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基于神经网络的炭气凝胶孔结构的预测与优化模型研究

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摘 要： 如何控制和预测孔结构是炭气凝胶研究的重要课题。然而，由于耗时耗财，导致实验方法研究控制和预测孔结构成为难题。本文提出一种基于神经网络的炭气凝胶孔结构的预测与优化模型，并采用遗传算法设计和优化模型，对六种典型训练算法模型性能进行比较分析。利用该模型对孔径和吸附容量进行预测，两者的预测相关系数分别为 0.992 和 0.981，预测均方根误差分别为 0.077 和 0.054。经测试，该模型与实验研究的结果相符，并有效的应用于预测和控制炭气凝胶实验参数。

关键词： 炭气凝胶；孔结构；神经网络；训练算法；模型

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Modelling and optimization of the pore structure of carbon aerogels using an artificial neural network

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Abstract： An intelligent simulation method for predicting and optimizing the pore structure of carbon aerogels is proposed by using an artificial neural network (ANN) algorithm. The ANN model has been optimized based on an improved genetic algorithm from six typical training algorithms. The volumes and diameters of pores in the simulated samples are predicted by the optimized ANN model, which shows correlation coefficients R^2 of 0.992 and 0.981 and root-mean-square prediction errors (RMSPE) of 0.077 and 0.054 between the predicted and experimental values for the volumes and diameters of pores, respectively. The proposed model is expected to have practical applications in the pore structure control of carbon aerogels.

Key words： Carbon aerogels; Pore structure; Neural network; Training algorithms; Modelling

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1 Introduction

Carbon aerogels have high ratios of surface or interface atoms owing to their particles in nanometer scale that form them[1]. Compared with conventional granular materials, carbon aerogels have a series of excellent physical and chemical properties such as low densities, high electrical conductivity, high special surface area, biocompatibility, and anticorrosion by acid and base[2,3]. It is considered as a promising material for various electrochemical applications, catalyst supports, adsorbents, and chromatography packings[4,5,6].

In this study, a new type of carbon aerogels was prepared by sol-gel polymerization method using phenol, melamine and formaldehyde as raw materials. Pore structure of carbon aerogels is essential to carbon aerogels because it will directly affect their performance. However, it is difficult to control practically pore structure parameters of carbon aerogels due to the constraints of time and cost.

In recent years, interest using artificial neural networks (ANNs) as a tool in material technology has increased. ANNs have been successfully used in several types of material applications like analysis, classifications, predictions or control and others[7,8].

ANNs are mathematical models that have the capabilities to relate input to output parameters. They

can learn from examples by iteration without requiring a prior knowledge of the relationships between process parameters and properties of materials[9].

The neural network is determined by the architecture, training algorithms and learning rule. The most often used ANN for material applications is a fully connected and supervised network with a back propagation learning rule. The neural network architecture is designed by means of a trial-and-error process with a human intervention. Although there are some studies carried out on the automatic design of architectures[10], how to design an appropriate architecture systematically and autonomously remains a challenging problem. The genetic algorithm (GA) is quite effective in solving optimization problems owing to its inherent property of implicit parallelism[11]. In this paper, we have established an optimal structure of ANN by GA. Plumb et al.[12] have shown that a proper selection of the training function has a significant effect on the predictive ability of a network. Therefore, one of the aims of this paper is to obtain an optimized ANN to control and predict the pore structure for carbon aerogels through selecting training algorithms. To do this, six training algorithms have been evaluated.

Performances of ANN have been optimized by varying the numbers of neurons in the hidden layer, optimizing the architecture of neural network and selecting a proper training algorithm. Then, the numerical simulation results from the optimal controlling and predicting model are compared with experimental ones. The purpose of this paper is to investigate the behaviors of pore structure for carbon aerogels and establish controlling and predicting model using the neural network method. The flowchart of this study is shown in Fig. 1.

