Prediction of Chemical Production Based on Neural Network

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

Review Article

ABSTRACT

As an important part of artificial intelligence and machine learning, artificial neural network (ANN) has been widely used because of its strong information processing and autonomous learning capabilities. In this paper, the development history of ANN is summarized, and the three common types of ANN are introduced: MLP neural network, BP neural network and recurrent neural network. Finally the practical application of ANN in chemical production forecasting are analyzed and an outlook on its development direction is prospected.

1. INTRODUCTION

Artificial neural network (ANN) is an algorithmic mathematical model that imitates the behavioral characteristics of animal neural networks for distributed parallel information processing. The artificial neural network refers to the animal brain neural network, and uses computer technology to process information. Its core is mathematical algorithm, and the calculation is realized by computer software and hardware [1]. The basic structure is shown in Fig. 1. The operation of the artificial neural unit simulates the operation of nerve cells, and the organizational structure of the neural network of the brain is also its inspiration [2]. Today, artificial neural network, as the core technology of artificial intelligence, has been widely used in face recognition, speech recognition, image recognition, automatic driving and other fields. With the development of artificial

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intelligence technology, its importance has become increasingly prominent, and it is worthy of further study.

In the chemical process, when it involves the interaction of various experimental factors and even human operations in a specific chemical reaction system, the traditional method may make the problem difficult to solve. The "black box" nature of artificial neural networks highlights great advantages. Starting from the development history and types of artificial neural network, this paper focuses on the application of neural network in chemical production forecasting, and forecasts the development prospect of artificial neural network in chemical industry.

2. THE DEVELOPMENT HISTORY OF ARTIFICIAL NEURAL NETWORK

In 1943, McCulloch and Pitts [3] published a paper called "A logical calculus of the ideas immanent in nervous activity", in which they proposed the concept of artificial neural networks and the mathematical model of artificial neurons (MP model). It is generally believed that the MP model is the starting point of the artificial neural network. In order to commemorate, the MP model is named after the initials of the two people's names. The original MP model did not have an algorithm for adjusting the weights. In 1949, Hebb proposed that information in neural networks is stored by connecting weights. Since then, the research on the adjustment algorithm of the weight has been carried out. The realization of the different functions of the current neural network is realized by adjusting the weight of the artificial neural network.

In 1957, Rosenblatt [4] proposed the concept of "perceptron". In fact, perceptrons still fall under the category of MP models, but introduce the concept of machine learning. The perceptron can manually adjust the weights through the error learning algorithm, and continuously optimize the output value, so that the predicted results gradually approach the actual results. The perceptron is arguably the first artificial neural network in the true sense. The proposal of the perceptron set off the first upsurge of neural network research in the 1960s. Constrained by the times, people simply believed that any problem could be solved as long as a large number of neural units were combined together. In 1969, Minsky and Pepert [5] pointed out that perceptrons can only solve simple linear problems, and multi-layer networks must be used

to solve nonlinear problems, and the actual role of multi-layer networks cannot be proved for the time being. Because of Minsky's huge influence in the field of artificial intelligence, this view has a direct impact on the research of artificial neural networks.

Hopfield [6,7] proposed the "Hopfield Neural Network" (HNN) and designed the electronic circuit of the network, providing a physical proof for the usability of the model. Rumelhart et al. [8] published Learning representations by back-propagating errors and discovered the BP algorithm (error back-propagation algorithm). The error back-propagation algorithm is still one of the very basic algorithms in artificial neural network, and it has been widely used in existing artificial neural network models.

The BP algorithm enables the artificial neural network to have the ability of self-learning and generalization, but it also has obvious defects, that is, when the number of network layers is large, it is easy to fall into the local optimal solution, and it is easy to produce overfitting. And the computer system at that time could not support the operation of huge data sets. In 1995, Cortez and Vapnik [9] proposed the "Support Vector Machine" (SVM). This method has no local optimum problem and can obtain ideal results with a small number of samples. Therefore, when the development of BP algorithm encounters a bottleneck, some researchers turn to the research of SVM. LeCun [10], the inventor of convolutional neural network, insisted on researching artificial neural network, and published "Deep Learning: Towards Building Truly Intelligent Machines" in 1998, so he is called the father of convolutional neural network.

