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A Novel Chaotic Sequence Optimization Neural Network for Concentration Estimation of Formaldehyde by an Electronic Nose

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***Abstract*—Electronic nose (E-nose), as an artificial olfactory system, can be used for quantification of odor concentration combined with a pattern recognition module. Backpropagation neural network (BPNN) has been recognized as the common pattern recognition in E-nose development. Considering the flaw of easily trap into a local optimal of BPNN, this paper presents a novel chaotic sequence optimization BPNN method for improving the accuracy in E-nose quantification prediction. Three chaos dynamic equations including logistic map, tent map and Gaussian map for chaotic queue with ergodic characteristic were applied in chaos based optimization. Through comparisons with standard particle swarm optimization, the experimental results demonstrate the superiority and efficiency of the chaos based optimization algorithm from the point of view of the search ability and robustness.**

***Keywords-* Electronic nose; artificial olfactory system; backpropagation neural network; chaotic sequence optimization**

I. INTRODUCTION

Chaos is a bounded unstable dynamic behavior that exhibits sensitive dependence on initial conditions and also unstable periodic motions in nonlinear systems [1]. Although it appears to be stochastic, it occurs in a deterministic nonlinear system under deterministic conditions. Chaotic sequences generated from many chaotic maps commonly possess certainty, ergodicity and stochastic property, and therefore they have been used instead of random sequences and somewhat good results have also been demonstrated when combined with particle swarm optimization [2] for global solutions search. In prediction, classification, and pattern recognition, hybrid forecasting models based on chaotic mapping have been presented together with Gaussian support vector machine, particle swarm optimization and genetic algorithm in [3, 4]. Similarly, chaos optimization has also been used in prediction of silicon content in hot metal [5] and faults classification [6, 7]. Chaos search immune algorithms have been presented in [8, 9] for neuro-fuzzy controller design and pattern recognition. The choice of chaotic sequences is justified theoretically by their unpredictability including spread-spectrum characteristic, non-periodic, complex temporal behavior, and ergodic properties.

Electronic nose, as an artificial olfactory system, includes a central process unit, chemical gas sensor array, other peripheral circuits and pattern recognition module [10]. It has been widely used for analysis of volatile organic compounds [11] and vapor chemicals [12]. Neural network, especially back-propagation neural network (BPNN), has been widely used for recognition and function approximation based its strong regression ability [13]. So, in this paper, BPNN is used for concentration estimation of formaldehyde in an electronic nose. However, BP neural network still posses some inherent problems. First, BP model can easily get trapped in local minima for the problems of pattern recognition and complex functions approximation [14], so that a local optimal solution is obtained. Second, the solutions are different for every train with the random initial weights. In this paper, we apply a novel mutative scale chaotic sequence method to optimize the weights of BPNN considering the characteristic of ergodic. Two kinds of chaotic mapping equations with tent map and logistic map have been used for generation of chaotic sequences.

II. MATERIALS AND METHODS

A. *Electronic Nose System*

Our sensor array in E-nose system consists of four gas sensors from the TGS series including TGS2602, TGS2620, TGS2201A and TGS2201B. In addition, a module (SHT2230 of Sensirion in Switzerland) with two auxiliary sensors for the temperature (T) and humidity (H) are also used for compensation. The sensors were mounted on a custom designed printed circuit board (PCB), along with associated electrical components. A 12-bit analog-digital converter is used as interface between the Field Programmable Gate Array (FPGA) processor and the sensors. FPGA can be used for data collection, storage and processing. The e-nose system is connected to a personal computer (PC) via a Joint Test Action Group (JTAG) port which can be used to transfer data and debug programs. An input vector with 6 variables can be obtained in each observation; the multidimensional response data set presents a nonlinear relation with the target gas concentration. Formaldehyde measurements were employed by an E-nose in the constant temperature and humidity chamber in which the temperature and humidity can be effectively controlled in terms of the target temperatures and humidity. Note that the precisions of the chamber for temperature and humidity are ±0.1   and ±5%RH.

