Learning Behaviors of Stochastic Gradient Radial Basis Function Network Algorithms for Odor Sensing Systems

Namyong Kim, Hyung-Gi Byun, and Ki Hyeon Kwon

Learning behaviors of a radial basis function network (RBFN) using a singular value decomposition (SVD) and stochastic gradient (SG) algorithm, together named RBF-SVD-SG, for odor sensing systems are analyzed, and a fast training method is proposed. RBF input data is from a conducting polymer sensor array. It is revealed in this paper that the SG algorithm for the fine-tuning of centers and widths still shows ill-behaving learning results when a sufficiently small convergence coefficient is not used. Since the tuning of centers in RBFN plays a dominant role in the performance of RBFN odor sensing systems, our analysis is focused on the center-gradient variance of the RBFN-SVD-SG algorithm. We found analytically that the steady-state weight fluctuation and large values of a convergence coefficient can lead to an increase in variance of the center-gradient estimate. Based on this analysis, we propose to use the least mean square algorithm instead of SVD in adjusting the weight for stable steady-state weight behavior. Experimental results of the proposed algorithm have shown faster learning speed and better classification performance.

Keywords: Odor, radial basis function network (RBFN), center-gradient, stochastic gradient (SG), least mean square (LMS).

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I. Introduction

There is demand for the development of instruments that emulate the human sense of smell, which is a sophisticated chemosensory system. An electronic odor sensing system comprises an array of conducting polymer sensors mounted on a ceramic substrate together with associated electronics. Extremely selective information for discrimination between adsorbed chemical species can be obtained by an analysis of the cross-sensitivities between sensor elements. The modulation of electrical conducting polymers by external physical and chemical interactions makes them attractive for use in chemical sensors [1], [2]. Using an electronic odor sensing system, it is desirable to discriminate between chemicals and compare one sample with another. The ability to classify pattern characteristics from relatively small pieces of information has led to growing interest in methods of sensor recognition. Radial basis function networks (RBFN) and other neural networks have recently been applied to odor classification problems [3], [4].

To use an RBFN as a classifier, parameters such as centers, widths, and weights have to be optimized in the training stage prior to the classification stage, in which classification is carried out using the RBFN with optimized and fixed parameters. Along with how well a sensor mechanism is used, how accurately (close to optimum) the parameters are acquired is one of the most important factors in classification performance. Usually, training RBFN parameters requires a lot of computation and time. This is another obstacle to cope with. Mean squared error (MSE) learning speed is an indicator showing how long a training time is needed, and a steady-state

MSE value indicates how close to the optimum values the adjusted parameters are. Though sensor drift can cause a little shifting of optimum parameters of an RBFN, acquiring the closest parameters to the optimum can be a solution for minimizing the loss of performance due to sensor drift.

The centers and widths of an RBFN are calculated by the fuzzy c-means algorithm and the distribution of input patterns. The weights of an RBFN are calculated by the singular value decomposition (SVD) method in a single shot process. This RBFN-SVD is considered superior to other learning algorithms, particularly in terms of processing speed and solvability of non-linear pattern responses in odor analysis [4]. But, the performance of an RBFN as a classifier is highly dependent on the choice of centers and widths in basis function. So, the fine-tuning of centers and widths is needed and the stochastic gradient (SG) method [5] is successfully applied for this purpose. The adaptive RBFN-SVD-SG algorithm has shown good classification performance for complex and mixed chemical patterns and has been confirmed by experimental trials [6]. In our study on MSE learning behavior in training parameters, however, the RBFN-SVD-SG algorithm shows ill-behaving MSE learning characteristics when a sufficiently small convergence coefficient is not used. However, a small value of the convergence parameter makes the learning speed of the algorithm slow. Improving the performance of an RBFN in terms of convergence speed and recognition error has become an important research area for many researchers [7]-[9]. An investigation into the causes of such performance degradation in the RBFN-SVD-SG algorithm is needed. Focusing on the choice of a convergence coefficient, we observed experimentally that learning curves of a center-gradient estimate of the RBF-SVD-SG algorithm increase and bounce if a sufficiently small value of convergence coefficient is not used. In this paper, we present a theoretical analysis of the factors contributing to center-gradient fluctuation of the RBFN-SVD-SG algorithm and propose a method to acquire faster convergence and better recognition performance.