In 2006, the research group of Hinton [11] (Who previously proposed the BP algorithm) proposed the concept of deep network and deep learning. Deep network is a multi-level artificial neural network. With the rapid development of computer technology, the computing speed of computers has been greatly improved, and big data and cloud computing have gradually become a reality. Since then, artificial neural networks have been increasingly used in many fields, including image recognition [12-14], traditional Chinese medicine processing [15-17], wireless signal processing [18-20], security risk assessment [21-23], process control and optimization [24-26], medical assisted treatment [27-29], forecasting [30-32], aquatic products, [33-35] intelligent driving [36-38], and so on.
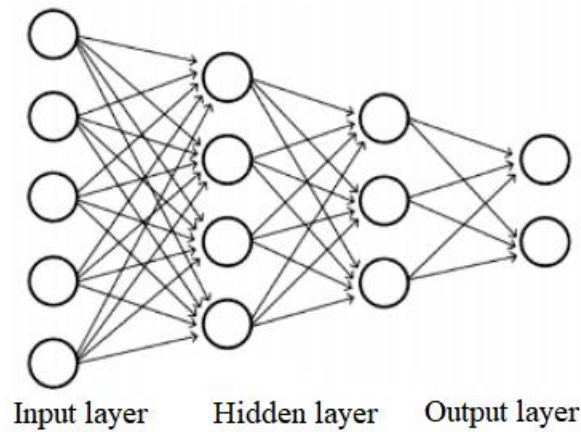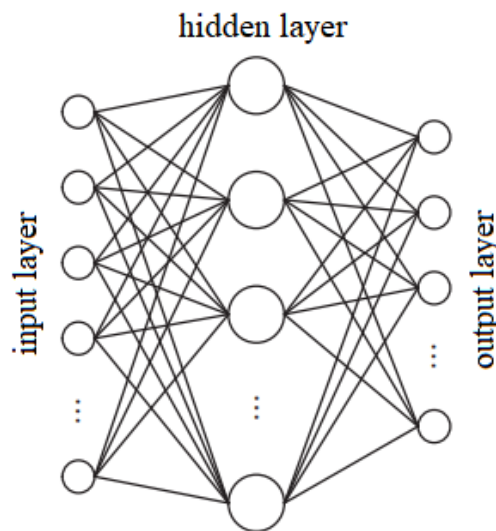
Fig. 1. Artificial neural network structure

Fig. 2. Schematic diagram of MLP structure

3. SOME KINDS OF COMMON ARTIFICIAL NEURAL NETWORKS

3.1 MLP Neural Network

MLP (Multilayer Perceptron) with excellent nonlinear matching and generalization capabilities is as shown in Fig. 2. Training the MLP with the backpropagation algorithm reduces the global error between the MLP output data and the actual desired data.

Although MLP architectures have many advantages, they are relatively inefficient in high-dimensional spaces, which can lead to over fitting in model training. And because the existence of the hidden layer increases the number of parameters, the training process needs to deal with a high amount of calculation when the convergence is slow. In the traditional MLP real-valued model, the data input that a single neuron can receive is a single real number, which usually fails to achieve satisfactory results when it performs multi-dimensional signal input [39]. At present, the cross-validation commonly used in MLP has high complexity and is limited by the total amount of data, resulting in insufficient generalization ability of MLP.Multilayer feedforward neural network. Chen et al. [40] applied it to the study of a large number of meteorological data, and obtained the MLP after training the observation point 1 data processed by the genetic algorithm. However, the accuracy of observation point 2 is significantly lower than that of observation point 1. This indicates that the generalization ability of MLP still needs to be improved.

3.2 BP Neural Network

The network architecture of the BP neural network model is multi-layered, which is essentially a gradient descent local optimization technique, which is related to the backward error correction of the network weights. The multi-layer structure of BP neural network makes the output of the model more accurate. The internal structure of BP neural network determines its good nonlinear mapping ability, self-learning ability and fault-tolerant performance. It can capture and store complex mapping relationships through learning when the mechanism of each factor is unclear. Therefore, when the BP neural network is applied to a complex reaction system, training and verification with an appropriate amount of experimental data can simplify the association process between the influencing factors and the target quantity [41]. The structure of BP neural network is shown in Fig. 3.