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B. Data Acquisitions

In terms of the indoor monitoring of the formaldehyde concentrations, formaldehyde was measured at the concentration range of 0~5 ppm, target temperatures of 15, 25, 30 and 35 and target humidity of 40%, 60%, 80%RH (relative humidity) in order to imitate the real environment indoor. For each measurement, the total measurement cycle time for one single measurement was set to 20 mins, i.e. 2 mins for reference air (baseline), 8 mins for gas sampling and 10 mins for cleaning of the chamber through injecting clean air before the next measurement begins. Totally, 116 observation samples were collected. For model building, 71 train samples, 25 test samples and 20 validation samples were divided from the whole sample set. The actual concentration of each sample was obtained through the spectrophotometer analysis of the chemical sampling using the air sampler. For each sample, a vector with 6 variables was extracted at the steady state response. Besides, a simple normalization method divided by 4095 was used for subsequent pattern analysis. Notice that 4095 is calculated as 212-1 with the principle of 12-bit A/D converter. The simplified experimental platform is illustrated in Fig.1.

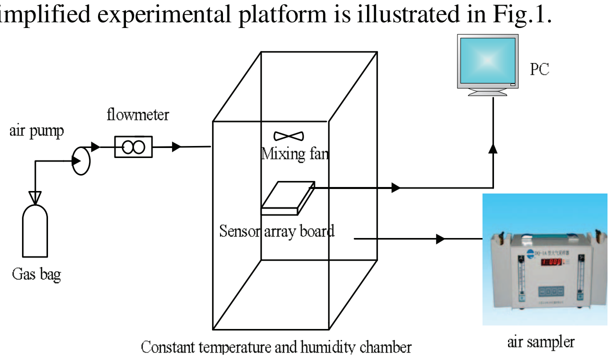

Figure 1. Experimental platform of formaldehyde by an electronic nose

C. Mutative Scale Chaotic Sequence Optimization Neural Network

Chaos optimization is developed using chaotic variables. Three chaos map equations were studied in this paper. The logistic map is shown by

$$z_k = \mu \cdot z_k \cdot (1 - z_k) \qquad (1)$$

where z_k is the k-th chaotic variable and k denotes the iteration number. Obviously, $z_k \in (0,1)$ under the conditions that the initial $z_0 \in (0,1)$ and the z_0 can not be the digits of {0, 0.25, 0.75, 1}. Here, μ=4 can be a completely chaotic state.

The tent map resembles the logistic map. It can also generate chaotic queue in (0, 1) in terms of the following form

$$z_k = \begin{cases} z_k/0.7 & , z_k < 0.7 \\ 10/3 \cdot z_k \cdot (1 - z_k), & z_k \geq 0.7 \end{cases} \qquad (2)$$

The Gauss map which can also generate a chaotic queue in (0, 1) can be represented by

$$z_{k+1} = \begin{cases} 0 & , z_k = 0 \\ 1/z_k - \lfloor 1/z_k \rfloor, & z_k \in (0,1) \end{cases} \qquad (3)$$

where $\lfloor x \rfloor$ denotes the largest integer less than x.

The algorithm procedure of mutative scale chaotic sequence optimization neural network can be concluded as follows

Step 1: Initialization g=0. Randomly generates one M-dimensional population $\mathbf{X}^0$ with N individuals within (0, 1) and determine the initial optimization boundary [$\boldsymbol{a}$, $\boldsymbol{b}$] in the optimization space.

Step 2: Map the variable $\mathbf{X}_i^k$ into the optimization space and obtain one new population $\mathbf{MX}_i^k$ using the following equation

$$MX_i^k = a_i^k + MX_i^k (b_i^k - a_i^k), i = 1, \ldots, N; k = 1, \ldots, M \qquad (4)$$

Step 3: Evaluate the new population **MX** using BPNN algorithm and find the best individual **Xgbest**. The cost function has been defined as the maximum absolute relative error of the train and test samples shown by

$$f = \max \left\{ 1/n_1 \cdot \sum_{i=1}^{n_1} |ytr_i - ttr_i|/ttr_i,\ 1/n_2 \cdot \sum_{j=1}^{n_2} |yte_j - tte_j|/tte_j \right\} \times 100 \qquad (5)$$

where n_1 and n_2 denote the number of train samples and test samples; **ytr** and **ttr** denote the predictive concentrations and actual concentrations of train samples; **yte** and **tte** denote the predictive concentrations and actual concentrations of test samples. Note that a decoding of **MX** for the initial weights and bias of the neural network is necessary, because each individual is encoded as the weights and bias.

Step 4: Mutative scale of chaotic variable search.