II. RBFN Algorithms

The architecture of an RBF network is simple and consists of input, hidden, and output layers. The basis functions in the hidden layer produce a localized response to the input and typically use hidden layer neurons with Gaussian response functions; in that case, the activation levels O_j of hidden unit j are calculated by

$$O_j = \exp[-\frac{\|x - c_j\|^2}{\sigma_j^2}], \quad (1)$$

where x is the input vector, c_j is the center associated with hidden unit j, and σ is the width coefficient for hidden unit j, which represent a measure of the spread of data. The outputs of the hidden unit lie between 0 and 1. The closer the input to the center of the Gaussian is, the larger the response of the node. The activation level O_j of an output unit is determined by

$$output(x) = \sum_{j=1}^{M} w_j O_j , \quad (2)$$

where w_j is the weight from hidden unit j to output .

The performance of an RBF network is highly dependent on the choice of centers and widths in basis function. For a minimum number of nodes, the selected centers should well represent the training data for acceptable classification. Most of the training algorithms for an RBF network have been divided into two stages of processing. First, as a clustering method the fuzzy c-means algorithm, which we found relatively good, is applied to the input patterns in order to determine the centers for hidden layer nodes. After the centers are fixed, the widths are determined in a way that reflects the distribution of the centers and input patterns. Once the centers and widths are fixed, the weights between the hidden and output layers are trained by block-processing using SVD. This two-stage method provides some useful solutions in the pattern classification problem. However, since the centers and widths are fixed after they are chosen, this method often results in an unsatisfying performance when input patterns are not particularly clustered. For the fine-tuning of centers and widths, the SG algorithm was applied and produced great performance improvement [6].

III. RBF-SG Algorithm for Center and Width Adaptation

The RBF-SG algorithm adapts all the free parameters of the network using the gradient descent of the instantaneous output error power. An input vector having L elements is defined as

$$x^{(n)} = [x(n), x(n-1), ..., x(n-L+1)]^T . \quad (3)$$

Let the error be denoted by $e^{(n)} = d^{(n)} - y^{(n)}$, where $d^{(n)}$ is the desired output and $y^{(n)}$ is the RBF output, all at training time n. For network parameter ϕ, the RBF-SG algorithm adapts its value $\phi^{(n)}$ at time n according to

$$\phi^{(n+1)} = \phi^{(n)} - \mu_\theta \frac{\partial e^{(n)2}}{\partial \phi^{(n)}} , \quad (4)$$

where μ_θ is the convergence coefficient. Among the localized basis functions, the Gaussian is the most popular choice for RBF-SG. The output of RBF-SG with M Gaussian basis

functions is

$$y^{(n)} = \sum_{j=1}^{M} w_j^{(n)} \exp[-\frac{\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)2}}]. \quad (5)$$

As a localized basis function, Gaussian is a fast decaying function. It can be assumed that not all the basis function units contribute significantly to the network output values. Hence, instead of training all the hidden nodes, one could train only a selected number of basis function nodes with the largest output values. This implies that each node output can be considered not greatly correlated with other node outputs due to a node's localized basis function.

The RBF-SG algorithm adapts the network parameters according to the following equations [5].

$$c_j^{(n+1)} = c_j^{(n)} + \mu_c e^{(n)} w_j^{(n)} \exp[\frac{-\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)2}}]\frac{[x^{(n)} - c_j^{(n)}]}{\sigma_j^{(n)2}} \quad (6)$$

and

$$\sigma_j^{(n+1)} = \sigma_j^{(n)} + \mu_s e^{(n)} w_j^{(n)} \exp[\frac{-\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)2}}]\frac{\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)3}}, \quad (7)$$

where $c_j^{(n)}$ is the j-th element of center vector $C^{(n)}$ at time n. Coefficients μ_s and μ_c are adaptation coefficients for widths and centers, respectively, and they control the speed of adaptation. The weights between the hidden and output layers are tuned by SVD calculation in the same iteration along with the centers and widths.