However, when using BP neural network, there may be a local minimum, which makes it impossible to find the global optimal solution, and in the face of large sample data, the mean square error is too large, which makes it difficult to converge. Based on this situation, it is a common solution to change the excitation function, add an adaptive learning rate and add a momentum term during each iteration of the network. It can be known from the derivation process of the error that its first derivative is related to the first derivative of the excitation function between each layer. Therefore, when optimizing the excitation function, in addition to determining the optimal combination of traditional excitation functions according to the actual problem, other functions such as trigonometric functions, bipolar functions and sigmoid functions with steepness factors can be added [42].

Based on considering the error gradient adjustment direction of the current cycle and the previous cycle at the same time, and adjusting the weight threshold to improve the network convergence speed, Rumelhart et al. [8] proposed the idea of adding a momentum term. At the same time, the learning rate is also an important parameter in the network adjustment process. It is adjusted according to the error of the network this time and the error of the previous cycle. The increase of the error reduces the learning rate to stabilize the network structure. On the contrary, the learning rate is increased to speed up the iteration speed, so it can effectively improve the efficiency of the network. In the process of BP neural network training, the simultaneous use of adaptive learning rate and momentum factor can not only reduce the number of training oscillations, but also improve the convergence speed.
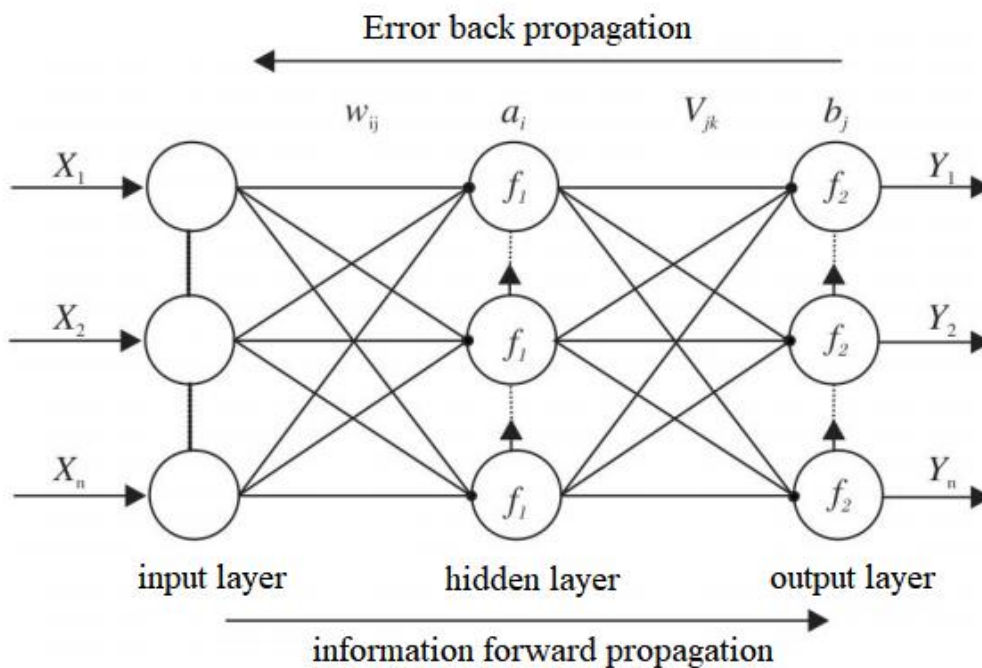

Fig. 3. BP neural network structure

3.3 Recurrent Neural Networks

Recurrent Neural Network (RNN) is an artificial neural network based on sequence modeling, which can transmit data information laterally between neurons and express the correlation between some data. Its structure is shown in Fig. 4. The characteristic of RNN is that the neurons in the hidden layer are connected to each other, so that the time-related input information in the sliding window can be sequentially transmitted, and the temporal correlation between distant events in the time dimension can be considered.

