Electronic Nose for the Vinegar Quality Evaluation by an Incremental RBF Network

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***Abstract*—Pattern classification was an important part of the RBF neural network application. When the electronic nose is concerned, in many cases it is difficult to obtain the entire representative sample; it requires frequent updating the sample libraries and re-training the electronic nose. In addition，the gas detected from the online environment is not always the known gas in the training samples. This paper proposes a RBF neural network model in order to identify gas. This model uses K-means clustering algorithm and has incremental learning ability, the network output node can be adjustable online to ensure the network with high generalization ability and some incremental learning ability. Finally, the classification system based on this algorithm is used to identify the vinegar online. The results show that this algorithm has faster convergence speed, good performance of the network's online classifieds.**

***Index Terms*—radial basis function; K-means clustering; incremental learning; electronic nose**

I. INTRODUCTION

Electronic nose is one of the applications in bionics; it used the gas sensor array to make a specific identification and analysis for gas molecules. It has been widely used in many fields, including food surveillance [1], medical test [2], environmental monitoring [3], explosives detection [4]. Currently, according to the research related to electronic nose, the accuracy of identification algorithm for a single gas which has been known has become to a considerable degree of (93 %to 95%), but for the test case of the gas is unknown gas are not yet effective algorithms. We intend to make unknown gas as an unclassified gas (the gas is not belong to any part of a training database), and design a clustering algorithm to identify it in order to improve the gas recognition accuracy. Compare to the traditional pattern recognition method, neural network classifiers have better performance in the case of the characteristics of the identified gases is unknown, and also has better generalization ability.

For a classifier, its performance largely depends on the training samples. The more representative training sample has the better performance of the classifier. But in many cases, it is difficult to obtain a representative sample. So it often need to use incremental learning techniques which means after use the trained samples to complete the study, obtained the new sample to training neural network classifiers in incremental learning approach. Actually neural network classifier has been used in a wide range of area. Therefore, the research about neural network algorithm which is based on the incremental learning is necessary. At present there are many neural network algorithms based on incremental learning [5-9]. Compare to the BP neural network, RBF is more suitable for incremental learning. The activation function of BP neural network is the S-function, which is a function of a global response, while the activation function of RBF neural network is Gaussian, the response is local. So that the weight coefficients and the hidden layer nodes of the RBF neural only link with parts of the region in the sample space. So the incremental learning of the RBF network only need to adjust the weight coefficients and the hidden layer nodes corresponding to the input sample space can achieve incremental learning RBF network. which means that the RBF network is suitable for incremental learning [10,11] Based on this consideration, this paper presents a incremental learning algorithm for RBF network based on K-means clustering algorithm and the number of the hidden layer nodes is adjustable. It has the following characteristics: a. the training samples first used the K-means cluster and then adjusted to make between different types of the subsets has no overlap. So in the incremental learning process of the new samples, it can avoid a lot of repetitive training to improve the efficiency of training; b. After the K-means clustering, the training samples become to a subset with the local clustering, RBF neural network only distribute hidden layer nodes to the center of subset, not generate hidden

doi:10.4304/jcp.7.9.2276-2282

layer nodes for every sample. So the size of the network can be controlled in some extent.

II. RBF NETWORK AND K-MEANS CLUSTERING ALGORITHM

A. RBF

Broom head and Lowe in 1988 proposed the RBF network, and then have been someone makes the RBF network extended and improved [12]. RBF network is usually a three-tier feed-forward network, the first layer is input layer, input the Eigen values of the input feature space mode, input nodes directly connect with the each neuron in the second layer; the second layer is the hidden layer in RBF network neuron, the number of hidden neurons can change with the complexity of the problem; the third layer is output layer [13].

B. K-means

Clustering method can generally be divided into partition-based methods [14], based on a layered approach [15], density-based method [16] and grid-based method [17]. Among them, the Partition-based clustering algorithm in pattern recognition are the most common type of clustering algorithm, which Mac Queen proposed a real-time unsupervised clustering algorithm K-means most widely used [18,19].