The RBF-SG algorithm can provide greater robustness to poor initial choices of parameters, especially the centers [10]. The fine tuning of centers by RBF-SG plays a dominant role in the performance of RBFN odor sensing systems. But the difference between center estimate and optimum center is fed back to center-gradient estimation and can induce performance degradation. We analyze the influence of the convergence coefficient on the center-gradient estimation noise of the RBF-SVD-SG algorithm.

IV. The Center-Gradient of the RBF-SG Algorithm

The performance of the stochastic gradient method is dependent on how accurately the MSE gradient is estimated [8]. In the RBF-SG algorithm, the center-gradient estimate is

$$\nabla_c^{\wedge}(n) = \frac{\partial e^{(n)2}}{\partial C^{(n)}}. \quad (8)$$

The center-gradient estimate for the j-th center becomes

$$\nabla_{cj}^{\wedge}(n) = \frac{\partial e^{(n)2}}{\partial c_j^{(n)}} = 2e^{(n)}[-\frac{\partial y^{(n)}}{\partial c_j^{(n)}}]. \quad (9)$$

Equation (9) can be written as

$$\nabla_{cj}^{\wedge}(n) = -4e^{(n)} w_j^{(n)} \exp[\frac{-\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)2}}]\frac{[x^{(n)} - c_j^{(n)}]}{\sigma_j^{(n)2}}. \quad (10)$$

Defining

$$O_j^{(n)} = \exp[\frac{-\left\|x^{(n)} - c_j^{(n)}\right\|^2}{\sigma_j^{(n)2}}], \quad (11)$$

(6) and (8) become (12) and (13), respectively.

$$c_j^{(n+1)} = c_j^{(n)} + \mu_c e^{(n)} w_j^{(n)} O_j^{(n)} \frac{x^{(n)} - c_j^{(n)}}{\sigma_j^{(n)2}}, \quad (12)$$

$$\nabla_{cj}^{\wedge}(n) = -4e^{(n)} w_j^{(n)} O_j^{(n)} \frac{[x^{(n)} - c_j^{(n)}]}{\sigma_j^{(n)2}}. \quad (13)$$

Notice that the difference between center estimate and optimum center is fed back to the center-gradient estimation and can induce error accumulation.

Assuming the centers in the steady-state (that is, as $n \to \infty$) are located close to the optimum centers, and the Euclidian distance between the input patterns and the cluster's center is less than the width, $\left\|x_n - c_j^{(n)}\right\|^2 << \sigma_j^{(n)2}$, $O_j^{(n)}$ in (11) closely approximates 1. Then, the variance of $\nabla_{cj}^{\wedge}(n)$ with the assumption that the expected value of the error is $E[e^{(n)}] = 0$ can be expressed as

$$\begin{aligned} Var[\nabla_{cj}^{\wedge}(n)] &= E[\{\nabla_{cj}^{\wedge}(n) - E[\nabla_{cj}^{\wedge}(n)]\}^2] \\ &= \frac{16}{(\sigma_j^{(n)})^4} E[e^{(n)2}] E[w_j^{(n)2}] \\ &\quad \cdot E[(x^{(n)} - c_j^{(n)}) \cdot (x^{(n)} - c_j^{(n)})]. \end{aligned} \quad (14)$$

Defining the difference between input pattern $x^{(n)}$ and the optimum center c_j^o as $v_j^{(n)} = x^{(n)} - c_j^o$, and center deviation $f_j^{(n)}$ as $f_j^{(n)} = c_j^{(n)} - c_j^o$, $x^{(n)} - c_j^{(n)}$ becomes

$$x^{(n)} - c_j^{(n)} = v_j^{(n)} - f_j^{(n)}. \quad (15)$$

Substituting (15) into (14) yields

$$Var[\nabla^{\wedge}_{cj}(n)]=\frac{16}{\sigma_j^{(n)4}}E[e^{(n)2}]E[w_j^{(n)2}]E[(v_j^{(n)}-f_j^{(n)})(v_j^{(n)}-f_j^{(n)})]$$
$$=\frac{16}{\sigma_j^{(n)4}}E[e^{(n)2}]E[w_j^{(n)2}]$$
$$\cdot(E[v_j^{(n)}\cdot v_j^{(n)}]-2E[f_j^{(n)}\cdot v_j^{(n)}]+E[f_j^{(n)}\cdot f_j^{(n)}]). \quad (16)$$

