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Simultaneous estimation of classes and concentrations of odors by an electronic nose using combinative and modular multilayer perceptrons

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Abstract

It is relatively suitable to take a simultaneous estimation problem of multiple odor classes and concentrations for multiple function approximation ones. To solve such problems, this paper decomposes a many-to-many approximation task into multiple single-output approximation ones, and correspondingly presents a kind of combinative and modular multilayer perceptrons (MLPs). Every module is made up of multiple one-to-one MLPs and one many-to-one MLP, and one MLP is regarded as an expert. One module consists of several such experts and implements a many-for-one approximation task. By means of enlarging the input components to the range of [0,6.0] and making the sigmoid activation functions $s(x) = 3(1 + \exp(-x/3))^{-1}$, the learning processes of MLPs are sped up. In an electronic nose, one MLP module is on behalf of a kind of odor, and determines how similar an undecided odor is to a known odor, namely its strength. The most similar module gives the class label and strength value of the odor. The experiment for simultaneously estimating the classes and concentrations of four kinds of fragrant materials, namely ethanol, ethyl acetate, ethyl caproate and ethyl lactate, 21 different concentrations in all, shows that the proposed combinative and modular approximation method is quite effective.

Keywords: Simultaneous estimation; Odor class and concentration; Electronic nose; Combinative and modular mulitlayer perceptrons

1. Introduction

It is said that an expert is able to recognize over 4000 kinds of odors, but is a little poor to exactly estimate odor strengths [1,2]. Compared with that, the capabilities of electronic noses are not worth mentioning. Up to now, electronic noses are only used to recognize limited kinds of odors, or to estimate the concentrations of a certain single-component odor, but few reported about simultaneously determining multiple odor classes and concentrations in the literature [1–8], which is far from man's expectation. It is reasonable to make an electronic nose undertake the task of simultaneously estimating odor classes and concentrations. The main obstacles are that the sensitivity and selectivity of gas sensors are not high enough, and that the classification and approximation abilities of data processing methods are not ideal. This paper focuses on the latter.

In the early stage of electronic noses, some data processing methods in common use were multivariate regression [3], partial least square (PLS) [1,2], cluster analysis (CA) [4], principle component analysis (PCA) [4,5], discriminant function analysis (DFA) [1,2], template matching [1,2], etc. Today, artificial neural networks (ANNs) [1,2,6–8], support vector machine (SVM) [9], independent component analysis (ICA) [10], and the others, are often used. Without a doubt, ANNs, particularly multilayer perceptrons (MLPs), are the most widely used.

From a long-term point of view, electronic noses will be required to carry out the tasks of simultaneously estimating

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odor classes and strengthens. The problems of this kind can be really treated as many-to-many function approximation problems. Unfortunately, up to now there are few reports about successfully solving high dimensional and multi-output approximation problems in literature [11]. Many-to-many MLPs, for example, cannot do so. One of the main difficulties is that a continuous function always provides an output for an arbitrary input. In principle, an MLP is able to approximate any complicated function with any accuracy under condition that it has sufficient hidden nodes and long learning time. In order to implement the tasks of simultaneously estimating odor classes and concentrations with MLPs, the following two approaches can be employed. (A) Transform a many-to-many approximation problem into multiple classification problems. The shortcoming to do like that is that too many classifiers are needed. It is especially impractical when a great quantity of strengths in a kind of odor needs to be estimated. (B) Take one multi-input multi-output MLP simultaneously, or many multi-input single-output MLPs, namely MLP modules, to fit the strength curves of multiple odors one after another. In fact, the effects are not ideal. The drawbacks of the former are that a multi-output MLP often is of complicated structure, long learning time, and low approximation accuracy. And the main defect of the latter is that MLP modules may give self-contradictory results for one multivariate response of the sensor array, because MLPs do not know to say "No". For example, what can we do if one single-output MLP says that an odor is 100 ppm (parts per million) of methanol, and another says it is 1000 ppm of ethanol?

The concept of classifier combinations or ensembles was presented in 1990s [12–15], because the capability of a single classifier is limited after all. For solving the large-scale learning problems, task decompositions and modular classifiers [16,17] are proposed. If each module is regarded as an expect, for a given pattern, we can determine its class label according to majority vote, weighted vote, sum, product, Borda count, maximum, minimum, and the other combinative rules [12–15]. With the help of combinative and modular idea, this paper decomposes a complex multi-output approximation task into multiple simple single-output approximation tasks, and correspondingly, proposes a kind of combinative and modular single-hidden-layer perceptrons for simultaneously estimating multiple odor classes and concentrations.

This paper is organized as follows. In Section 2, we briefly introduce an experimental system. The task decomposition method, the structures of combinative and modular single-hidden-layer perceptrons as well as the combination strategies, are formulated in Section 3. In Section 4, the presented method is applied to simultaneous estimation of classes and strengths for such fragrant materials as ethanol, ethyl acetate, ethyl caproate and ethyl lactate, 21 kinds of concentrations altogether. Finally, Section 5 comes to our conclusions.