The hidden layer structure of the recurrent neural network RNN makes it widely used in time series prediction. Wei et al. [43] applied the recurrent neural network and several other artificial neural network models to the experimental data of pore water pressure respectively. The conclusion that the model with RNN structure is more accurate when targeting time series data is obtained. In particular, the LSTM and GRU structures in the recurrent neural network can describe the time-delay effect between the input and the response, which is more accurate and reliable than the standard recurrent neural network. Ling et al. [44] applied RNN to the fault prediction of nuclear power machinery, and proposed an intelligent fault prediction method. The data after PCA dimensionality reduction was passed to the complete RNN model, and an alarm was generated in advance according to the speed and vibration signals. The experimental results show that the RNN model can effectively identify faults during creep.

The recurrent neural network also has the following shortcomings: the traditional RNN will produce gradient disappearance, and the accuracy will be greatly reduced when dealing with long-term data dependence, the input and output data sequences do not match, and the missing information caused by the parameter sharing of the model may have an impact on the time series features. RNN encodes the previous hidden state of each node as the historical information of the whole model, but ignores the independent relationship between each node. In view of the limitations of traditional models, improved structures such as LSTM and GRU are proposed [45], which will not be introduced in this paper due to space limitations.

4. APPLICATION OF NEURAL NETWORK IN CHEMICAL PRODUCTION FORECASTING

4.1 Electrodialysis Desalination Prediction

The experimental study found that the change of the desalination rate of the electrodialysis unit has strong nonlinear characteristics [46]. To make a more accurate prediction, a prediction method that can capture the nonlinear change law needs to be adopted. Artificial neural network is an adaptive nonlinear dynamic system composed of a large number of neurons through extremely rich and perfect connections. It does not need to understand the relationship between input and output, and is very suitable for modeling research of nonlinear systems. Therefore, Li et al. [47] used the improved BP algorithm to predict the desalination value of electrodialysis.

270 groups of experiments were carried out under the conditions of different inlet NaCl solution concentrations, different voltages across the plates and different experimental temperatures. The conductivity of 270 thin chamber solutions was measured with a conductivity meter, and the conductivity measured experimentally was converted into concentration. Measure the NaCl concentration in the fresh room, and use the Equation (1) to calculate the desalination rate SP.

$$SP = \frac{(C_0 - C)}{C_0} \times 100\%$$

(1)

According to these data, the BP algorithm is used to predict the separation rate of the model under different conditions, then there are 4 input vectors of BP, namely concentration C, voltage V, temperature T and flow rate Q, then the output vector is 1, namely the model desalination rate SP . 220 groups were selected as training data, and the remaining 50 groups were used as test data.

Using a single hidden layer BP neural network to predict, since the input sample is a 4-dimensional input vector, there are 4 neurons in the input layer. The network has only 1 output data, so the output layer has only 1 neuron. Calculate the number of neurons in the hidden layer z by Equation (2).
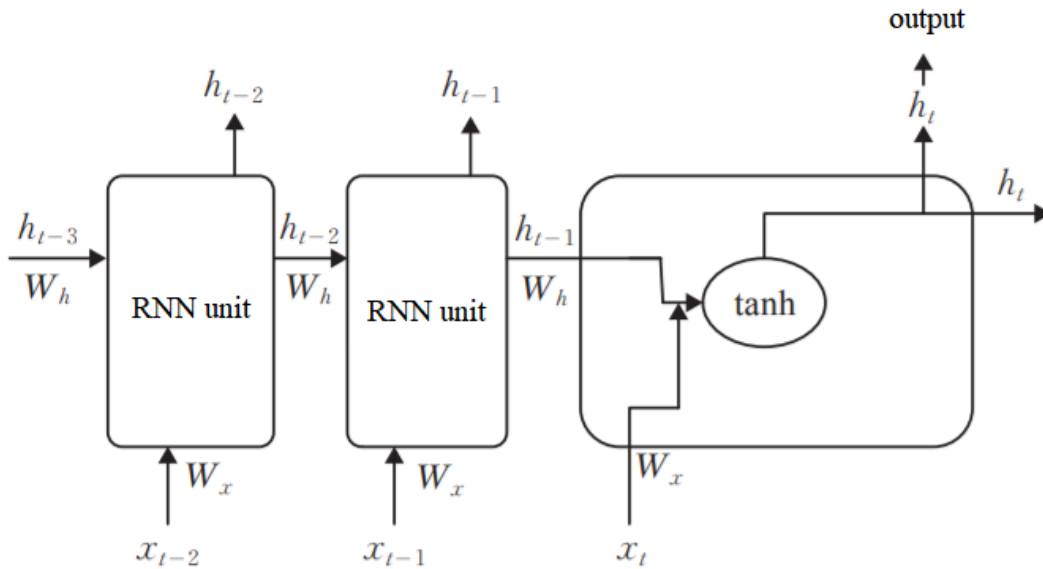
Fig. 4. Schematic diagram of RNN structure