It can be assumed that $v_j^{(n)}$ and $f_j^{(n)}$ are uncorrelated and $E[f_j^{(n)}\cdot v_j^{(n)}]=0$. By defining the variance of input patterns $E[v_j^{(n)}\cdot v_j^{(n)}]$ as V_j,

$$Var[\nabla^{\wedge}_{cj}(n)]=\frac{16}{\sigma_j^{(n)4}}E[e^{(n)2}]E[w_j^{(n)2}](V_j+E[f_j^{(n)}\cdot f_j^{(n)}]). \quad (17)$$

Using $f_j^{(n)}=c_j^{(n)}-c_j^{o}$, (12) can be expressed as

$$f_j^{(n+1)}=f_j^{(n)}+\mu_c e^{(n)}w_j^{(n)}\frac{v_j^{(n)}-f_j^{(n)}}{\sigma_j^{(n)2}}$$
$$=f_j^{(n)}-\mu_c e^{(n)}w_j^{(n)}\frac{f_j^{(n)}}{\sigma_j^{(n)2}}+\mu_c e^{(n)}w_j^{(n)}\frac{v_j^{(n)}}{\sigma_j^{(n)2}} \quad (18)$$
$$=f_j^{(n)}[1-\mu_c e^{(n)}w_j^{(n)}\frac{1}{\sigma_j^{(n)2}}]+\mu_c e^{(n)}w_j^{(n)}\frac{v_j^{(n)}}{\sigma_j^{(n)2}}.$$

For the sake of convenience, we define

$$B=\mu_c e^{(n)}w_j^{(n)}/\sigma_j^{(n)2}. \quad (19)$$

Taking the Z transform of (18), the transfer function for the variance of the *j*-th center-gradient is the system $A(j, z)$ with input $v_j^{(n)}$ and output $f_j^{(n)}$ as

$$A(j,z)=\frac{Bz^{-1}}{1-(1-B)z^{-1}}. \quad (20)$$

Since in the steady-state (that is, as $n\to\infty$) the variance of $f_j^{(n)}$, $E[f_j^{(n)}\cdot f_j^{(n)}]$, equals the sum of the squares of the impulse response of $A(j, z)$ times the variance of the input, $E[f_j^{(n)}\cdot f_j^{(n)}]$ is given by

$$E[f_j^{(n)}\cdot f_j^{(n)}]=V_j\Phi_j, \quad (21)$$

where

$$\Phi_j=\sum_{n=1}^{\infty}[(1-B)^{n-1}B]^2=\frac{B^2}{1-(1-B)^2}=\mu_c e^{(n)}w_j^{(n)}/2\sigma_j^{(n)2} \quad (22)$$

for $\mu_c e^{(n)}w_j^{(n)}/2\sigma_j^{(n)2}<<1$.

Substituting (22) into (17) and using $E[e^{(n)2}]=MSE_{\min}$ in the steady state leads us to

$$Var[\nabla^{\wedge}_{cj}(n)]=\frac{16MSE_{\min}}{\sigma_j^{(n)4}}E[w_j^{(n)2}]\cdot[V_j+\mu_c e^{(n)}w_j^{(n)}/2\sigma_j^{(n)2}]. \quad (23)$$

In (23), we can find that steady-state weight fluctuation and large values of μ_c can lead to a large fluctuation of the center-gradient estimate. For stable steady-state weight behavior, we propose to use the least mean square (LMS) algorithm [11] instead of SVD for adjusting the weight, without decreasing μ_c. Because the center deviation is fed back to the center-gradient estimation as in (13), error accumulation can be produced. The SVD, which can be considered as a method of a matrix-inverse process in a single-shot process, can induce instability due to these accumulated errors. The LMS algorithm, which calculates weights iteratively pattern by pattern, is known to be slow but robust. The experimental results when using the LMS algorithm for adjusting weights in the RBFN (RBFN-LMS-SG) are presented in the following section.