2. Experimental

Fig. 1 is the schematic diagram of a practical electronic nose, which is mainly made up of a test box, a thermostatic cup and a personal computer (PC). The test box consists of the gas sensor array, the three-channel high-precision direct constant power sources (5 ± 0.01 V for the sensor heaters, 10 ± 0.001 V for the sensor working circuits, 12 ± 0.1 V for the others), the gas sampling and flow control units, waste gas exhauster, thermostatic unit, etc. The sensor array is composed of 16 TGS sensors, namely TGS800, TGS812,

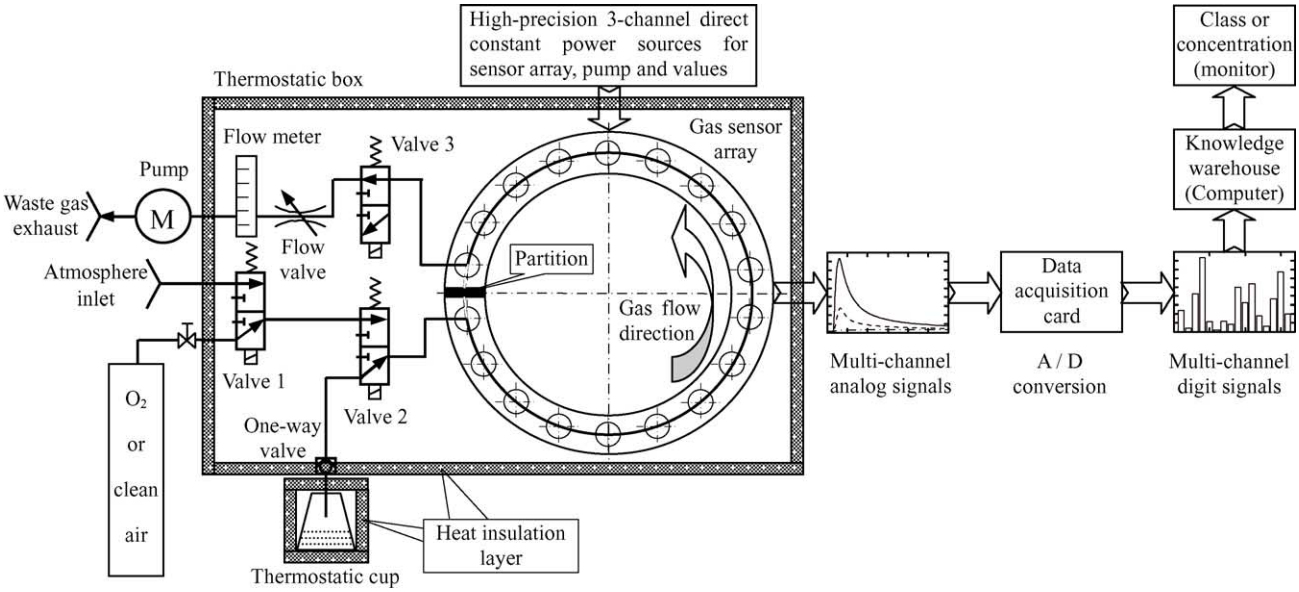

Fig. 1. Schematic diagram of a practical electronic nose.

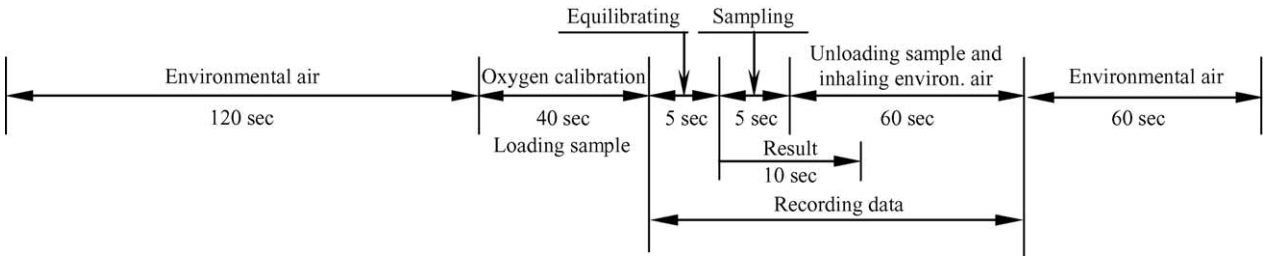

Fig. 2. Flow chart of a sampling procedure.

TGS813, TGS816, TGS821, TGS822, TGS823, TGS824, TGS825, TGS826, TGS830, TGS831, TGS832, TGS842, TGS880, TGS883T, all provided by Figaro Engineering Inc., Japan. The array is set up within a 200 ml circular chamber. The 16-bit high-precision data acquisition system card is inserted in the expansion slot of the motherboard of the PC [18].

In order to ensure that every measurement is under the same condition, the following steps are adopted.

