the interferences, such that the accurate sensing is seriously affected. Therefore, it is urgent to face with this thorny problem. However, there are so many kinds of interferences appeared in real scenarios, such that the discrimination of target and interferences gas cannot be defined as a general pattern recognition problem because there are no interference data. For solutions of the discrimination, two artificial intelligence learners were developed for discrimination of unwanted odor interferences in [18]. Another interference discrimination method was also proposed based on the invariant target gases information [19].

The existing methods to distinguish the targets and interferences depend on the enough collection of the interferences samples. To this end, we propose to use the prior knowledge of the targets in modeling. According to the characteristics between targets and backgrounds, if an unknown gas can be correctly expressed by target samples set, then the unknown gas will be recognized to be some target. Otherwise, it would be discriminated as background. With the ELM theory, more formally, we name the proposed olfactory target and background detector as Self-expression Extreme Learning Machine (SeELM). The basic idea of SeELM is illustrated in Fig.1, which is simply divided into two steps. First, SeELM is modeling on the obtained target gas dataset, thus, a self-expression coefficient matrix is computed. Second, for abnormality detection, each new pattern is represented by using the well-learned self-expression coefficient matrix and the representation error is computed for abnormality (i.e. background) detection.

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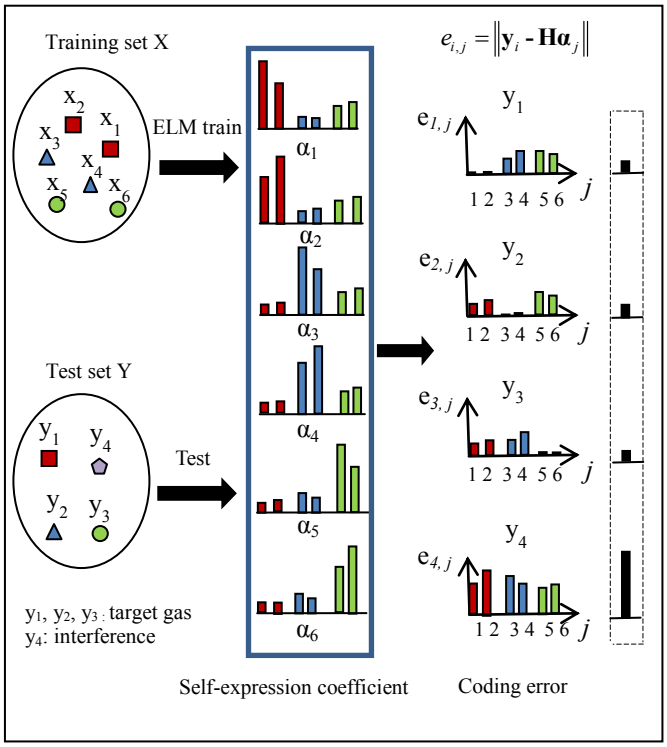

Fig. 1 Overview of the SeELM method

II. Related Works

Extreme Learning Machine (ELM) is a single-hidden-layer feedforward neural network learning algorithm (SLFN) [1], which can be used for feature extraction, clustering, multi-class classification and regression problems. The superiority compared to other methods (e.g. SVM) is that the training speed of ELM is extremely fast. In ELM, the input layer parameters (linking the input layer and the hidden layer) including the input weights and hidden biases are randomly chosen, and do not require computationally intensive tuning upon the data. The activation function can be any type of piecewise continuous nonlinear hidden neurons, including sigmoid function, Fourier function, RBF function, etc. In learning process, hidden layer nodes (number of neurons) can be tuned in terms of the actual situation and naturally do not require an iterative adjustment.

In the case of clean data, the output function of ELM for generalized SLFNs is presented as

$$f(\mathbf{x}) = \sum_{i=1}^{L} \boldsymbol{\beta}_i G(\mathbf{a}_i, b_i, \mathbf{x}) \qquad (1)$$

where $\mathbf{x}$ is the input vector, L is the number of hidden nodes, $\mathbf{a}_i$ is the input weights, b_i is the bias of the hidden nodes, $\boldsymbol{\beta}_i$ is the output weights between the hidden layer with L nodes and the output nodes, $f(\mathbf{x})$ is the respective target output vectors, and