The steps of the k-means clustering algorithm [20]

(1) From n data objects arbitrary choice k objects as initial cluster centers;

(2)According to each cluster object means (central object), calculated the distance between the each object and the object of these centers; and according to the minimum distance re-classification of the corresponding object, each object is (re) assigned to the closest class.

(3) re-calculated for each (change) clustering means (central object)

(4) Repeat (2) and (3) until no further change in each cluster, k-means algorithm attempts to find the k-clustering which make the value of the squared error function to be minimum; it is defined as follows:

$$E = \sum_{i=1}^{k} \sum_{p \in ci} \left| p - mi \right|^2 \tag{2}$$

E is the sum of squared error of all of the objects in the database, p is the point in space ,which express a given data object, mi is the average of cluster Ci (p and mi are multi-dimensional).This criterion make the results clusters generated compact and separate as much as possible.

C. Improved K-means Clustering Algorithm

First we can use the improved hierarchical clustering method get the k division from the sample data. By calculating the means in each division object from the k classified sample data, you can get the k initial cluster centers.

The basic idea of the improved k-means clustering algorithm is as follows:

(1) Use the sample data makes analysis by hierarchical clustering method, get k division;

(2) Calculate the k-hierarchical clustering analysis divided each division means, and the clustering algorithm as k-means initial cluster centers;

(3) According to means in each cluster object (central object), calculated the distance between each object and these center object; and according to the minimum distance to divide the corresponding object;

(4) Re-calculated means (central object) in each (change) clustering

(5) Repeat (3) and (4) until there is no further change in the class of each object

First to sample data use improved hierarchical clustering method can effectively ruled out the random factors in clustering center from the random initial in k-means clustering algorithm. Make this algorithm get stable clustering results. And because the initial clustering center has very good represents the cluster, make the iterative times in this algorithm decreased significantly and improve the running speed of the algorithm; the initial way also can make use of the structure information in the hierarchical clustering method. Make clustering quality improved significantly relative to the average quality of random initially.

III. IMPROVED RBF NEURAL NETWORK MODEL

In the applications of pattern recognition, in many cases one-time get all of the data to train neural network is not only time-consuming, arduous, and sometimes is not realistic; in addition, when the sample size is large, it is often not feasible to use all of the samples to make the training because of the limitation of the system memory, then you need neural network to make incremental learning. Incremental learning neural network can learn new sample information, while maintaining the original sample of knowledge, the learning process do not need the original sample. Incremental learning neural network can be achieved by adjusting the parameters; you can also adjust the network topology to achieve. As the radial basis function network (RBF) with a hidden layer restructuring potential, attracting researchers study its incremental learning ability [21, 23].

The RBF network model used in this paper use the K-means algorithm to make sure the cluster center and the right .Make use of the incremental learning algorithm to achieve the output of the network nodes online adjustable. The structure of network model is shown in Figure 1.

For incremental learning can be divided into two steps the learning process and the recognition process, the specific algorithm is described as follows:

A. The Learning Process

1) Unsupervised learning algorithm

Make use of the improved K-means algorithm to achieve the dynamic adjustment of hidden nodes, the number of samples for the input set Xp, p = 1, 2 …N.

(1) Set the number of initial hidden nodes is K (0) and the initial cluster centers, and set the hidden layer initialized weights is W1.j (0), W1.j (0), j=1, 2 …K (0);