(A) Purge the gas array by O_2 or dry air in the speed of 60 mm/s for about 40 s before sampling.
(B) Pour a 30 ml liquid sample in a 250 ml flask and keep it within the thermostatic cup for 30–60 min. The cup is wrapped with heat insulation materials and heated by a semiconductor heater. The thermostatic accuracy is $55 \pm 0.1\,^{\circ}C$.
(C) Keep the gas array, the inlet pipes and three electromagnetic values in a thermostatic box. The test box is wrapped with heat insulation materials and heated by a resistance heater. The thermostatic accuracy is $55 \pm 0.1\,^{\circ}C$.

Fig. 2 gives an all-round sampling procedure, which takes 290 s. All the procedure is automatically controlled by the computer. What an operator needs to do is only to load or unload an awaiting sample according to the computer's order. The detailed operating principle and procedure are given in [18]. The maximum value from the response curve of a sensor is taken as a feature component. Because the array is made up of 16 sensors, the input dimensionality is 16. Such a 16-dimensional pattern is then transformed into the category, strength, concentration of odors or the results in agreement with human perceptions by means of appropriate classification and non-linear mapping methods.

3. Combinative and modular multilayer perceptrons

3.1. Combinative and modular MLPs

In order to simultaneously determine the classes and concentrations of odors, it is quite ideal to employ the divide-and-conquer and combinative strategies. A panel or module is on behalf of a kind of odor and made up of several experts, and correspondingly the number of panels is equal to the number of kinds of odors. It is natural that the most consistent panel ought to be taken to determine the class and concentration of a sample. For the purpose of clarity, let us suppose that there are three modules and three experts in every panel. For sample $\boldsymbol{x}$, the predicted results of the three panels are shown in Table 1. According to the table, the relative standard deviation (RSD) of *Module* 1 is the smallest, or the three experts in the first panel have the most identical views, so one can make such a decision that $\boldsymbol{x}$ belongs to the odor represented by *Module* 1 and its concentration is 1000 ppm.

The relationship between strengths or concentrations of an odor with only a kind of changing component and responses of the sensor array is a hyper-dimensional curve, and the points on the curve are in the name of odor strengths. The change of responses of the sensor array means the change of odor strengths. A lot of experiments show that the relationship is logarithmic [1,2]. Because the changes of response curves are not fiercely undulate [1–8], it is suitable to use single-hidden-layer perceptrons to implement such function approximation tasks. In other words, an MLP is able to play the role of an expert.

As stated above, multi-output MLPs are unable to effectively cope with multi-output approximation problems. Therefore, we have to resort to multiple single-output MLPs. Does a many-to-one MLP trained with the data set from odor j have a real output for a sample $\boldsymbol{x}$ from odor k? Yes! And

Table 1
Comparison of predicted concentrations of sample x by three 3-member panels (ppm)

Predicted result	Module 1			Module 2			Module 3		
	Expert 1	Expert 2	Expert 3	Expert 1	Expert 2	Expert 3	Expert 1	Expert 2	Expert 3
Predicted concentration	1000	1050	950	1500	2500	500	500	2000	500
Average concentration		1000			1500			1000	
RSD (%)		4.08			54.43			70.71	

the reverse is true. For instance, three many-to-one MLPs, called MLP1, MLP2 and MLP3, are used to predict the class and concentration of a sample $\boldsymbol{x}$. MLP1 maybe takes $\boldsymbol{x}$ for a 1000 ppm ethanol, MLP2 for a 750 ppm methanol, and MLP3 for a 1500 ppm acetone. The embarrassing situation shows that the class and concentration of $\boldsymbol{x}$ can be not certainly decided by only many-to-one MLPs, which looks just like the lack of selectivity of a single sensor. So we turn to one-to-one MLPs for help.

Our basic idea is as follows. A module consists of one many-to-one MLP and multiple one-to-one MLPs, and stands for a kind of odor. And n modules are behalf of n kinds of odors. In one module, the many-to-one MLP is used to imitate the total behaviors of the sensor array, and a one-to-one MLP the behaviors of a single sensor. If a sample $\boldsymbol{x}$ is indeed from odor j, the outputs of the MLPs in module j, regardless of many-to-one and one-to-one, will simultaneously be close in on a certain concentration point, otherwise their outputs will be quite divergent. In this way, the class label and concentration of a sample are determined by multiple MLP modules according to a certain kind of combinative rule, not by only one MLP. In other words, the module with the highest similarity determines the class label of an undecided sample, and the average outputs of all MLPs in the module determine its concentration or strength.