$$z = \sqrt{x + y} + a \qquad (2)$$

Where *x* is the number of input units, y is the number of output neurons, and *a* is a constant between [1, 10]. The number of neurons in the hidden layer is 8, so the network is a 4×8×1 structure. The experiment was performed multiple times under Matlab 7.8.0, and a set of

data with the smallest average error and the best training result was obtained. The error after 2000 training runs is shown in Fig. 5.

After calculating the normalized data, plot the predicted and experimental values as shown in Fig. 6 where "+" is the actual value, and "o" is the predicted value.
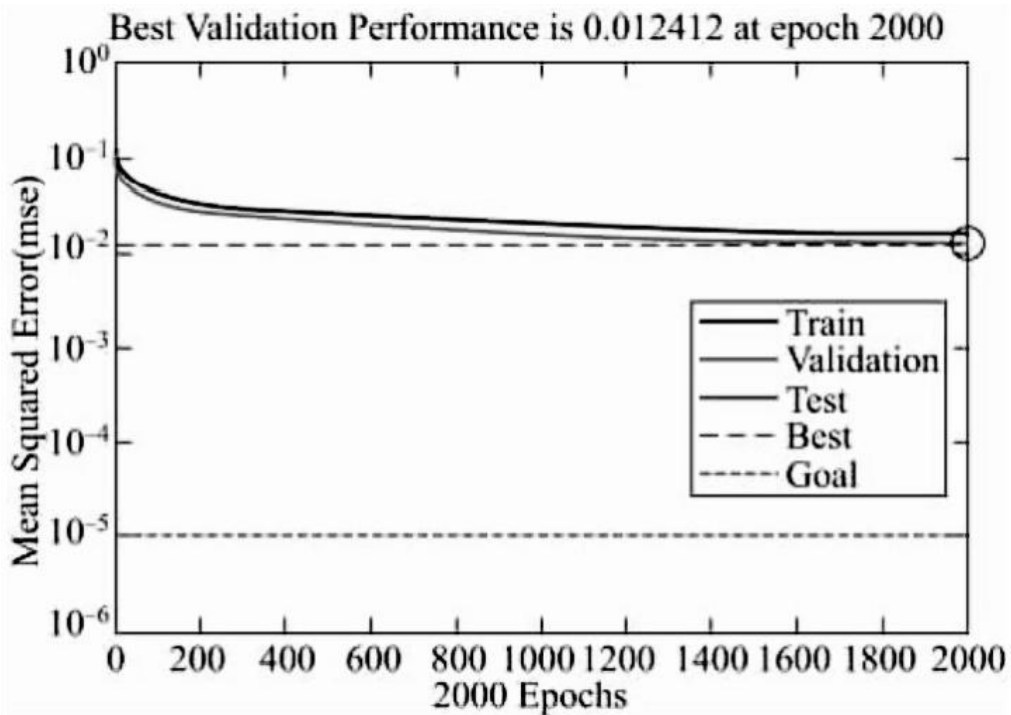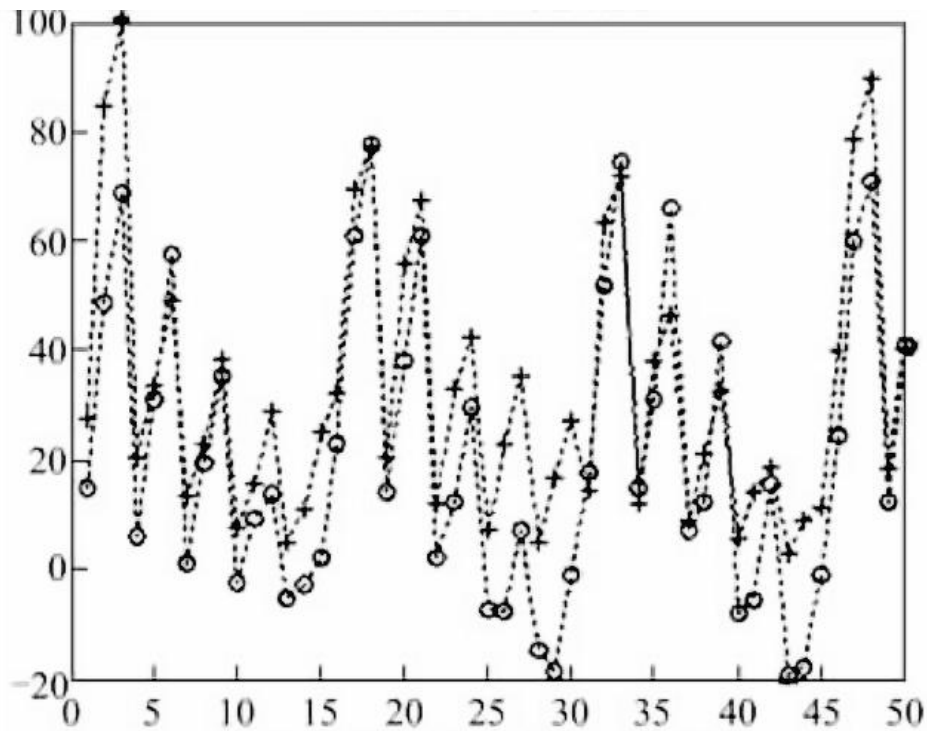