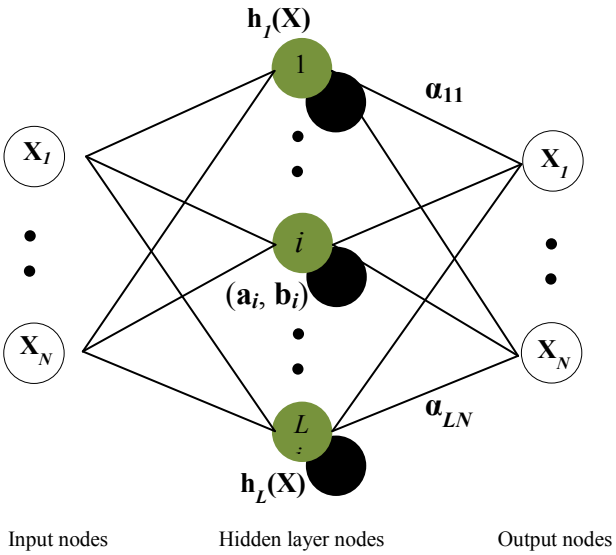

Fig. 2. The schematic diagram of self-expression procedure via ELM

$G(\mathbf{a}_i, b_i, \mathbf{x})$ is the output vector of the i-th hidden neuron, respectively. The Eq.(1) can also be compactly written as

$$f(\mathbf{x}) = \mathbf{h}(\mathbf{x})\boldsymbol{\beta} \qquad (2)$$

where $h_i(\mathbf{x})=G(\mathbf{a}_i, b_i, \mathbf{x})$ is the output vector of the i th hidden neuron, thus $\mathbf{h}(\mathbf{x})=[h_1(\mathbf{x}), h_2(\mathbf{x}),\ldots, h_L(\mathbf{x})]$ is the output vector of the hidden layer, $\boldsymbol{\beta}=[\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_L]$ is the output weights. In order to minimize the norm of the output weights, the minimal norm least square method is employed in ELM instead of the standard optimization methods [1]. Thus, the output weights vector $\boldsymbol{\beta}$ is determined analytically using Moore–Penrose (MP) generalized inverse as

$$\boldsymbol{\beta} = \mathbf{h}(\mathbf{x})^{+}\mathbf{T} \qquad (3)$$

where $\mathbf{T}=f(\mathbf{x})$, $\mathbf{h}(\mathbf{x})^{+}$ is the Moore–Penrose generalized pseudo-inverse of the hidden layer output matrix, $\boldsymbol{\beta}$ has the smallest norm among all the optimization solutions, and this is the reason why ELM has better generalization performance and higher learning accuracy. According to Bartlett's neural network generalization theory, in addition to achieving smaller training error, the smaller the norms of weights are, the better generalization performance the networks tend to have, the regularized ELM [8] is expressed as

$$\min_{\boldsymbol{\beta}} \|\boldsymbol{\beta}\|_F^2 + C\|\mathbf{H}\boldsymbol{\beta} - \mathbf{T}\|_F^2 \qquad (4)$$

Then the solution can be written as

$$\boldsymbol{\beta} = \mathbf{H}^{\mathrm{T}}\left(\frac{\mathbf{I}}{C} + \mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{T}, \quad if\ N<\mathrm{L} \qquad (5)$$

where N is the number of training samples, and L is the number of hidden nodes. When the number of training samples N is huge and larger than that of nodes L, then we can have

$$\boldsymbol{\beta}=\left(\frac{\mathbf{I}}{C}+\mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{T},\ \ if\ N>\mathrm{L} \tag{6}$$

Therefore, the ELM output function is represented as follows

$$f(\mathbf{x})=\mathbf{h}(\mathbf{x})\boldsymbol{\beta}=\mathbf{h}(\mathbf{x})\mathbf{H}^{\mathrm{T}}\left(\frac{\mathbf{I}}{C}+\mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{T},\ \ if\ N<\mathrm{L} \tag{7}$$

$$f(\mathbf{x})=\mathbf{h}(\mathbf{x})\boldsymbol{\beta}=\mathbf{h}(\mathbf{x})\left(\frac{\mathbf{I}}{C}+\mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{T},\ \ if\ N>\mathrm{L} \tag{8}$$