Suppose an array is made up of m gas sensors, $m+1$ MLPs, perceptrons 0 through m, are needed to constitute a module j, as shown in Fig. 3. Let $\boldsymbol{x}_p = (\boldsymbol{x}_{p1}, \boldsymbol{x}_{p2}, \ldots, \boldsymbol{x}_{pi}, \ldots, \boldsymbol{x}_{pm})^T \in R^m$ be the preprocessed response of a sensor array for sample p, which is taken as the real input of perceptron 0, and x_{pi} is the response of the ith sensor, which is taken as the real input of perceptron i ($i = 1, 2, \ldots, m$). The real output of module j for $\boldsymbol{x}_p$ from a known odor ω_j is the similar degree ζ_{pj}, given according to the sum and average combinative rules. Fig. 4 shows that the class label and strength of $\boldsymbol{x}_p$ are determined by the most similar module j according to the minimum combinative rule. Concretely speaking, perceptron 0 in module j fits the relationship between the response $\boldsymbol{x}_p$ of a sensor array and the concentrations C_{pj} of odor ω_j, and perceptron i ($i = 1, 2, \ldots, m$) fits the relationship between the response x_{pi} of sensor i and the concentrations C_{pj} of odor j, as shown in Fig. 5. In the learning stages of module j, the target outputs $d_{pj} = f(C_{pj})$ of perceptrons 0 through m are the same, namely the logarithmic concentration values of odor ω_j. At the moment, only the samples that belong to ω_j take part in learning. In the test stages, for a certain sample $\boldsymbol{x}_p$, the minimum ζ_{pj} given by module j shows that $\boldsymbol{x}_p$ belongs to odor j and its concentration is the function $C_{pj} = f^{-1}(\bar{y}_{pj})$ of the average output of perceptrons 0 through m.

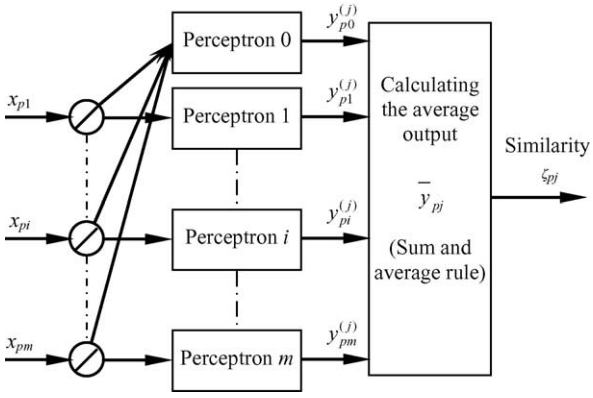

Fig. 3. Block diagram of perceptron module j.

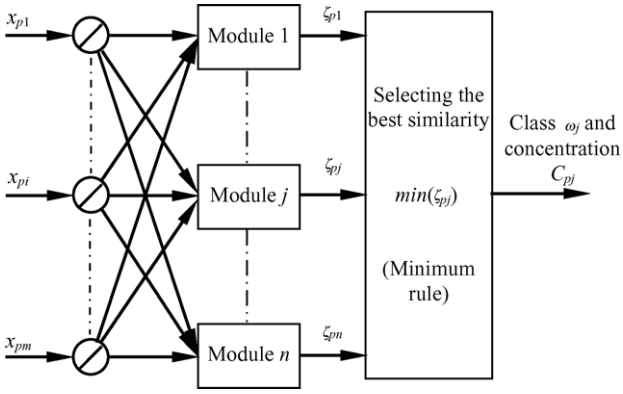

Fig. 4. Block diagram of combinative modular perceptrons.

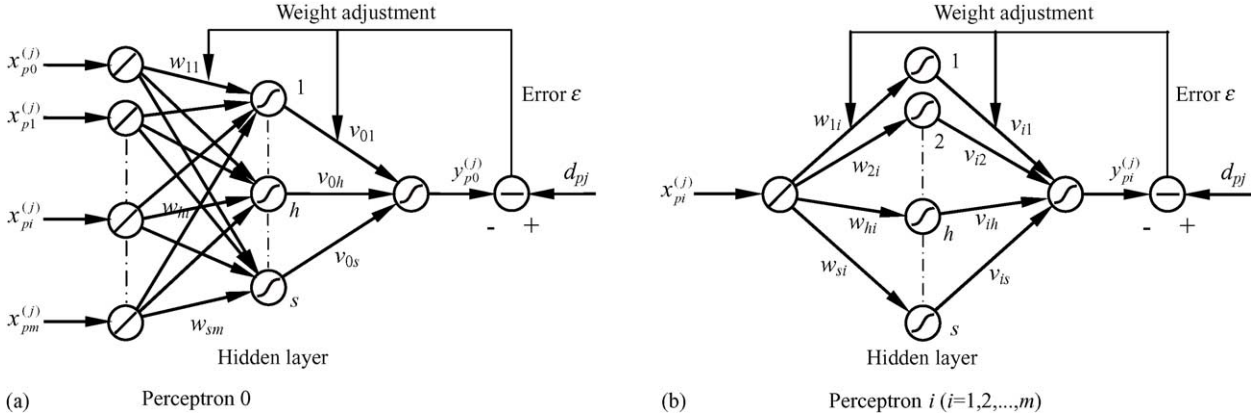

Fig. 5. Structure of perceptron module j in the learning stage.

Because an MLP always gives an output for any input, no matter how absurd it may be, this paper presents the following combinative and modular methods to simultaneously determine odor classes and concentrations.