(2) For j = 1, 2 …k; p = 1, 2, N, calculate

$$d_{jp} = \left\| x_p - W_{1,j}(t) \right\|, \tag{2}$$

$$\mu_{jp} = 1 \Big/ \sum_{i=1}^{k} \left(d_{jp} / d_{ip} \right)^{\left(\frac{2}{m-1}\right)}, \tag{3}$$

$$W_{1,j}(t) = \sum_{p=1}^{N} \left(\mu_{jp}\right)^m x_p \Big/ \sum_{p=1}^{N} \left(\mu_{ip}\right)^m, \tag{4}$$

$$\overline{x} = \sum_{p=1}^{N} \left(x_p\right) \Big/ N, \tag{5}$$

m is the weighting factor, usually take 2, μ_{jp} is the first p samples belonging to the j-th membership function in the fuzzy sets, $W_{1,j}(t)$ is the j-th cluster center, d_{jp} is the center distance between x_p and fuzzy set j;

(3) Calculate

$$E = \sum_{j=1}^{c(t)} \left\| W_{1,j}(t) - W_{1,j}(t-1) \right\|^2, \tag{6}$$

If $E > \varepsilon$, then turn to step (2) continue learning;

(4) Calculate the clustering index function

$$S(k) = \sum_{p=1}^{N} \sum_{j=1}^{c} \left(\mu_{jp}\right)^m \left(\left\| x_p - W_{1,j} \right\|^2 - \left\| W_{1,j} - \overline{x} \right\|^2 \right), \tag{7}$$

If $S > \tau$, then k (t +1) = k (t) +1, re-learn, otherwise, stop learning. Also, make sure the number of cluster k and cluster centers $W_{1,j}$, turn to step (5);

(5) Calculate the radius of the kernel function

$$\sigma_j^2 = \frac{1}{m_j} \sum_{x_p \in j} \left\| x_p - W_{1,j}(t) \right\|^2, j = 1, 2, \cdots\cdots, c \tag{8}$$

Which, m_j as the number of samples belonging to the j-th cluster?

2) Supervised learning algorithm

Adjust the weights vector between the output layer and hidden layer. Make solve by the gradient descent and minimum mean square error method. In the iterative process, the learning rate η and the momentum factor a are automatic adjustments

(1) Initialize the connection weights $W_{2,i}(0)$ between the hidden layer and output layer to the random number, i as the number of the sub-network output layer node, i = 1, 2... m;

(2) Provide training on (x, t), j-th hidden layer neuron's output is:

$$u_j = \exp\left(-\left\| x - W_{1,j} \right\|^2 \Big/ \left(2\sigma^2\right) \right) j = 1, 2 \cdots\cdots, k \tag{9}$$

$$u = (u_j)_{c \times 1} \tag{10}$$

(3) The output of i-th output layer neurons:

$$y_i = W_{2,i}(t) \cdot u, i = 1, 2, \cdots\cdots, m \tag{11}$$

(4) Calculate the output error:

$$e_i = t_i - y_i, i = 1, 2, \cdots\cdots, m \tag{12}$$

(5) Correct the weight

$$W_{2,j}(t+1) = W_{2,j}(t) + \Delta W_{2,j}(t+1) \tag{13}$$

$$\Delta W_{2,j}(t+1) = \eta \cdot e_i \cdot u' + a \cdot \Delta W_{2,j}(t), i = 1, 2, \cdots\cdots m \tag{14}$$

(6) Return to Step (2) until the end of iteration

B. *Recognition Process*

Make use of the RBF network which have been trained and have M output node to identify the input sample. When found the input sample belongs to a new class, the network in accordance with k-means clustering algorithm to add a hidden layer node and output node. And then use the samples from the new class train the network; make it learn a new classification of knowledge, to meet the requirements of incremental learning.

Step 1 initialization process: Make use of the sample set A as training set for learning and establish the RBF neural network classifiers S. In this process use the K-means algorithm mentioned earlier. Make cluster analysis for the initial sample set, the number of clustering is the number of initial hidden layer in RBF networks, the number of cluster centers is the basis function centers, according to the cluster variance to get the smoothing parameters in base function, and get the connected weights value by using the least square algorithm calculate. Finally, get the initial RBF network structure.