III. Proposed SeELM method

A. Notations

In this paper, the training phase is divided into two parts: First, computing the self-expression matrix $\boldsymbol{\alpha}$. Second, determine the representation error threshold T. $\mathbf{X}\in\Re^{D\times N}$ is the target gas data. To obtain the coding coefficient matrix α, the training data of target gases is denoted as $\mathbf{X}_{\boldsymbol{\alpha}}\in\Re^{D\times N}$. To obtain T, the training data of the target gases is denoted as $\mathbf{X}_{Tt}\in\Re^{D\times N_{Tt}}$ and the training data of a very few interference gas data is denoted as $\mathbf{X}_{Td}\in\Re^{D\times N_{Td}}$, respectively, where D is the number of dimensions, N, N_{Tl} and N_{Td} are the number of training samples, $\boldsymbol{\alpha}\in\Re^{L\times N}$ is the self-expression coding coefficient matrix. $\|\cdot\|_F$ denotes Frobenius norm of a matrix. Throughout this paper, matrix is written in capital bold face, vector is presented in lower bold face, and variable is in italics.

B. Formulation of the Proposed SeELM

The proposed SeELM consists of two parts: 1) computing the self-expression coding coefficient matrix $\boldsymbol{\alpha}$; 2) computing the representation error threshold T for discrimination.

- Self-expression coding

There are numerous types of interferences in real scenarios, which can produce serious effects on the performance of electronic nose systems. Obviously, people cannot obtain all of them in experiments. Luckily, the several types of target gases that we need to detect by using electronic noses are known, thus we attempt to use the prior information of the target gases. Compared to the variable backgrounds, the target gases are invariant information. Therefore, for constructing a model based only on the target gases, it is rational to imagine that a self-expression model can be designed for capturing the internal relationship of the target gases. The relationship within targets can be used to detect the backgrounds by exclusion. Instinctively, the relationship can be modeled by formulating

$$\mathbf{X}=\mathbf{X}\boldsymbol{\alpha} \tag{9}$$

While the self-expression formula may cause the problem of over-fitting. From the network of ELM, which contains a nonlinear activation function, the self-expression matrix $\boldsymbol{\alpha}$ shows sparsity and achieves a good generalization ability. As illustrated in Fig. 2, ELM is introduced for representing the relationship between the target gases $\mathbf{X}_{\alpha}$ by using itself. Through the ELM network, we aim to learn a self-expression coefficient matrix $\boldsymbol{\alpha}$. Therefore, the optimization problem can be formulated as

$$\min_{\boldsymbol{\alpha}}\|\boldsymbol{\alpha}\|_F^2+C\|\mathbf{H}\boldsymbol{\alpha}-\mathbf{X}_{\alpha}\|_F^2 \tag{10}$$

where $\mathbf{H}$ is the dictionary for coding each sample $\mathbf{x}_i$ (i=1,2,…,N) via the self-expression matrix $\boldsymbol{\alpha}$. Compactly, the training data (target gas) being coded is expressed as $\mathbf{X}_{\alpha}=(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)^{\mathrm{T}}$. The coding matrix $\boldsymbol{\alpha}$ in Eq. (10) can be written as

$$\boldsymbol{\alpha}=\mathbf{H}^{\mathrm{T}}\left(\frac{\mathbf{I}}{C}+\mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{X}_{\alpha},\ \ if\ N<\mathrm{L} \tag{11}$$

$$\boldsymbol{\alpha}=\left(\frac{\mathbf{I}}{C}+\mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{X}_{\alpha},\ \ if\ N>\mathrm{L} \tag{12}$$

The procedure for solving $\boldsymbol{\alpha}$ is outlined in Algorithm 1.

- Coding error threshold search

The expression error (coding error) of the target gases can be calculated by

$$e_{tj}=\frac{1}{N}\sum_{i=1}^{N}\left\|\mathbf{x}_{Tt\,j}-\mathbf{H}\boldsymbol{\alpha}_i\right\|,\ \ j=1, 2, \ldots, Tt \tag{13}$$

Similarly, the expression error of the very few interference samples can be calculated by

$$e_{dj}=\frac{1}{N}\sum_{i=1}^{N}\left\|\mathbf{x}_{Td\,j}-\mathbf{H}\boldsymbol{\alpha}_i\right\|,\ \ j=1, 2, \ldots, Td \tag{14}$$

We know that larger coding errors will be obtained by using the learned self-expression matrix $\boldsymbol{\alpha}$ in coding the samples with different patterns from the target data. Therefore, to distinguish the target and interference gases, a coding error threshold T can be used for target/background detection,

$$label=\begin{cases}0\ , & e\le T\\ 1\ , & e>T\end{cases} \tag{15}$$

Note that the *label* "0" denotes target patterns (i.e. target gases), and *label* "1" denotes the background patterns (i.e. interferences). Specifically, the procedure for searching the threshold T is outlined in Algorithm 2.