V. Experiments and Results

1. Apparatus for Odor Measurement

For the measurement, we used an odor sensing system that has an array of conducting polymer sensors mounted on a ceramic substrate together with associate electronics developed by Prof. Krishna C. Persaud at University of Manchester, U.K. [1]. Along with this instrument, a sampling apparatus consisting of a compressed air cylinder, activated charcoal filter, flow meter, water bath, Teflon tubing, and Duran bottles has been designed for laboratory use to collect samples under highly controlled conditions. Figure 1 shows the simple configuration of the measurement system.

The experiment preparation started by passing clean air through the system for several minutes before sampling. This

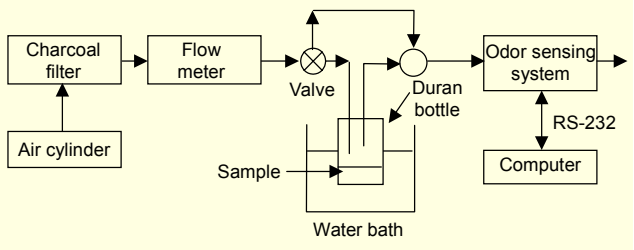

Fig. 1. Apparatus configuration for odor measurement.

gave enough time to heat up the sensor array for a stable condition as well as flushing out any unwanted odors that may have been present in either the connected tubing or equipment. Each sensor responded very quickly when the two-way valve was opened to allow an analysis of the chemical vapor; this response is due to chemical and electrical effects of the chemicals on the surface of polymer sensors.

Figure 2 illustrates the way the sensors operate. When a volatile chemical is presented, all the sensors respond with a reversible change of resistance. The intensity of response is dependent on the affinity of chemical species for individual sensors, and is proportional to the concentration present. The steady-state response of each sensor to the absolute sum of the response of the entire array is taken, and the raw data between the two cursors can be transformed into a pattern that is unique so that particular chemical species, or a mixture, can be used as 'fingerprints' to identify it.

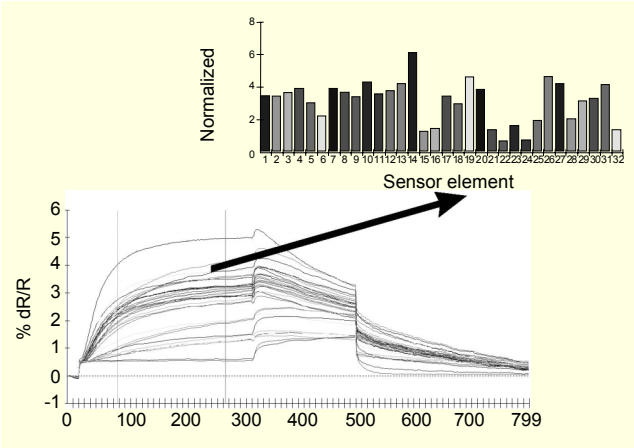

Fig. 2. Raw response of conducting polymer sensor array and extraction pattern.

Measurements of the chemicals were repeated to collect patterns from solvent vapors over a period of four weeks. Figure 3 shows that there was some variability in the responses of the sensor array during the four-week measurements, which may be due to causes including drift.

2. Results and Discussion

For testing the center-gradient behavior and MSE performance of the classifier based on the adaptive RBFN-SVD-SG algorithm on drifting data, a conducting polymer sensor array consisting of 32 sensors (L=32) was used to collect patterns from solvent vapors measured over a period of four weeks. For network training, eight centers for each class (M = 8) were chosen from a total of 520 patterns in data sets from weeks 1 and 2. After having trained the adaptive RBFN-SG using weeks 1 and 2 data sets obtained from 1% acetonitrile (ac1), 10% acetonitrile (ac10), 1% acetone (ae), 1% butanone (bu), 10% methanol (me), 1% propanol (pr1), 10% propanol (pr10), and water (wa), the RBFN was applied to the previously unseen data of 528 patterns (66 patterns for each gas) from weeks 3 and 4 to evaluate odor prediction under drift effects. Previous works on RBFN odor sensing systems have not analyzed MSE learning behaviors. We observed that MSE bouncing and fluctuations of the center-gradient estimate occur when a sufficiently small μ_c is not used. Center-gradient behaviors are compared for different values of μ_c in Fig. 4. For convenience, μ_c is expressed as u in Figs. 4, 5 and 6.