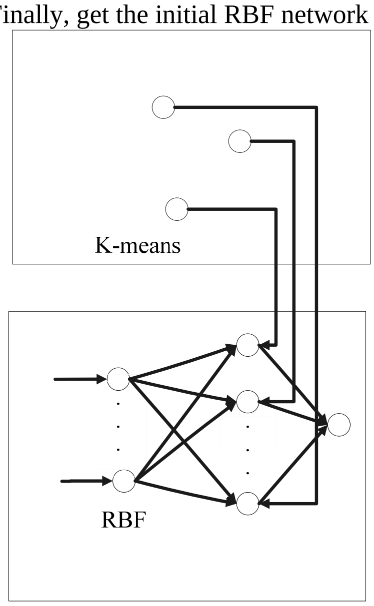


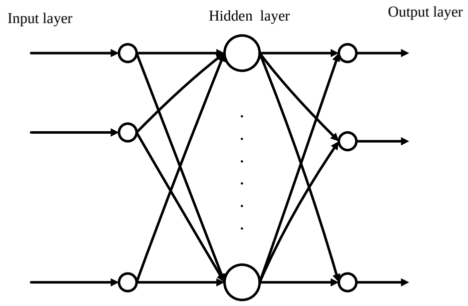
Figure 1. Network structure

Step 2 incremental process: after loading the incremental data set B, not only the normal data sample in B, but also there may be many types of heterogeneous data sample. Because the multi-class problems can be transformed into more second-class problem, here only consider the basic second-class problem. Which means if there are heterogeneous sample in B, only considered B as a set contains normal samples and a class of heterogeneous sample. Specific incremental training process is as follows:

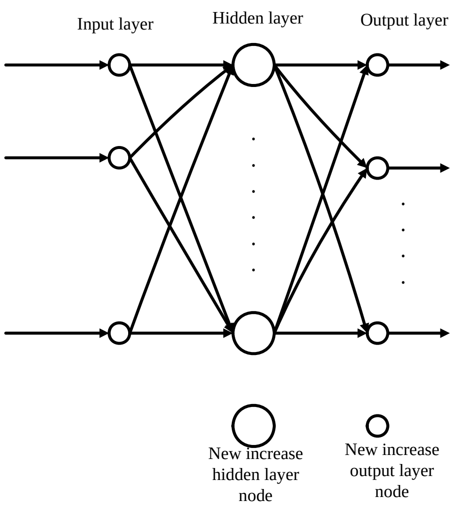
(1) Inspection sample set B whether have heterogeneous sample. If it does not exist, the algorithm stops, S is the incremental learning outcomes; If it exists, according to test results divide sample set B into B1 and B2, B1 as the heterogeneous sample set and B2 as the normal sample set, turn to step (2).

(2) Based on the original RBF neural network classifier S, increase an output node, make M = M +1.According to K-means algorithm make effective clustering to the sample set B1, make sure the number of the added hidden layer nodes and the corresponding added center and width parameters .Meantime random initial the added connection weights between the hidden layer and the output layer. Using the steepest descent method to learn new class samples, and correct the new increase weights value.

After the online learning network the change of hidden layer nodes shown in Figure 2.



a. RBF network structure before incremental learning



b. RBF network structure after incremental learning

Figure 2 RBF network output before and after incremental learning

IV. SIMULATION

Test samples are 5 kinds of Chinese vinegar: vinegar River White City, River City Rice vinegar, Liubiju vinegar, apple vinegar, Zilin Old vinegar. The system uses the TGS-8 series of six metal oxide gas sensors come from Figaro company, the specific model are TGS822, TGS813, TGS821, TGS830, TGS831, TGS832. The experiment equipment used the signal regulating circuit of divider-type. Through the sensor voltage reflects the gas concentration. Use the quantitative liquid sampling methods, sample volume set at 5ml. The system selects the time between the data rapidly increasing and slow decrease to collect the data. Generally, after the sample put into a container 2min later, the significant changes a lot. In order to avoid the impact of environment on the test results, we carried out for two weeks of intermittent testing. Before each sample being measured, use built-in fan make the sensor come to usual.