To this end, an unknown sample can be discriminated as target/background by using the self-expression matrix $\boldsymbol{\alpha}$ and the coding error threshold T. For example, given a sample $\mathbf{y}$ being recognized, we can obtain the average coding error by $e_y=\frac{1}{N}\sum_{i=1}^{N}\|\mathbf{y}-\mathbf{H}\boldsymbol{\alpha}_i\|$. If $e_y<T$, the unknown y is the target. Otherwise, interference is observed. This idea implies that the invariant information of the fixed dataset $\mathbf{X}_{\boldsymbol{\alpha}}$ has been memorized in the learned prediction network, such that it is easy to label the unknown gas as target or background.

IV. Experiment Data

The electronic nose system and experimental setup developed in this paper were described previously in [18]. The

Algorithm1. Self-expression coding

Input: $\mathbf{X}_{\alpha} \in \Re^{D\times N}$, input weights $\mathbf{A} \in \Re^{N\times L}$, hidden biases $\mathbf{B} \in \Re^{D\times L}$

Procedure:

1. **A** and **B** are chosen randomly;
2. calculate **H=XA+B;**
3. **if** $N<L$, compute

$$\boldsymbol{\alpha} = \mathbf{H}^{\mathrm{T}}\left(\frac{\mathbf{I}}{C} + \mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{X}_{\alpha}$$

if $N>L$, compute

$$\boldsymbol{\alpha} = \left(\frac{\mathbf{I}}{C} + \mathbf{H}^{\mathrm{T}}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{X}_{\alpha}$$

Output: **α**, **H**

E-nose system is composed of an array of sensors, consisting of TGS2602, TGS2620, TGS2201A and TGS2201B. In this paper, six kinds of target gases are monitored by this E-nose, including formaldehyde (HCHO), benzene (C_6H_6), toluene (C_7H_8), carbon monoxide (CO), ammonia (NH_3) and nitrogen dioxide (NO2). In experiments, the number of target samples for formaldehyde, benzene, toluene, CO, NH3, NO2 are 188, 72, 66, 58, 60, 38, respectively. Additionally, 48 samples of alcohol (background) were also obtained. Besides, we also collect two extra real-time sequences, including interference sequence without target gas and interference sequence with target gas.

A. Experimental data

- Dataset 1 for training and testing of the self-expression coding model

This dataset aims to learn the self-expression coding coefficients and the error threshold by using the proposed SeELM with six target gases: formaldehyde, benzene, toluene, carbon monoxide, ammonia, nitrogen dioxide. In the self-expression model, the whole target gases dataset was divided into three parts, the data for training **α**, the data for training T and the test data. The details have been illustrated in Table I. The alcohol dataset (i.e. interference) was divided into two parts: the data for training T and the test data. Each of them includes 24 samples.

- Dataset 2 of real-time interference without target gas

Dataset 2 was obtained by exposing electronic nose to the environment only under the odor interferences. That is, no target gases were presented. An observation vector with length of 2400 points for each sensor was obtained in continuous sampling way. This dataset is developed under two odor interferences, i.e. perfume and floral water. In detail, we present the approximation positions for each object as follows. Perfume exists in two approximated regions 95-308 and 709-958; floral water exists in two approximated regions 1429-1765 and regions 2056-2265.

- Dataset 3 of real-time interference with target gas

Dataset 3 was obtained by exposing electronic nose to interference and some concentration of the target gas, simultaneously. Similar to dataset 2, dataset 3 with length of

Algorithm 2. Coding error threshold search

Input: $\mathbf{X}_{Tt} \in \Re^{D\times N_{Tt}}$, $\mathbf{X}_{Td} \in \Re^{D\times N_{Td}}$, $\mathbf{H} \in \Re^{D\times L}$, $\boldsymbol{\alpha} \in \Re^{L\times N}$

Procedure:

1. For the target gases

$$e_{tj} = \frac{1}{N}\sum_{i=1}^{N}\left\|\mathbf{x}_{Tt\,j} - \mathbf{H}\boldsymbol{\alpha}_i\right\|, \quad j=1, 2, \ldots, Tt$$

Then $e_t=[e_{t1}, e_{t2}, \ldots, e_{tTt}]$;

For the interference gases

$$e_{dj} = \frac{1}{N}\sum_{i=1}^{N}\left\|\mathbf{x}_{Td\,j} - \mathbf{H}\boldsymbol{\alpha}_i\right\|, \quad j=1, 2, \ldots, Td$$