2 Experimental

2.1 Preparation and experimental design

In the present experiments, the total reactant concentration is 20%, and the molar ratio of phenol and m-cresol is 1∶2. The catalyst concentration is 100 mmol/L. We investigate the effect of the reactant concentration, the molar ratio of phenol and m-cresol in the solution on pore structure of carbon aerogels. The reactants are mixed in propyl alcohol to form transparent solutions. The solutions are poured into sealed glass ampoules (8 cm×2 cm, internal diameter, each filled with 20 mL solution) and heated at 90 ℃ for 48 h in a water bath. Then, the black organic gels are moved into a pressure vessel and supercritically dried at 270 ℃ and 8 MPa. Finally, with a heating rate of 5 ℃/min, the carbon aerogels are formed by pyrolysis of the organic aerogels in a horizontal tube furnace at 800 ℃ for 3 h under nitrogen protection. As a comparison, phenol-furfural (m-C/P=0) and m-cresol-furfural (m-C/P=∞) are polymerized in 1-propanol under the same conditions[13].

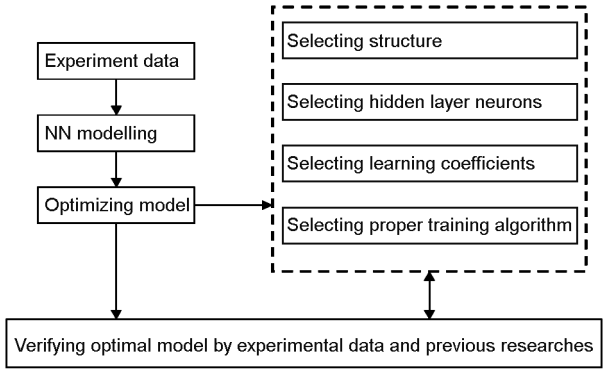

Fig. 1 Flowchart of this study.

Samples are named MP/RC/CC in accordance with preparation conditions, in which MP is melamine/phenol molar ratio, RC is the concentration of the reactants and CC is the catalyst concentration. Under certain conditions (solvent exchange, supercritical drying and pyrolysis), the influences of different reaction temperatures, reaction times, various melamine/phenol molar ratios (M/P) on pore structure of carbon aerogels are studied.

2.2 Analysis and characterization

Main analysis and characterization methods of this paper are as follows:

Laser particle size analyzer. Particle size distribution and average particle size were measured by a laser particle size analyzer.

Nitrogen adsorption. Adsorption and desorption isotherms of nitrogen were measured at 77 K using a commercial adsorption apparatus (ASAP2020M, Micromeritics). Samples were degassed at 200 ℃ under vacuum for 12 h. The BET surface areas (S_{BET}) were analyzed by the Brunauer-Emmett-Teller (BET) method from the adsorption isotherm of nitrogen at p/p_0 from 0.05 to 0.2. Micropore volumes (V_{mic}), micropore surface areas (S_{mic}), and external surface areas (S_{ext}) were obtained by the t-plot method using an adsorption branch of the isotherms. Mesopore size distributions, mesopore volumes (V_{mes}) and average pore diameters (D_p) were obtained with the BJH (Barrett-Johner-Halendar) model using the desorption branch of the isotherms.

3 ANN description

An ANN concept, which is from artificial intelli-

gence family, has been developed to model nonlinear processes in many areas. An ANN is a parallel-distributed information processing system. It stores the samples with distributed coding, thus forming a trainable nonlinear system. The main idea of the neural network resembles the functions of human brains. It is self-adaptive to the environment so as to respond different inputs rationally[14].

An overview of neural network algorithms was provided by McCulloch[15]. A neuron as a unit with process of stimulus and reaction is generalized in this system. A set of training data for learning is performed with weight (connection strength), transfer function and biases. In this study, a back-propagation (BP) algorithm is used for the neural network, which is simple from the viewpoint of structure and easy analysis with mathematics. The back propagation neural network scheme, which has a great learning ability in training and mapping the relations between inputs and outputs, is the most commonly used network models[16,17]. The basic structure of BP neural network is shown in Fig. 2.