(1) Decompose a multi-input multi-output approximation task f: $\boldsymbol{X} \rightarrow \boldsymbol{D}$ into multiple multi-input single-output approximation sub-tasks f: $\boldsymbol{X}^{(j)} \rightarrow \boldsymbol{d}_j$. Here $\boldsymbol{X} \in \boldsymbol{R}^{N\times m}$, $\boldsymbol{X}^{(j)} \in R^{N_j\times m}$, $\boldsymbol{D} \in R^{N\times n}$ and $\boldsymbol{d}_j \in R^{N_j\times 1}$, N is the total number of learning samples. Each subset is only composed of N_j samples that belong to odor ω_j, and learned by a many-to-one MLP.
(2) Decompose a multi-input single-output fitting task f: $\boldsymbol{X}^{(j)} \rightarrow \boldsymbol{d}_j$ into multiple single-input single-output fitting tasks f: $\boldsymbol{x}^{(j)} \rightarrow d_j$. Here $\boldsymbol{x}^{(j)} \in R^{N_j\times 1}$. Each one-to-one MLP realizes a certain fitting task.
(3) Use an m-to-1 MLP, called perceptron 0 as shown in Fig. 5(a), to realize f: $\boldsymbol{X}^{(j)} \rightarrow \boldsymbol{d}_j$, and m one-to-one MLPs, called perceptron i ($i = 1, 2, \ldots, m$) as shown in Fig. 5(b), to realize f: $\boldsymbol{x}^{(j)} \rightarrow d_j$. In one module, the target outputs of all the MLPs are the same, the preprocessed continuous values in a certain interval.
(4) Predetermine the concentration of an odor by all members in each module according to the average combinative rule:

$$\bar{y}_{pj} = \frac{1}{m+1}\sum_{i=0}^{m} y_{pi}^{(j)} \tag{1}$$

The similarity to odor ω_j is given by

$$\zeta_{pj} = \frac{1}{\bar{y}_{pj}}\sqrt{\frac{1}{m+1}\sum_{i=0}^{m}\left(y_{pi}^{(j)} - \bar{y}_{pj}\right)^2} \times 100\% \tag{2}$$

In fact, ζ_{pj} is similar to the R.S.D. and $\bar{y}_{pj}$ to the mean value.
(5) Determine the final class label ω_j and concentration C_{pj} of an undecided odor $\boldsymbol{x}_p$ by all the modules with the help of the minimum combinative rule:

$$x_p \in \omega_j \quad \text{and} \quad C_{pj} = f^{-1}(\bar{y}_{pj})$$
$$\text{if } \zeta_{pj} = \min_{1\le k\le n}(\zeta_{pk}) \quad j = 1, 2, \ldots, n \tag{3}$$

3.2. Fast learning of MLPs

The so-called error back-propagation (BP) algorithm is, in fact, that the weight adjustment $\Delta w(t)$ is equal to its negative error gradient $-\partial E(\tau)/\partial w(\tau)$ multiplied by the step factor η. Here $E(\tau)$ is the root-mean-square (RMS) error of a network at iteration epoch τ. On the premise that the network is not caught into local points or does not oscillate, a larger $-\partial E(\tau)/\partial w(\tau)$ is favorable for its convergent improvement [18–20].

The types of activation functions have important influences on MLPs' learning speed, classification and approximation accuracy. The relationship between output $s_0(x)$ and input x for the standard sigmoid activation function is

$$s_0(x) = (1 + \exp(-x))^{-1} \tag{4}$$

Its general form [20] may be written as

$$s(x) = \gamma(1 + \exp(-\beta x))^{-1} \tag{5}$$

where γ is the strength parameter, which limits $s(x)$ in the range $(0, \gamma)$, and β is the gain factor, which controls the steep or slope degrees of sigmoid functions. Let $\gamma = 3.0$ and $\beta = 1/3.0$, a real activation function is $s_1(x) = 3(1 + \exp(-x/3))^{-1}$. The ratio ρ between the first-order partial derivatives of $s_1(x)$ and $s_0(x)$ is

$$\rho = \frac{\partial s_1/\partial x}{\partial s_0/\partial x} = \frac{\partial(3(1 + \exp(-x/3))^{-1}/\partial x}{\partial(1 + \exp(-x))^{-1}/\partial x} \tag{6}$$

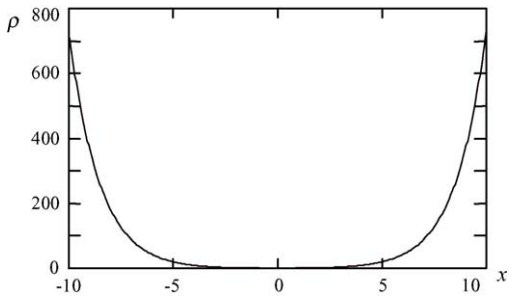

Fig. 6. Ratio $\rho = [3\partial(1 + \exp(-x/3))^{-1}/\partial x]/[\partial(1 + \exp(-x))^{-1}/\partial x]$.