The magnitude of the center-gradient for $\mu_c = 0.00005$ shows stable behavior, but center-gradients for larger μ_c's, that is, $\mu_c = 0.00009$ and $\mu_c = 0.0001$, show unstable fluctuations

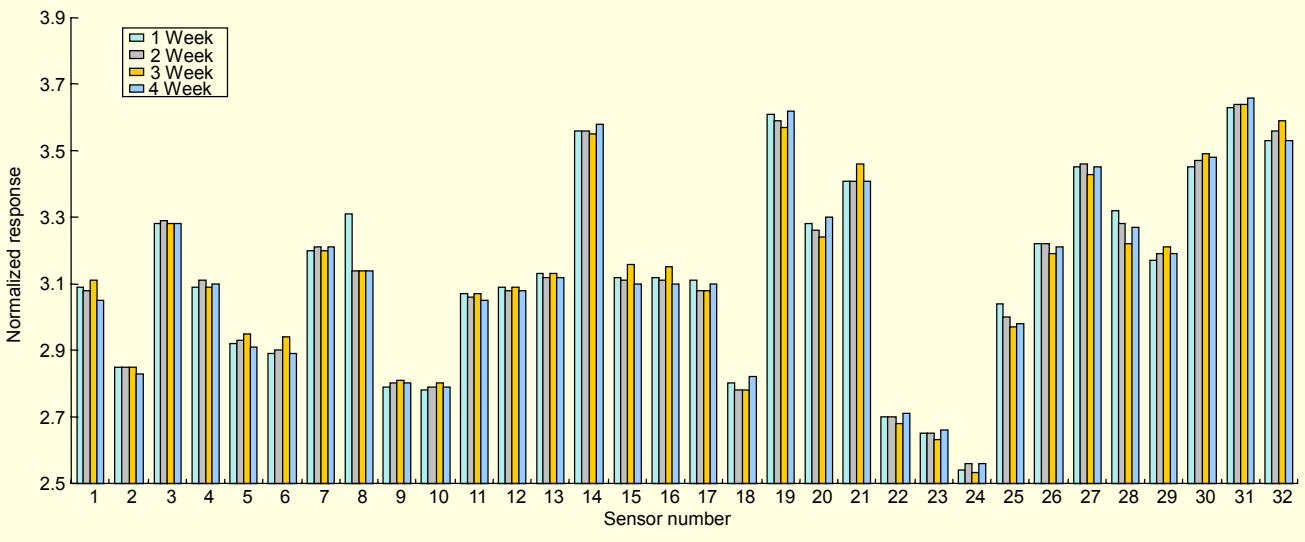

Fig. 3. Normalized response patterns from 32-sensor array for 10% methanol.

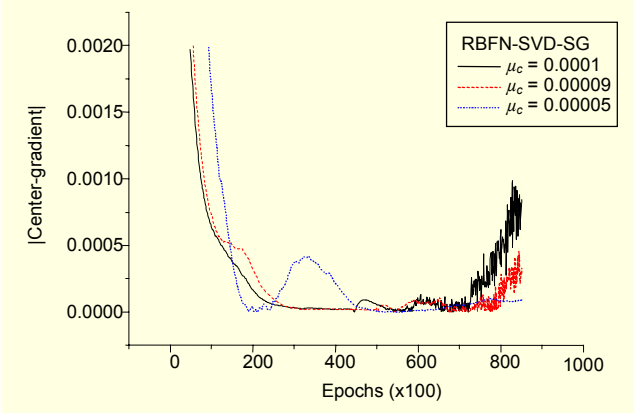

Fig. 4. Center-gradient curves of RBF-SVD-SG.