Fig. 5. Error results [47]

Fig. 6. Deviation between predicted value and true value [47]

According to the experimental data obtained from the electrodialysis model, BP and improved BP neural network can be established to predict the NaCl desalination rate of the electrodialysis model. Applying it to the actual production is used to predict the desalination rate of the electrodialysis unit, so that managers can adjust the operating conditions in time according to the desalination rate value to ensure the normal and stable operation of the desalination unit.

4.2 Prediction of Particle Size by Cyclone Separator

As a commonly used centrifugal gas-solid separation equipment, cyclones are widely used in industrial scenarios such as solid dust collection, circulating fluidized bed, petroleum catalytic cracking, and aerosol sampling [48-50]. The fractional particle size is an important parameter for evaluating the separation performance of a cyclone, and a small fractional particle size generally means high separation performance [51]. Liu [52] et al. constructed a segmentation particle size prediction model based on BP neural network (BPNN) by correlating the global size parameters and operating parameters of the cyclone separator. The BPNN model is optimized by comparing the combined prediction performance of different

algorithms and the number of neurons in the hidden layer. Finally, the prediction performance of the BPNN segmentation particle size model is evaluated and compared with other theoretical models, semi-empirical models and multiple regression models.

4.2.1 Parameter selection

The cyclone separator mainly includes 8 structural size parameters, as shown in Fig. 7, which are the inlet height a, the inlet width b, the diameter De of the exhaust core pipe, the insertion depth S of the exhaust core pipe, the height of the cylinder body h, and the total height H , Dust outlet diameter B, cylinder diameter D. Their changes have different degrees of influence on the segmentation particle size [53]. Since too many input parameters will increase the complexity of the BP neural network model, it is necessary to reduce the data dimension to improve the quality of the model. In addition, the dimension of the input and output parameters is 1 to further simplify the model. After a series of simplification processing, finally choose Re_{ann}, D_s/D, S/D as the input parameters of BP neural network and $\Psi_{0.5}$ as output parameters.