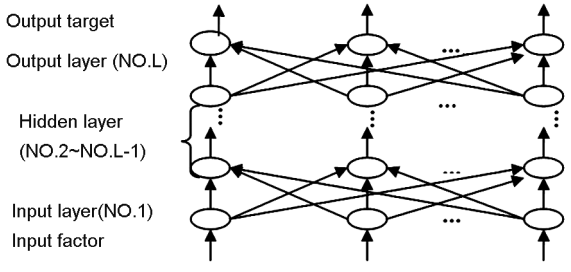

Fig. 2　Basic structure of BPNN.

The neuron shown in Fig. 2 can be classified into three types, input, output and hidden neurons. Input neurons are the ones that receive input signal from external sources. Output neurons are those that send the signals to external sources. Neurons, which have inputs and outputs, are called hidden neurons. There are one or several nodal points in the output layer, which generate output data.

In this network, each input value is connected to each input neuron by the weight matrix. Usually, BP neural network is represented by the following model (Eq. (1)),

$$\begin{cases} N_j = \sum W_{ji} I_i \\ H_j = f(N_j + B_j) \\ O_k = f(\sum W_{kj} H_j + B_k) \end{cases} \quad (1)$$

where I_i and O_k are input and output values, H_j is the output of activation function of the j_{th} neuron in the hidden layer, W_{ji} and W_{kj} are weights, f is the transfer function and B_j and B_k are biases.

The optimal ANN configuration is selected from various ANN configurations based on their predictive performance. Mean square prediction error (MSE) defined as Eq. (2) is used to evaluate prediction accuracy of the model:

$$\mathrm{MSE} = \sum_{k=1}^{N} (O_k - T_k)^2 / N \quad (2)$$

where N is the number of prediction data, T_k is the actual value of the k_{th} experimental data and O_k is the k_{th} estimated value of the prediction model. MSE is easily computed and it can give a precise description of the predictive performance of the network.

Also, the linear regression coefficient R^2 between the predicted values of the ANN model and the desired output is used to evaluate the predictive ability of the network.

MSE and R^2 are frequently calculated until error is acceptable. Finally, the test data are used to verify the nonlinear relationship between the input and output data sets. Steps of optimization procedure and learning algorithm are listed in detail in Ref. [18].

ANN is self-adaptive to the environment so as to respond different inputs rationally. In other word, a designed neural network can give a rapid response for any given input. Some advantages of a neural network are adoption, learning, generalization, easy to implementation, and self-organization.

Implementation of a neural network needs a decision of two main features, the structure in other word topology of the network and the type of learning algorithm. In this article, the topology of the network is optimized by an improved genetic algorithm. Six different training algorithms are tested by comparing predicting results.

4　Methodology design of the neural network

In this study, the neural network is used to predict diameters and volumes of pores in the MP/RC/CC carbon aerogels. There are 24 experimental data in training and test sets (Table 1). Six different training algorithms are used to predict experimental results.

A neural network is implemented with a three layer feed-forward structure, an input layer, a hidden layer and an output layer. The designed neural network has 3 input and 2 output neurons as shown in Fig. 3.

Table 1 The experimental data used to form the training and test sets.

Samples	Input 1 of NN	Input 2 of NN	Input 3 of NN	Output 1 of NN	Output 2 of NN
	M/P	Reactant content (g/100mL)	Catalyst content (mol/L)	Pore diameter(nm)	Volume adsorbed (cm^3/g)
S(1)	0.05	5	0.02	10.3	1.5
S(2)	0.05	10	0.05	9.5	1.3
S(3)	0.05	15	0.1	7.5	1.1
S(4)	0.05	20	0.2	6.9	0.9
S(5)	0.1	5	0.02	8.7	1.4
S(6)	0.1	10	0.05	7.6	1.1
S(7)	0.1	15	0.1	5.4	0.75
S(8)	0.1	20	0.2	3.8	0.68
S(9)	0.2	5	0.02	14.1	1.9
S(10)	0.2	10	0.05	11.2	1.6
S(11)	0.2	15	0.1	8.1	1.0
S(12)	0.2	20	0.2	7.3	0.96
S(13)	0.4	5	0.02	8.6	2.1
S(14)	0.4	10	0.05	15.3	1.9
S(15)	0.4	15	0.1	11.9	1.6
S(16)	0.4	20	0.2	8.1	0.79
S(17)	0.6	5	0.02	20.8	2.6
S(18)	0.6	10	0.05	19.2	2.4
S(19)	0.6	15	0.1	17.1	2.1
S(20)	0.6	20	0.2	15.4	1.6
S(21)	0.8	5	0.02	28.6	2.9
S(22)	0.8	10	0.05	24.2	2.6
S(23)	0.8	15	0.1	22.1	2.5
S(24)	0.8	20	0.2	16.5	1.3