Fig. 6 gives the change of ρ. $\rho = 732.6$ when $x = \pm 10.0$. According to Fig. 6, we can predict that a single-hidden-layer perceptron with activation functions $s_1(x) = 3(1 + \exp(-x/3))^{-1}$ has faster convergence than the one with standard sigmoid activation functions $s_0(x) = (1 + \exp(-x))^{-1}$ does. Therefore, in our experiment, the activation functions are $s_1(x) = 3(1 + \exp(-x/3))^{-1}$, the input variables are transformed in proportion to the range of [0.0, 6.0], and the target outputs to the range of [0.0, 3.0] [21].

4. Experimental results

Four kinds of fragrant materials are ethanol, ethyl acetate, ethyl caproate and ethyl lactate, and each of them is diluted with distilled water into 4–6 kinds of concentrations, as shown in Table 2.

The measurement method is just the same as stated in Section 2. Fifty samples for each concentration are collected, and 40 of them are used as a part of the training set, and the others as a part of the test set. Therefore there are $40 \times 21 = 840$ samples in the training set, and $10 \times 21 = 210$ patterns in the test set. Fig. 7 shows the difference of responses between distilled water and 1.0 ppm ethyl caproate in liquid. Fig. 8 is the principle component analysis result for all the original data set. The reproducibility of data is comparatively good. It is

Table 2
Concentrations of fragrant materials in water (ppm)

Ethanol (distilled water)	Ethyl acetate (distilled water)	Ethyl caproate (distilled water)	Ethyl lactate (distilled water)
		1	
100	10	5	100
2500	100	10	2500
5000	1000	100	5000
7500		1000	7500
10000	10000	10000	10000

obvious that the fitted curves are different from each other. The linear regression method fails to solve the problems effectively, and the multivariate polynomial regression method will give some unreasonable results.

It is not feasible to directly change the concentration values into the range of [0.0, 3.0], because that will further lead to the reduction of target distinction between low-concentration samples. Therefore, we suppose the concentration of distilled water is 1.0×10^{-7}, namely 0.1 ppm, and apply the common logarithmic transformation to the real concentrations. Let the real concentration be C_{pj} for sample $\boldsymbol{x}_p$, the target of an MLP in module j is given by:

$$d_{pj} = (1 + \log\ C_{pj})\frac{3.0}{5.0} \tag{7}$$

In consideration of the cut-off and saturated states of sigmoid activation functions, the range of target outputs is further cut down, namely $d_{pj} = 0.15$ corresponds to the distilled water ($C_{pj} = 0.1$ ppm) and $d_{pj} = 2.85$ to $C_{pj} = 10{,}000$ ppm. Therefore, (7) is revised to be:

$$d_{pj} = (1 + \log\ C_{pj})\frac{2.7}{5.0} + 0.15 \tag{8}$$

In addition, we must take the following two situations into accounts:

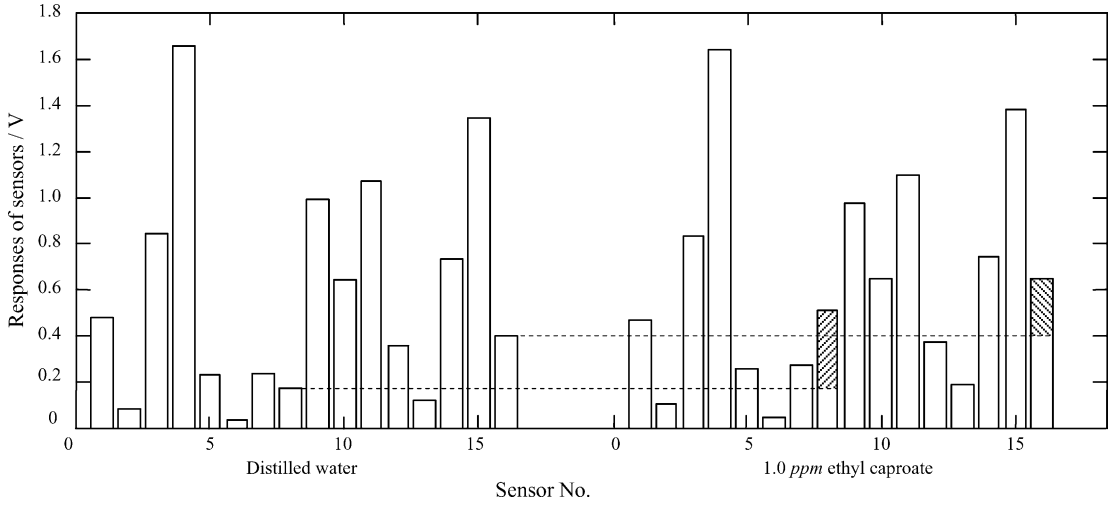

Fig. 7. Responses of sensors for distilled water and 1.0 ppm ethyl caproate.