$$Re_{ann} = \frac{\rho_g Q(D-D_e)}{\mu a b} \tag{3}$$

$$\Psi_{0.5} = C^{1/2}d_{p0.5}/D \qquad (4)$$

$$\frac{D_s}{D} = \left\{ \frac{\frac{h}{D}+\frac{1}{3}\left(\frac{H}{D}-\frac{h}{D}\right)\left[1+\frac{B}{D}+\left(\frac{B}{D}\right)^2\right]^{0.5}}{\frac{H}{D}} \right\} \qquad (5)$$

4.2.2 Model establishment

In order to compare the influence of different number of neurons and training algorithm on the prediction performance of BP neural network, L-M algorithm, quasi-Newton algorithm and Bayesian regularization algorithm are used to compare the prediction performance. Each training algorithm predicts $\Psi_{0.5}$ with 6, 7, and 8 neurons in the hidden layer. In order to avoid the influence of the randomness of the initial weights and thresholds of the network, the BP neural network of each combination is run 10 times continuously, and the 10-time mean of the evaluation index is selected for evaluation. The E^2 mean predicted for the training set and the test set is shown in the Fig. 8.

It can be seen that under the same training algorithm, the use of different numbers of neurons in the hidden layer has an impact on the prediction accuracy of the training set and the test set. By comparison, when the number of neurons in the hidden layer is 6 and 8, the E^2 of

each training algorithm is greater than the E2 when the number of neurons is 7. Therefore, 7 is the optimal number of neurons in the hidden layer. Among them, the Bayesian regularization algorithm shows the best prediction performance. Therefore, the Bayesian algorithm with adaptive regularization parameters can better avoid the problems of under-fitting and over-fitting during network training, thereby ensuring the robustness and generalization performance of the BP neural network. Therefore, when the number of neurons in the hidden layer is 7, the BP neural network based on the Bayesian regularization algorithm is selected to establish the BR-BPNN segmentation particle size model.

4.2.3 Prediction results

The assignment of initial weights and thresholds of BPNN is random, which will result in different weights and thresholds for the final iteration of each run. In order to determine the optimal weights and thresholds of the BP neural network, the BR-BPNN segmentation particle size model was used to predict the training set and the test set for 10 consecutive times. Comparing the E^2 obtained each time, as shown in Fig. 9, it can be seen that the E^2 obtained by the ninth prediction of the training set and the test set is the smallest among the 10 times, which are $1.73×10^{-10}$ and $8.639×10^{-11}$ respectively.
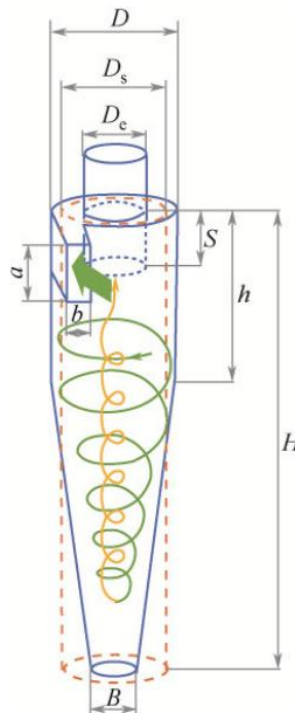

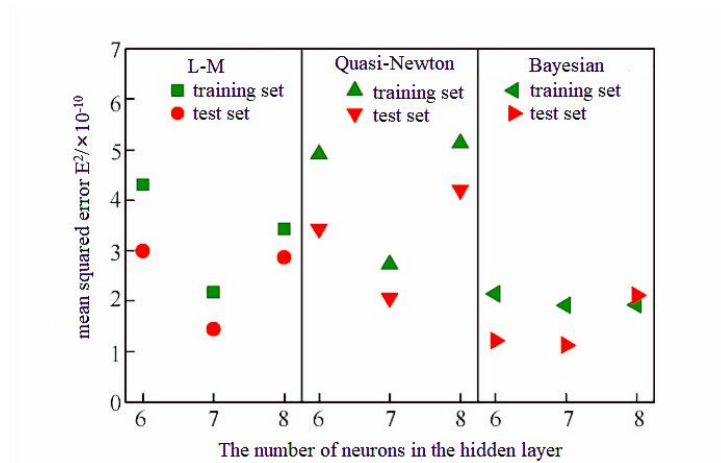
Fig. 7. Structure and dimensions of the cyclone separator [52]