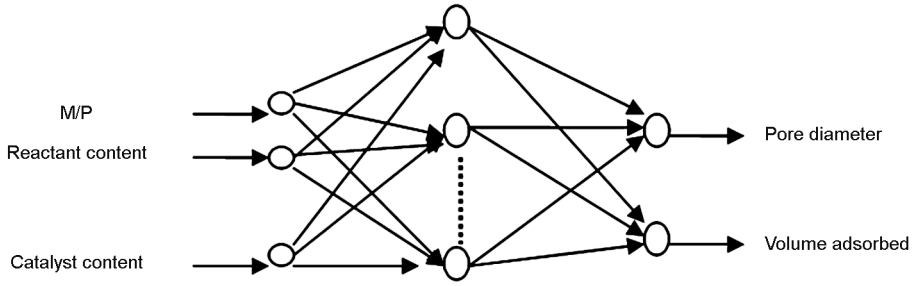

Fig. 3 The topology of involved neural network.

4.1 Architecture optimization of neural network

In the neural network based model, too few hidden neurons will hinder the learning process and too many will depress the predictive abilities of the ANN owing to the overtraining. To make the model computationally efficient, experiments show that a constant bias added to the input signal can affect learning time.

Bias is set up to improve the accuracy and speed of convergence. For choosing the best bias, the MSE of network simulation and actual results are tested. According to the demand of material design accuracy, MSE is less than 0.2. Normally, bias should be set to a small value, and the smaller is the value, the higher is the precision, but too small of the value would affect the convergence speed. However, if bias is too big, it will speed up convergence at the beginning of the simulation, but when it is near the optimum point of 0.37, it will produce an oscillation and a reduce convergence. Therefore, bias is chosen as 0.37 in this paper.

In this paper, bias is added to the input signals that are near the centers of the training functions, where the learning rate is highest. Another way to

make the model computationally efficient is to search for a theoretical optimal number of hidden units.

The coefficient of the learning rate (μ) and its corresponding decrease factor (μ_d) are two important parameters and play an important role in the design of a structure based on diameters and volumes of pores in the prediction model. In general, the architecture of a neural network in the model is predetermined based on a prior knowledge of nonlinear system or designer's experience. In this section, a GA-based method is developed to optimize the architecture of neural network based models. The aim of this section is to search for the feed-forward network architecture with an optimal hidden layer neuron number and other structure parameters by GA.

4.1.1 Genetic algorithm

GA, based on a direct analogy to Darwinian natural selection and genetics in biological systems, is a promising alternative to conventional heuristic methods. Based on the Darwinian principle of 'survival of the fittest'[19,20], one of the most important problems of GA is, as in the ANN case, the premature convergence to local minima due mainly to the tendency of the best individuals to maintain their genetic information across generations. In this paper, to avoid this problem, genetic algorithm is improved as following. N individuals are ranked from the best to the worst. The best and worst individuals (1-N) cross over, and then the second best and next-to-the-worst individuals (2-[N-1]) are selected. GA allows the characteristics of the 'bad' solutions to survive from one generation to another, giving more variability to the populations. So, the search space is wide and results are not easily fallen into premature convergence.

4.1.2 Optimization process of genetic algorithm neural network

In the present work, the flowchart of GA-based neural network optimization model is shown in Fig. 4.