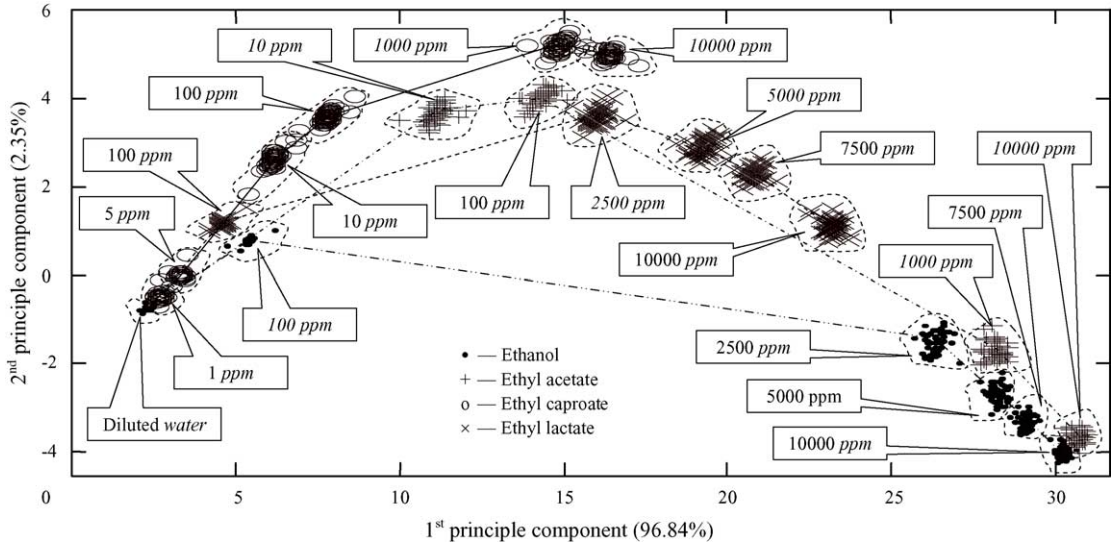

Fig. 8. Principle component analysis for the original data set.

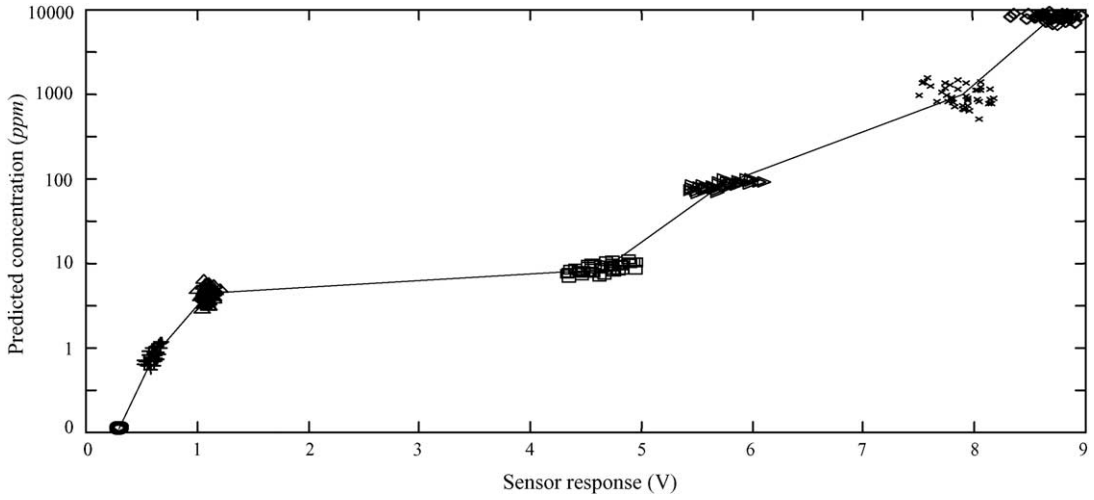

Fig. 9. Concentration estimation of the MLP corresponding to Sensor TGS826 for ethyl caproate in the training set.

(A) If the predicted concentration of an odor $\boldsymbol{x}_p$ by module j is over 10,000 ppm, the odor is considered not to belong to class ω_j. And similarly, an MLP steps down from decision if its real output is over 2.85.
(B) If the lower limit of sensitivity of a sensor for a certain odor is C_θ, the corresponding one-to-one MLP withdraws from decision when the predicted concentration is below C_θ.

There are four modules in the combinative function approximation machine, and 16 one-to-one MLPs and plus one 16-to-1 MLP in every module, because there are 16 sensors in the array and four kinds of odors.

All the perceptrons are single-hidden-layered and with sigmoid activation functions $s_1(x) = 3(1 + \exp(-x/3))^{-1}$. Let the structures of all one-to-one MLPs be 1-4-1, the learning factor $\eta = 0.25$, and the momentum parameter $\alpha = 0.075$, each MLP learns 2000 epochs and takes 1.904, 1.688, 1.904, 2.176 s in different modules respectively (PIV860 CPU time, the same below). Each 16-5-1 MLP learns 25,000 epochs and takes 66.32 s. Fig. 9 shows the estimation results of the one-to-one MLP corresponding to TGS826 for ethyl caproate. Fig. 10 gives the final predicted results for ethyl caproate. Obviously, the performance of the proposed method is satisfactory.