Then $e_d=[e_{t1}, e_{t2}, \ldots, e_{tTd},]$;

2. Initialize T=min e_t, Set a small delta;
3. Calculate $p=p_t+p_d$;

3.1 Count the number Nt of $e_{tj}<T$, the classification accuracy of target gases is

$$p_t = \frac{Nt}{Tt}$$

3.2 Count the number Nd of $e_{dj}>T$, then the classification accuracy of interference gases is

$$p_d = \frac{Nd}{Td}$$

4. $T=T$+delta; **if** $T<$max e_{dj}, return to Step 3, **else break**;

Output: T

2400 points for each sensor was also obtained in continuous sampling way. This dataset is developed under reference formaldehyde gas and four odor interferences, respectively. Briefly, formaldehyde exists in three approximated regions 102-250, 719-880 and 1380-1580; ethanol exists in region 260-410; floral water exists in region 881-1064; a hybrid interference of perfume and orange is located in region 1599-1899. Results and discussion

B. Recognition accuracy of target gas by using SeELM

The training result of self-expression extreme learning machine is relevant to the data amount for training **α** and T. In experiments, for observing the impact of training **α** caused by the number of training samples, 10, 15, 20, 25, 30, 35 and 40 samples per class are explored, respectively. The recognition accuracy is shown in Table II, in which sigmoid function and RBF function are used in this self-expression method. From the results, we can see the best performance (i.e. target/background recognition accuracy is 90.91% and 91.67%) when 30 samples per class are used.

Similarly, for observing the impact of searching T caused by the number of training samples, 10, 15, 20, 25, 30, 35 and 40 samples per class are explored, respectively. The recognition accuracy is shown in Table III, in which sigmoid function and RBF function are used in this self-expression method. We can observe that the best detection result for both target/background is 91.7% when 30 samples per class are used. It turns out that when the self-expression coding behaves well enough, this model can show the best performance with fewer training samples.

Through the comparisons shown in Table IV, we can observe that the results based on simple binary classification between targets and some interference are not that good. Besides, binary classification based method should rely on a number of interferences, which is not realistic. Therefore, the

TABLE I

TARGET GAS SAMPLES FOR MODEL LEARNING

Target gas	formaldehyde	benzene	toluene	CO	NO_2	NH_3
Number of Samples	188	72	66	58	38	60
Number of samples for training **α**	75	29	27	23	15	24
Number of samples for training T	75	29	27	23	15	24
Number of test samples	38	14	12	12	8	12

TABLE II

RECOGNITION ACCURACY OF TARGET/BACKGROUND UNDER DIFFERENT NUMBER OF SAMPLES PER CLASS

Number of samples per class		40	35	30	25	20	15	10
sigmoid	Target gas	100	92.93	90.91	80.81	72.73	34.34	15.15
	alcohol	66.67	83.33	91.67	100	100	100	100
	Average accuracy	83.34	88.13	**91.29**	90.4	86.37	67.17	57.57
RBF	Target gas	100	91.92	90.91	76.77	57.58	52.53	5.05
	alcohol	66.67	83.33	91.67	100	10	100	100
	Average accuracy	83.34	87.63	**91.29**	88.39	78.77	76.27	52.53

TABLE III

RECOGNITION ACCURACY OF TARGET/BACKGROUND UNDER DIFFERENT NUMBER OF SAMPLES PER CLASS

Number of samples per class		40	35	30	25	20	15	10
sigmoid	Target gas	81.82	81.82	89.9	90.91	81.82	81.82	80.81
	alcohol	100	100	91.67	91.67	100	100	100
	Average accuracy	90.91	90.91	90.79	**91.29**	90.91	90.91	90.41
RBF	Target gas	81.82	81.82	85.86	80.81	81.82	80.81	80.81
	alcohol	100	100	100	100	100	100	100
	Average accuracy	90.91	90.91	**92.93**	90.41	90.91	90.41	90.41

TABLE IV

RECOGNITION ACCURACY BASED ON BINARY CLASSIFICATION

Number of samples per class		10	20	30
sigmoid	Target gas	89.08	79.3	40.8
	alcohol	84.8	62.5	35.6
	Average accuracy	86.94	70.9	38.2
RBF	Target gas	84.67	77.45	52.8
	alcohol	82.86	62.5	37.6
	Average accuracy	83.77	69.9	45.2

proposed SeELM method is significant by using one kind of reference interference for searching the threshold *T*. Another important advantage is that in learning the coding coefficient α, only targets data is necessary.