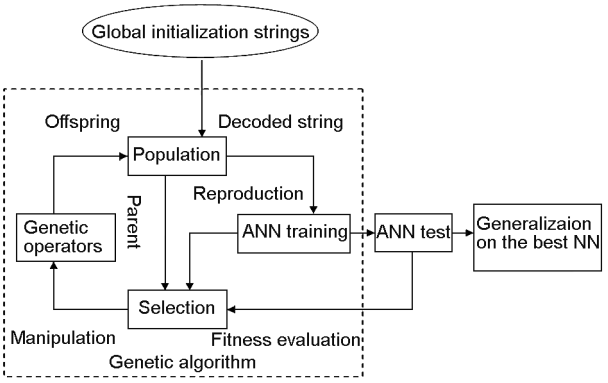

Fig. 4　A GA-based NN optimization model.

Many important issues for optimizing a topology, learning coefficient and learning coefficient decrease are as follows:

(1) Encoding

Before we apply a GA operation to find out the optimal architecture of neural network, an effective neural network encoding is needed to represent neural networks as a chromosome. We selected a binary coded system.

The numbers of hidden neurons and training parameters are represented by haploid chromosomes consisting of 'genes' of binary numbers. Each chromosome has three genes. The first gene represents the number of neurons in the middle layers of the network. The second and third genes represent the learning rate and learning coefficient decreasing factor.

(2) Crossover and mutation

In this study, crossover and mutation operators are used and the probabilities of the crossover and mutation operator are set to 0.85 and 0.01, respectively.

(3) Population size

There are no unified rules for determining the population size, but a population of 50-100 is typically used in GA. Once the population size is chosen, the initial population is randomly generated. So here, 80 random initial values are used to generate chromosomes. Hence in this study, the initial population pool value is set to 80 chromosomes.

(4) Fitness function

The structures of neural network are evaluated by the fitness function-mean square error. The optimal network architecture is obtained by helping to minimize the fitness function:

$$E = \sum_{k=1}^{N} e_k^2 / N \qquad (3)$$

where N is the number of training samples, e_k is the error between the actual and desired value of the k_{th} training sample.

4.2 Training algorithms

4.2.1 Description of Training algorithms

There are a few learning algorithms such as gradient-descent and Levenberg-Marquardt. It is difficult to predict which of these training algorithms will be the best one for any problem. Generally, it depends on some factors, the structure of the networks, in other words, the number of hidden layers, weights and biases in the network, aimed error at the learning. However, the datum structure and uniformity of the training set are also important things that can affect accuracy and performance. In this study, the prediction of pore diameter and volume of the MP/RC/CC carbon aerogels have been analyzed by using six different training algorithms. The used training algo-

rithms are Levenberg-Marquardt (LM), Bayesian Regularization Algorithm (BRA), Batch Gradient Descent with Variable Learning Rate and Momentum (VLM-BGD), Resilient Back Propagation (RBP), Normalized Least Mean Square (NLMS) and Recursive Least Squares (RLS).

The training and test data are used to evaluate each of training algorithms. The fundamental principles of six training algorithms are given in Table 2. During the training process, the weights and biases of the network are adjusted to obtain a minimized error and a high-performance solution.

Table 2 Training algorithms description.

Training function	Description
Trainlm	Levenberg-Marquardt(LM)
Trainbr	Bayesian Regularization Algorithm(BRA)
Traingdx	Batch Gradient Descent with Variable Learning Rate and Momentum(VLM-BGD)
Trainrp	Resilient Backpropagation Algorithm(RBP)
Trainnnnlms	Normalized Least Mean Square (NLMS)
Trainnnrls	Recursive Least Squares (RLS)

4.2.2 Evaluation of the training algorithms

Generally, for each neural network using various training algorithms, the decision-making process involves the following steps: (i) constitute a database for each neural network; (ii) analysis and normalization of data; (iii) train neural network using each training algorithm and (iv) test the trained networks.

Each of the training algorithms is tested by these ways: (i) the data, which are not used during the training procedure, are used to test training algorithm; (ii) MSE is used to analysis the error; (iii) the neural network predicting data are compared with the experimental data to evaluate the learning performance.

At the beginning of the training phase, the learning coefficient is set to 0.02. The weights of the ANN are randomly initialized between 0 and 1. For the given input data, the response of each neuron in the output layer is then calculated and compared with the corresponding real output response. Then, the prediction error associated with the output response is computed and sent back to the previous layers, and the weights are adjusted to reduce the prediction error using the six training algorithms.