If the best solution keeps invariant within T iterations, the shrink of the search boundary [a, b] can be performed using the following strategy for specific search in a smaller space

$$a^{g+1} = Xgbest - \gamma^g \cdot (b^g - a^g) \qquad (6)$$

$$b^{g+1} = Xgbest + \gamma^g \cdot (b^g - a^g) \qquad (7)$$

$$\gamma^{g+1} = \beta_1 \cdot \gamma^g \qquad (8)$$

where a^{g+1} and b^{g+1} denote the new search boundary, γ is the radius of search, β_1 denotes decay coefficient less than 1.

Step 5: The constraints process of the boundary using the following strategy

If a_i^k<-C^g, a_i^k=-C^g; if b_i^k>C^g, b_i^k=C^g (9)

$$C^{g+1} = \beta_2 \cdot C^g \qquad (10)$$

where C denotes the maximum boundary and β_2 denotes the attenuation coefficient similar to simulated annealing.

Step 6: if the current solution satisfies the termination criteria, stop; else go to step 7.

Step 7: Generate the new population **X** using the chaotic map equations, and go to step 2.

D. Parameter Settings

In this paper, a two hidden layered neural network whose structure is 6-10-10-1 was used. The log-sigmoid function and pure linear function were used in the hidden layers and output layer, respectively. In terms of the network structure, the length N of one individual can be calculated as N=6×10+10+10×10+10+10×1+1=191.

The size M of population is set as 50, the maximum iterations G=100 and the permissible iterations T=10 for stagnation.The initial boundary [a, b] is set as [-20, 20] and C=20. Besides, the decay coefficient β_1 and attenuation coefficient β_2 are set as 0.98 and 0.95, respectively. The initial search radius γ is set as 0.2.

III. Results and Discussion

The results for the experiments analyzed using the chaotic sequence optimization neural network and standard particle swarm optimization (PSO) have been presented in this section. The model building is based on the train samples and test samples. The role of the test samples is used to control the possible overfitting of training samples, because the information of test samples has been considered in the training process. We apply the maximum relative error of train and test samples to improve the robustness of the model. The validation samples are only used to verify the efficiency of the model. Fig.2 illustrates the prediction results of the validation samples using four optimization methods combined with BPNN. From the trace of predictions and actual concentrations, we can find that the four methods can track the actual concentrations. The predicted curve using chaos with logistic map can approach the actual curve better. For quantification of the prediction error, table 1 presents the relative prediction error using four optimization methods. From this table, we can find that the chaotic sequence optimization with logistic map has the minimum prediction error of validation samples. It also proves that the chaos queue with logistic map has the best performance.

TABLE I. RELATIVE PREDICTION ERROR USING DIFFERENT OPTIMIZATION METHODS

Optimization methods	Relative prediction error		
	Train	Test	Validation
Logistic map	28.35%	28.89%	**32.34%**
Tent map	29.78%	30.27%	**49.49%**
Gaussian map	30.06%	23.06%	**50.64%**
Standard PSO	29.94%	29.56%	**47.06%**

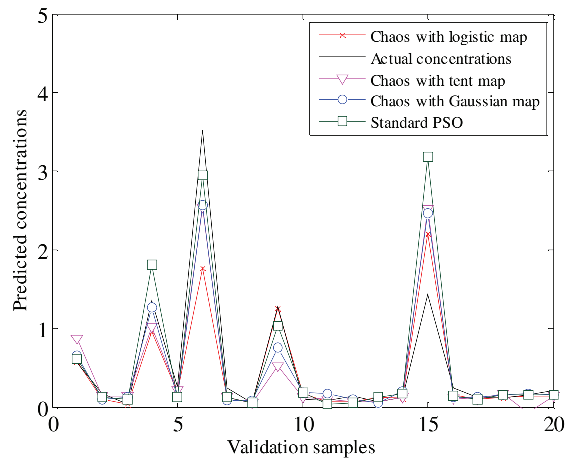

Figure 2. Prediction results of the validation samples using four methods

IV. Conclusions

This paper presents a novel chaos sequence optimization neural network method for concentration prediction of formaldehyde by an electronic nose. A detail of chaos optimization procedure has been provided. Through formaldehyde samples obtained in experiments using an electronic nose, we built the neural network prediction model combined with the chaos optimization. By comparison of the accuracy of models based on chaos sequence and particle swarm optimization, the chaos based method proposed in this paper has the best prediction performance.

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