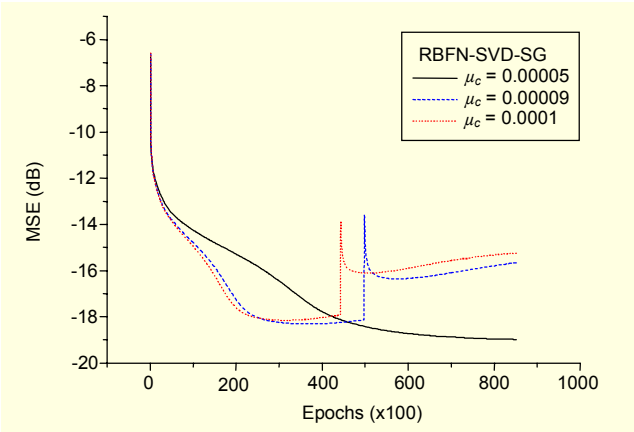

Fig. 5. MSE learning curves of RBF-SVD-SG.

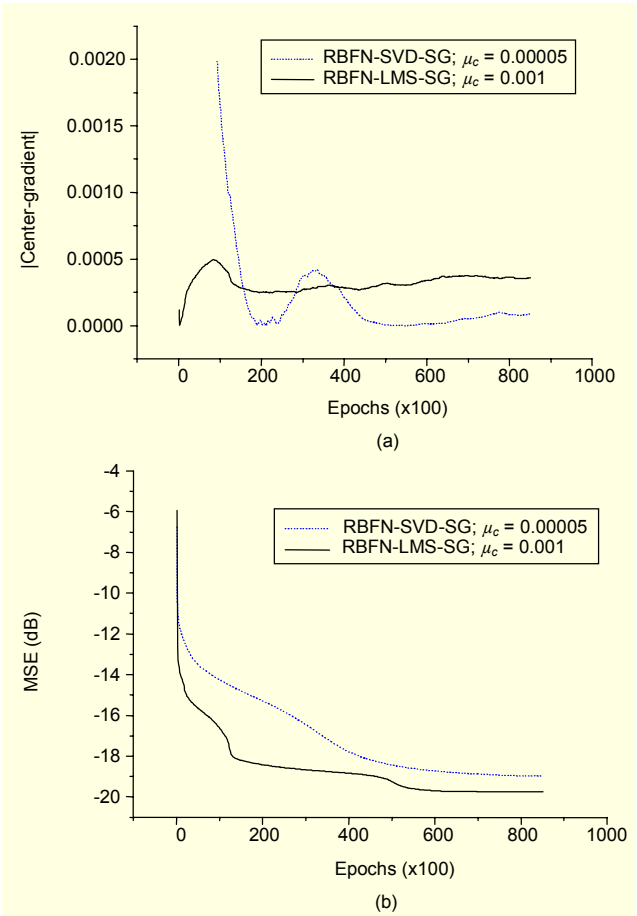

Fig. 6. (a) The center-gradient behaviors and (b) MSE performances.

in proportion to μ_c. That is, the larger μ_c the algorithm adopts, the bigger fluctuation shown. Figure 5 shows MSE learning curves of RBF-SVD-SG for different values of μ_c.

We observed that MSE-bouncing can occur even after converging at about the epoch of 45000 when $\mu_c = 0.0001$ and around the epoch of 50000 when $\mu_c = 0.00009$. In Fig. 4, we can also notice that the beginning of the bouncing is at about the epoch of 45000 when $\mu_c = 0.0001$ and around the epoch of 50000 when $\mu_c = 0.00009$. This implies that ill-behaving MSE learning curves can occur according to the fluctuation of the center-gradient. A method of avoiding the problems is to use a very small value of μ_c, such as $\mu_c = 0.00005$ in Fig. 5, but this produces a slow convergence.

The center-gradient behaviors of the proposed RBFN-LMS-SG using $\mu_c = 0.001$ and the conventional RBFN-SVD-SG using $\mu_c = 0.00005$ are shown in Fig. 6(a). The MSE performances of the proposed RBFN-LMS-SG using $\mu_c = 0.001$ and the conventional RBFN-SVD-SG using $\mu_c = 0.00005$ are in Fig. 6(b). The value of the convergence coefficient for the LMS algorithm is set to the same value, 0.001.