C. Real-time interference recognition with/ without target gas

As expressed in the part of experimental data, dataset 2 and 3 are collected and analyzed in real time. There are four sensors (TGS2602, TGS2620, TGS2201A/B) in total, all the sensors have similar response to interferences. With SeELM method, Fig. 3 is the background detection result on dataset 2 without target gas. From the result, the response curve of each sensor in dataset 2 has been presented, where the rectangular windows are represented as detected interference regions by using the SeELM method. It is obvious that four actual regions of interferences have been correctly recognized. Similarly, Fig. 4 illustrates the result on dataset 3 with target gas. From the figure, four actual regions of interferences have also been correctly recognized (i.e. the Rectangular windows). Notably, the target gases are not wrongly recognized.

D. Discussion

In the proposed SeELM model, a self-expression coding based on target data self and the coding error threshold based on a very few interference samples (i.e. reference) are studied. The key idea behind the proposed method is to construct an internal relationship based on targets, such that the non-targets (i.e. interference) can be detected if the relationship is violated. The rationality is that it is impossible to collect all kinds of interference in real application scenarios. That is, the discrimination between targets and backgrounds may not be recognized to be a binary classification problem simply. From the real-time interference recognition experiment, the interferences such as perfume, floral water, and mixture of perfume and orange, the target and interferences can be discriminated accurately.

V. CONCLUSION

In this paper, an olfactory target/background detection via self-expression Extreme Learning Machine (SeELM) method is proposed to discriminate target and unknown interferences in e-nose. This method consists of two parts: learn the self-expression coding coefficient matrix **α** and search the coding error threshold T. The advantage of this proposed method is

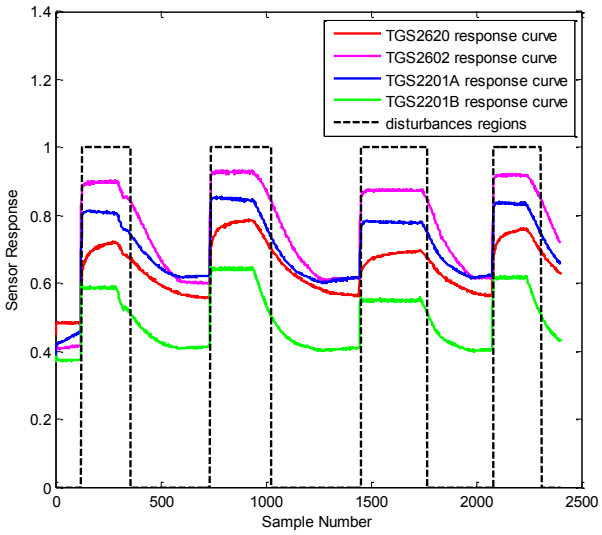

Fig. 3. The disturbance recognition of Dataset 2.

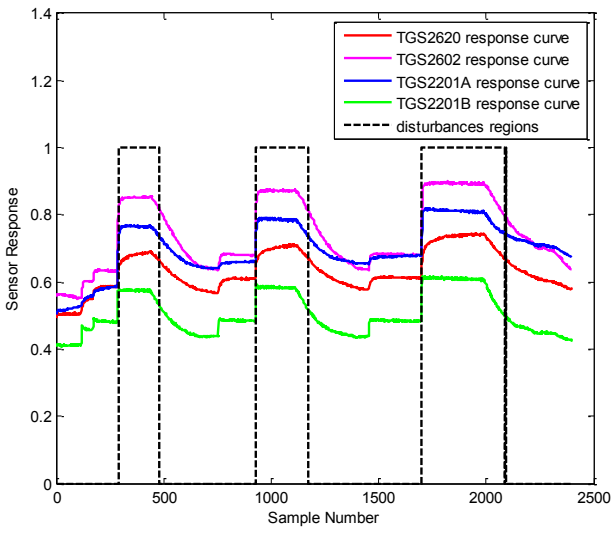

Fig. 4. The disturbance recognition of Dataset 3.

that in background detection, the target gases are considered as invariant information for coding. Only a very few background samples are used for determining the error threshold T. By comparing with ELM to binary classification in experiments, the proposed SeELM method shows better performance in discriminating the target and interferences in E-nose in real application scenarios.

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