The simultaneous estimation correct rate of odor classes and concentrations is 99.05% using the proposed combinative and modular MLPs, but only 62.38% using four such 16-5-1 MLPs, all for the test set. A 16-8-4 MLP is not able to converge to the required accuracy even after 50,000 iterating steps. Table 3 is the final estimation results of different methods. Obviously, the presented method is quite effective for simultaneously estimating many odor classes and concentrations. It has been made clear in Section 3.1 that we cannot depend upon only a kind of single-output MLPs to determine the class label and concentration of a sample. Therefore the predicted results of a certain 16-5-1 MLP in Table 3 only mean to be a little closer to the memorized concentration

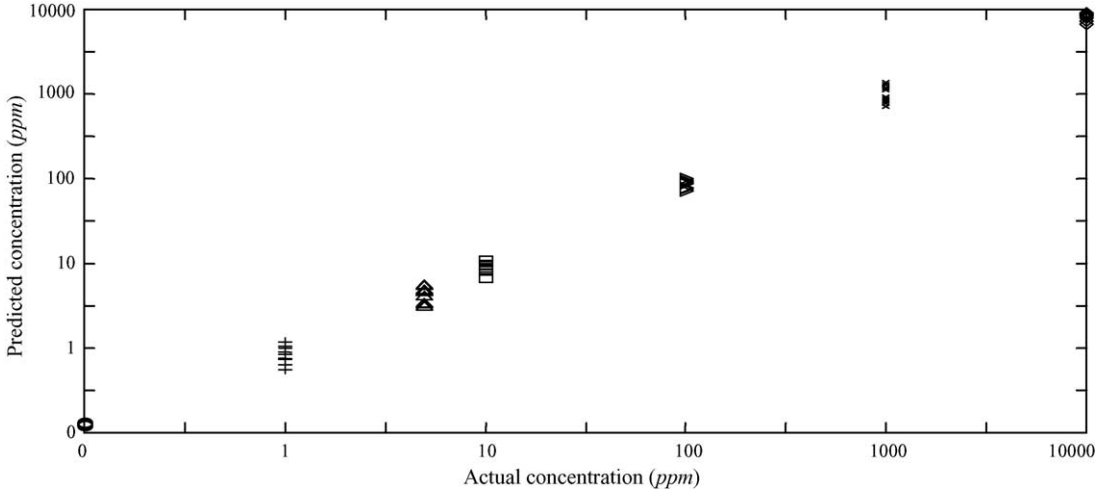

Fig. 10. Predicted results for ethyl caproate in the test set by the combinative modular perceptrons.

Table 3
Comparisons of predicted results between different methods

Activation function	Method	RMS error range for the training set	Learning epochs	Accuracy for the training set (%)	Accuracy for the test set (%)
$S_0(x) = (1 + \exp(-x))^{-1}$	16-8-4 MLP	No convergence	50000	No convergence	–
	16-5-1 MLPs	0.207–0.259	4×50000	85.71	53.33
	Combinative MLPs	0.031–0.259	$4 \times 25000 + 4 \times 16 \times 10000$	91.26	85.52
$S_1(x) = 3(1 + \exp(-x/3))^{-1}$	16-8-4 MLP	No convergence	50000	No convergence	–
	16-5-1 MLPs	0.011–0.024	4×25000	100	62.38
	Our method	0.008–0.024	$4 \times 25000 + 4 \times 16 \times 2000$	100	99.05

points than those of the other 16-5-1 MLPs do. In other words, the predicated results of a single kind of many-to-one MLPs are not so convincing as those of combinative and modular MLPs. If the input and target components are scaled in the range of [0.0, 1.0], and the structures and learning parameters of networks keep unchanged, the predicting accuracy of the combinative and modular MLPs is only 91.26% for the training set and 85.52% for the test set. The result shows that the presented combinative and modular MLPs with the improved activation functions $s_1(x) = 3(1 + \exp(-x/3))^{-1}$ have fast convergence and good non-linear approximation performances. In order to accurately predict an odor whose class is known but whose concentration is not included in the training set, the memorized concentration interval ought not to be too large.

Of course, the above problem can still be solved in the viewpoint of classification. The advantage of the proposed method will be further incarnated when there exist more concentrations, say over 16 grades in our experiment, for a certain kind of odor.

5. Conclusions

This paper decomposes a many-to-many approximation task into multiple one-to-one approximation tasks and a many-to-one approximation task, and takes multiple MLP modules to implement such approximation tasks. We employ multiple one-to-one MLPs and one multi-to-one MLP as the basic components of one module, and use the average and minimum combinative rules to determine the final classes and strengths of odors. The convergence of MLPs is sped up with the help of changing the standard sigmoid activation functions, input and output variables to some suitable extent. An example for estimating four kinds of fragrant materials in 21 grades of concentrations shows that the proposed method is quite effective for simultaneously determining the class labels and strengths of multiple odors, so improves the recognition performances of electronic noses. With the above combinative and modular approximation method, an electronic nose can well cope with the simultaneous class and concentration estimation problems of multiple odors on condition that each of them is either single-component or complicated but with only a kind of changeable component.

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