The weights are modified for each set of the training data. That is, the weights are optimized 500 times and every time the input data set is fed to the ANN. This process is repeated many times until the prediction error is reduced to around 5%.

4.2.3 Simulation results of training algorithms

Comparative studies of pore diameter between the neural network simulation results from different training algorithms and experimental ones are carried out. From Table 3, the predictive results obtained from BRA, VLM-BGD, RLS agree well with experimental results, and their predictive errors are slightly lower than RBP and NLMS. On the other hand, the predictive results from LM training algorithm are better than others.

Comparative studies of pore volume between the neural network simulation results from different training algorithms and experimental ones are carried out. From Table 4, the error of the RBP and NLMS training algorithm are larger than the others. VLM-BGD training method has a much smaller error than the others. Predictive results of LM are closer to those of the BRA method.

Table 3 Comparison of pore diameter between predictive results and experimental results of the different training algorithms.

Samples	Experimental	Neural network predictive results to various training algorithms					
	Pore diameter(nm)	LM	BRA	VLM-BGD	RBP	NLMS	RLS
S(1)	10.3	10.32	10.47	10.44	10.58	10.53	10.41
S(3)	7.5	7.48	7.64	7.68	7.74	7.65	7.56
S(5)	8.7	8.66	8.54	8.57	8.49	8.56	8.78
S(7)	5.4	5.34	5.25	5.24	5.36	5.21	5.50
S(9)	3.8	3.85	3.63	3.56	3.67	3.55	3.59
S(11)	8.1	8.07	8.24	8.21	8.39	8.19	8.22

S(16)-S(24) and the other twenty independent data are used to test ANN. MSE is a good criterion to evaluate of neural network model. Errors of training and test sets are computed and compared in Fig. 5, where the change of MSE values for each training method is given for 600 iterations. The accuracy of

the Levenberg-Marquardt method is evidently seen. Normally, it has the computational complexity, however it can give the results with a much great accuracy.

So, Levenberg-Marquardt back propagation is selected as the optimal training algorithm.

Table 4 Comparison of volume adsorbed behaviours between predictive results and experimental results of different training algorithms.

Samples	Experimental	Neural network predictive results to various training algorithms					
	Volume adsorbed behaviours(cm^3/g)	LM	BRA	VLM-BGD	RBP	NLMS	RLS
S(1)	1.5	1.46	1.48	1.52	1.48	1.57	1.44
S(3)	1.1	1.05	1.06	1.07	0.96	1.01	0.93
S(5)	1.4	1.47	1.43	1.42	1.57	1.45	1.43
S(7)	0.75	0.80	0.79	0.76	0.82	0.79	0.78
S(9)	1.9	1.81	1.84	1.85	1.74	1.80	1.88
S(11)	1.0	0.97	1.03	1.02	1.11	1.12	0.95

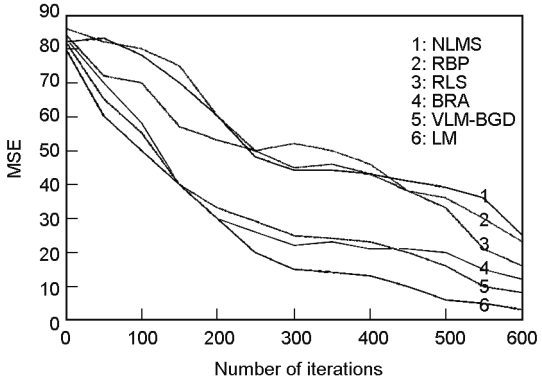

Fig. 5 Comparison of MSE curves versus number of iterations for training methods.

4.3 Optimization results of GA neural network

Once the training algorithm (Levenberg-Marquardt backpropagation) is selected, we need to optimize the topology of the network and other parameters. Optimum values of the number of hidden neurons, learning coefficient and decrease factor have been obtained after using GA. The optimized number of hidden neurons is 7, and the optimized learning coefficient and decrease factor are selected as 0.02 and 0.9, respectively.