Experimental data set are a total of 600 samples, which have five classes and each class have 120 samples. We extract 53, 53, 54, 53 samples in the four class as the training sample set, the rest as the test sample. The process of training the network, the sample is provided to the network one after another. After every training sample input RBF neural network, according to the actual output from the RBF neural network whether achieves the desired accuracy to decide whether to re-adjust the network parameters.

RBF network use four categories of vinegar samples as training sample set, five categories of vinegar samples as testing sample set. Table 1 shows the test results of sample data. After the RBF neural network structure re-learning, re-test the testing sample set. Comparative analysis of test results listed in table 1 show that all five categories of vinegar samples were correctly identified. In particular through incremental learning, the new increase categories of vinegar samples (e.g. samples 5, 6) are correct identification. This proves that the proposed improvement of K-RBF network with incremental learning ability can continue to improve gradually with practice, enhance the system's ability to identify.

In order to understand the network training condition, we recorded the adjustment number of RBF neural network parameters (Figure 3) for the fifth categories of vinegar samples. In the initial phase, the network does not adapt to the training samples. Performance in the RBF neural network parameters are frequently and greatly adjust; in the late stages of training, the network gradually adapt to the training sample, fluctuations tends to smooth, the adjust number of parameters are average 5 times. In order to observe the convergence performance of this algorithm, we selected the very representative of the fifth categories of vinegar samples as a research object. Because the initial RBF network is used the initial parameters, the network output error is greater in the initial phase. Through the adaptive adjust network parameters, the error between the network output and the actual value gradually reduced. After 31 times re-tune the network parameters, the output desired to requirements, shown as Figure 4. Figure 5 shows after the training of the RBF network, the approximation capability of 50 test samples; the red line is the target value, the blue line for the network's actual output value.

TABLE I
RBF NETWORK OUTPUT BEFORE AND AFTER INCREMENTAL LEARNING

Sample number	RBF network output before incremental learning	Category	RBF network output after incremental learning	Category
1	(1.015 0.007 0.006 0.002)	River City White vinegar	(1.015 0.007 0.006 0.002 0.001)	River City White vinegar
2	(0.011 0.978 0.005 0.011)	River City Rice vinegar	(0.011 0.978 0.005 0.011 0.004)	River City Rice vinegar
3	(0.020 0.006 0.932 0.002)	Liubiju vinegar	(0.020 0.006 0.932 0.002 0.010)	Liubiju vinegar
4	(0.002 0.003 0.013 0.998)	Apple vinegar	(0.002 0.003 0.013 0.998 0.009)	Apple vinegar
5	(0.009 0.002 0.001 0.001)	New Category	(0.009 0.002 0.001 0.001 1.009)	Zilin Old vinegar
6			(0.007 0.004 0.003 0.004 0.974)	Zilin Old vinegar