The RBF-LMS-SG has shown an earlier steadiness of center-gradient than the RBF-SVD-SG in Fig. 6(a), and this produces the rapid convergence in MSE performance shown in Fig. 6(b). The RBF-SVD-SG converges in about 80000 epochs, while the RBFN-LMS-SG reaches the same MSE in about 20000 epochs. Also, the RBFN-LMS-SG shows a lesser minimum MSE value by 1 dB than RBF-SVD-SG at an epoch of 80000.

Figures 7(a) and 7(b) show gas prediction performances for 10% propanol (pr10, 400-466 pattern) and water (wa, 467-528 pattern), in which most big errors occur, at the epochs of 20000 and 80000, respectively.

For pr10 (target level is 7), the prediction error of the RBFN-LMS-SG at the epoch of 20000 is a little bigger than the RBFN-SVD-SG at the epoch of 80000, but for wa (target level is 8), the RBFN-LMS-SG at the epoch of 20000 already shows a smaller prediction error than RBFN-SVD-SG at the epoch of 80000. On average, this result is in accordance with the MSE results in Fig. 6(b). The improvement of classification performance of the RBFN-LMS-SG after convergence is also shown in Fig. 7(b).

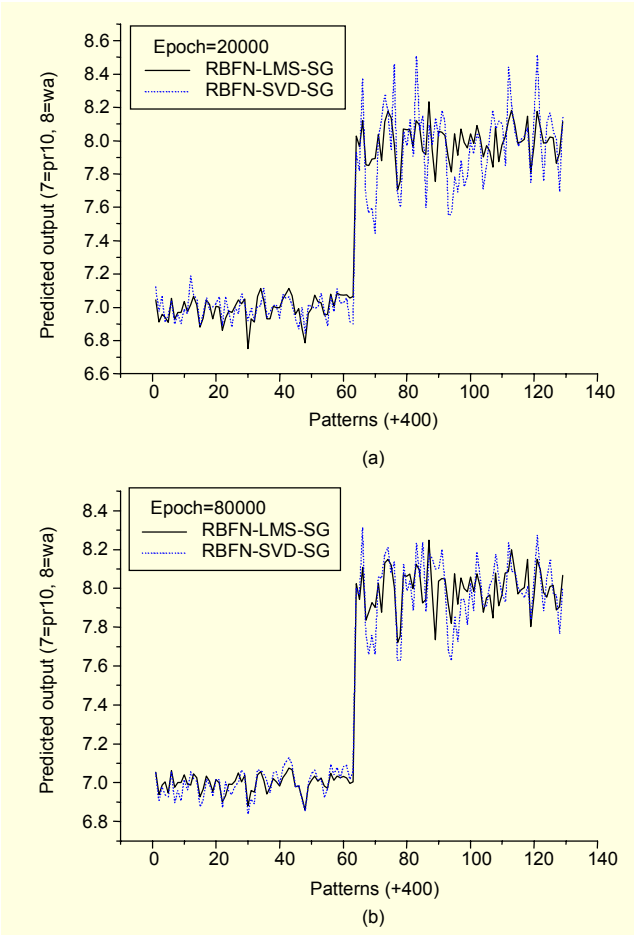

Fig. 7. Odor prediction results for 10% propanol (pr10) and water (wa) at (a) epoch = 20000 and (b) epoch = 80000.

VI. Conclusions

This paper presents an analysis of the center-gradient behavior of the RBFN-SVD-SG algorithm for an odor sensing system with conducting polymer sensor array. The center-deviation can have a negative effect on the RBF hidden node output. We found theoretically that the steady-state weight fluctuation and large values of μ_c can lead to an increase of variance of the center-gradient estimate. We also observed that the center-gradient for a small convergence coefficient shows stable behavior, but center-gradients for larger convergence coefficients show unstable fluctuations in proportion to the size of the convergence coefficient. The MSE learning curves of the RBF-SVD-SG algorithm can show bounces in accordance with the instable behavior of the center-gradient. From the theoretical results, methods for a stable steady-state weight, rather than decreasing μ_c, can be reasonable solutions. The proposed RBFN-LMS-SG using the LMS algorithm instead of SVD for adjusting the weight shows faster convergence speed and lower minimum MSE. Odor classification can be performed with good accuracy with the proposed method when it is used for odor sensing systems.

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