For checking on the validity of the optimized number of hidden neurons, 6-12 neurons in the hidden layer are tested. Different trainings are carried out for seven topologies by using the optimized μ and μ_d. Fig. 6 shows how the correlation coefficient decreases by 6-12 hidden neurons, from which the minimum errors are obtained using the topology of 3, 7, 2 (3 nodes in the input layer, 7 hidden neurons and 2 neurons in the output layer). In order to evaluate the optimized learning coefficient and decrease factor, how the predictability of the pore diameter and volume changes with learning coefficient (from 0.001 to 1) and learning coefficient decrease factor (from 0.1 to 1) is discussed. When the number of hidden neurons is 7, Fig. 7 shows how the predictability of the pore diameter changes with μ and μ_d, and Fig. 8 shows how the predictability of the pore volume changes with μ and μ_d, from which the prediction errors of pore diameter and volume are minimal when the optimized learning coefficient and decrease factor are selected as 0.02 and 0.9, respectively.

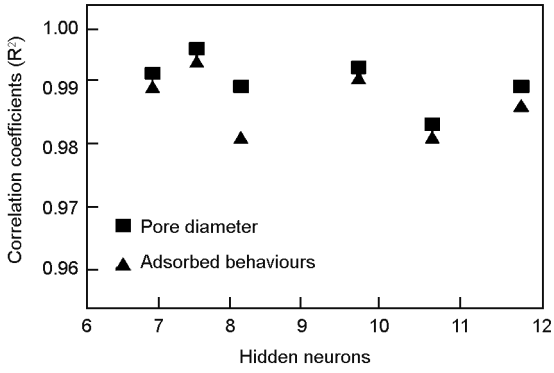

Fig. 6 Correlation coefficients (R^2) for pore diameter and adsorbed behaviors predictions depending on the number of neurons in the hidden layer.

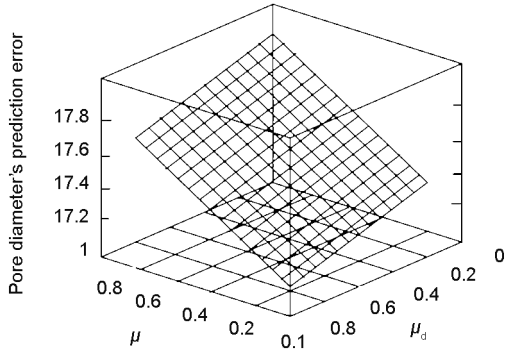

Fig. 7 Pore diameter's prediction error surfaces of the learning coefficient and its decrease factor.

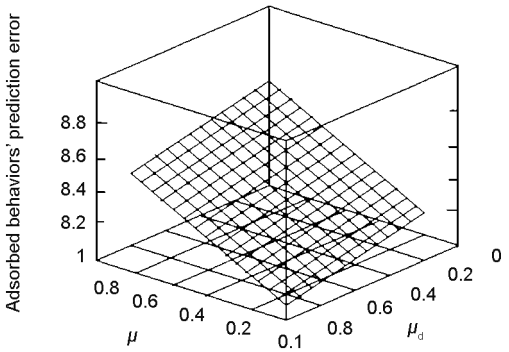

Fig. 8 Adsorbed behaviors' prediction error surfaces of the learning coefficient and its decrease factor.

5 Prediction and verification results of GA neural network model for MP/RC/CC carbon aerogels

To evaluate the neural network architecture, parameter and optimal algorithm, the prediction data (S (1)-S (16)) and validation data (S (16) -S (24) and the other twenty independent test data are selected as appraisal test data. In this step, the optimized topology (3, 7, 2) and the selected μ (0.02) and μ_d (0.9) are used.

Fig. 9 shows pore diameter (Fig. 9a) and volume (Fig. 9b) versus the corresponding predicted data.

In Fig. 9, the prediction results are in good agreement with experimental data. Moreover, the prediction performance of the model for pore diameter and volume are evaluated by the correlation coefficients (R^2) between the predicted and experimental values and root-mean-square prediction error (RMSEP).