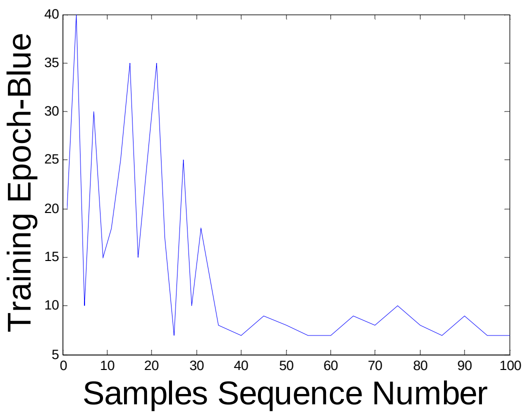


Figure 3. The training condition of the network

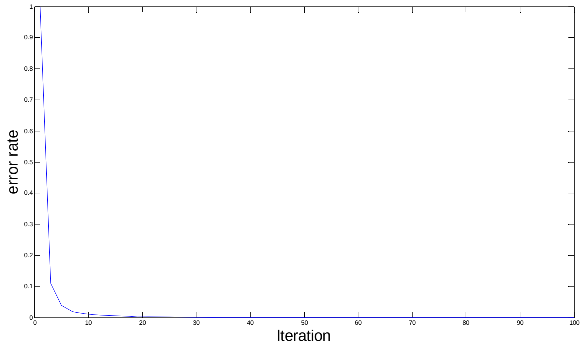


Figure 4 Algorithm convergence

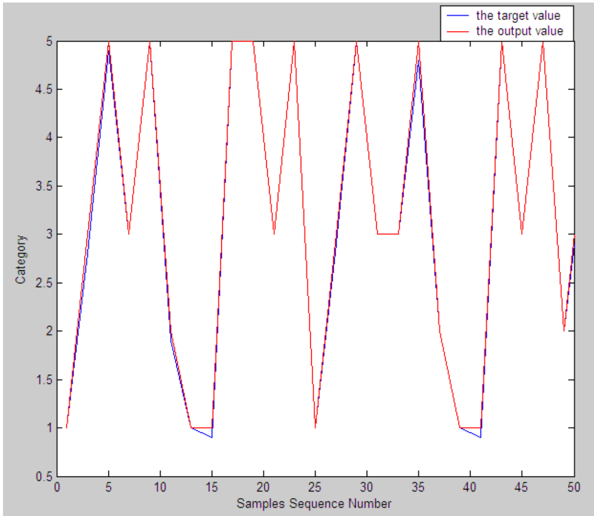


Figure 5.The approximation capability

As can be seen from Table 2, the former four known categories of vinegar samples have 91%, 93%, 95%, 90% recognition rate after RBF network training. After incremental learning to the fifth categories of vinegar samples, RBF recognition rate has not changed. That means the incremental learning algorithm model not only can accurately predict the new category, but also can not forget the original knowledge.

TABLEII
THE CORRECT RATE OF THE ELECTRONIC NOSE IDENTIFY THE NEW SAMPLE DATA

	before incremental learning	after incremental learning
River City White vinegar	91%	91%
River City Rice vinegar	93%	93%
Liubiju vinegar	95%	95%
Apple vinegar	90%	90%
Zilin Old vinegar		97%

As can be seen from Figure 6, the incremental learning algorithm performance is not very sensitive for the initial sample volume and the total amount of incremental data, when the initial sample volume of data changes from 50 to 100, the average recognition algorithm rate has not changed. When the total amount of incremental data changes from 50 to 100, the algorithm samples the greatest change in the average recognition rate of about 1%.

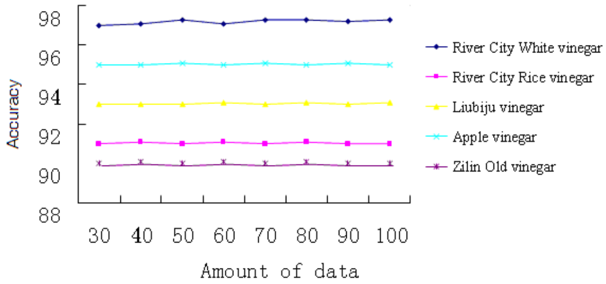


Figure 6 .Different amounts of data and algorithm performance

V. CONCLUSION

In this paper an incremental RBF neural network model based on K-means clustering is studied. This model make K-means clustering algorithms combined with the incremental learning algorithm, so the network can effectively learn new sample mode and keep the original memory of the old sample pattern, have progressive learning ability. Clustering initialization reduced training sequence of the initial data set sample effect on the RBF incremental learning network. The dynamically adjust strategy of the hidden layer nodes makes incremental RBF network has the ability to learn new information. Preliminary experimental results demonstrate the validity of the model.

ACKNOWLEDGMENT

This work was supported by Jilin Province Education Department Research Program of China (2011，NO.79) to Hong Men and Haiping Zhang.

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