A good model should be with a high R^2 value and a low RMSEP value. RMSEP is calculated by Eq. (4).

$$\mathrm{RMSEP}=\sqrt{\sum_{i=1}^{n}(y_{\mathrm{pi}}-y_{\mathrm{ni}})^2/(n-1)} \qquad (4)$$

Where y_{pi} is prediction value of the model, y_{ni} is experimental value and n is the number of predicted samples.

According to Eq. (4) and Fig. 9 (a), (b), the correlation coefficients of pore diameter and volume of MP/RC/CC carbon aerogels are 0.992 and 0.981, respectively, and the root-mean-square prediction errors of RMSEP are 0.077 and 0.054, respectively.

It is found that the predicted data of the model are in good agreement with the experimental data. A high correlation between experimental data and neural network model data of pore diameter and volume is obtained. Meanwhile, the network prediction has less root mean square error. Through the above analysis, it is revealed that the neural network model has good performances such as high accuracy and easy to implement by choosing adapted training function, optimized structure and parameters.

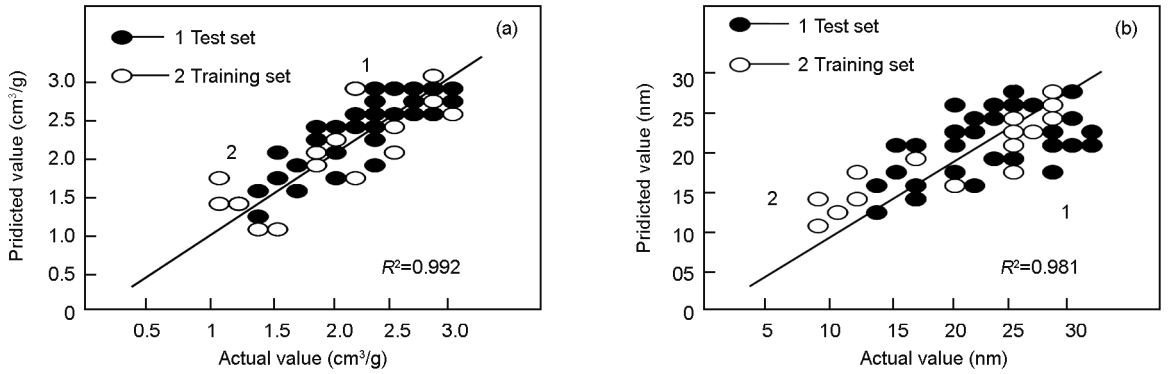

Fig. 9 Correlation plots between prediction and actual values for the MP/RC/CC carbon aerogels: (a) Pore diameter versus predicted values and (b) adsorbed behavior versus predicted values.

6 Conclusions

Quantitative data on the pore structure such as the diameter and volume of pores are essential to carbon aerogels. Traditional experimental design method is inefficient, costly and cannot meet pore structure controlling and predicting requirements.

In this paper, a kind of neural network is proposed to predict and optimize pore structure of carbon aerogels. To obtain an optimized ANN, ANN topology and learning coefficients are discussed. Then, various training algorithms based on learning performance of the controlling and predicting neural network model are investigated. The conclusions of this study are as follows.

GA NN-based model is adopted to select the ANN topology and to optimize the learning coefficient

and learning coefficient decrease factor. It is shown that ANN topology can be designed successfully.

An artificial neural network for carbon aerogels preparation has also been optimized through a proper selection of the training algorithms. Different ANNs, trained with different learning functions, have been assessed on their predictive ability. It is confirmed that the Levenberg-Marquardt is the optimal training algorithm.

Sixteen experimental data are used to train the neural network based model, and thirty-six validation tests are used to verify the effectiveness and robustness of the neural network architecture. The root-mean-square prediction errors for pore diameter and volume are 0.077 and 0.054, respectively. Also, the correlation coefficients (R^2) clearly show that the optimized neural network model has a precise predictability. Furthermore, comparisons between experimental data and numerical simulation results reveal that the predicted data agree well with experimental ones. It is proved that the pore structure of carbon aerogels can be simulated by the neural network model, which can be used to guide scientific and engineering research.

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