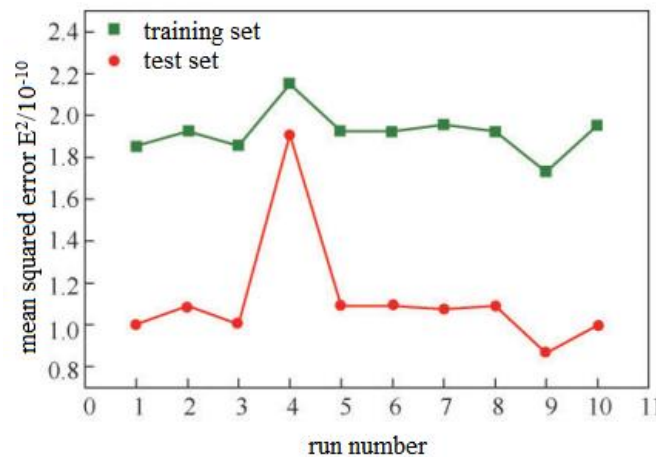**Fig. 8. Comparison of different BP neural network models E^2**

Fig. 9. Comparison of different BP neural network models E^2 [52]

Fig. 10 shows the comparison between the predicted value of the BR-BPNN segmentation particle size model and the measured value of the cyclone segmentation particle size. It can be seen from the figure that the prediction R^2 of $\Psi_{0.5}$ in the training set and the test set is 0.972 and 0.987, and the BR-BPNN segmentation particle size model shows high prediction accuracy. The R^2 predicted for the test set is higher than the training set, which indicates that the neural network trained on the training set is successfully extended to the test set, and the reliability of the network is confirmed. At the same time, the reduction of the data dimension improves the quality of the BR-BPNN segmentation particle size model, and the data features can be effectively learned during the training process, thereby providing better prediction ability for new data. In summary, this model can be used as a new prediction model to predict the particle size of cyclone separators.

4.3 Risk Prediction of Hazardous Chemicals Production

Building a scientific and effective early warning indicator system is the premise and core content of establishing a risk early warning model for the safe production of hazardous chemicals. Through the comprehensive analysis of each effective early warning index, the weight of different early warning indicators is obtained. Each index contains multiple factors, which play different roles in early warning work. Some factors cannot be quantified and can only be evaluated qualitatively. In order to realize the quantification of key indicators and factors, it is necessary to comprehensively evaluate them with appropriate methods, so that the indicators can quantitatively express the safety status of hazardous chemicals reflected by the safety production risk early warning model as much as possible.

Artificial neural network (ANN) can simulate human thinking for logical reasoning, and can effectively solve nonlinear and linear prediction and early warning problems [54]. The BP algorithm can carry out supervised learning, and has super self-learning ability and nonlinear computing ability. Combined with computer technology, it can quickly realize comprehensive evaluation of multiple evaluation indicators [55]. In addition, BP neural network has rich application experience and has been successfully used in many monitoring and management systems, which can greatly improve system accuracy and logical fault tolerance. Its self-learning and adaptive characteristics can help it be effectively applied in risk early warning systems. Zhang et al. [56] applies the BP neural network computing method to establish a safety risk early warning model, which plays a positive role in the dynamic monitoring and early warning of hazardous chemicals.

4.3.1 Sample data selection

The accuracy of the risk early warning model is mainly related to the selection of early warning indicators, which can reflect the risk early warning level. Therefore, selecting reasonable early warning indicators is helpful to achieve accurate early warning. The risk warning of hazardous chemical production safety mainly starts from the physical and chemical properties of hazardous chemicals, storage status, detection parameters, meteorological parameters, environmental vulnerability and emergency rescue capabilities. Select multiple quantitative indicators such as temperature, pressure, liquid level, flow rate, fire alarm volume, fire alarm time, material risk, toxic and harmful gas concentration, ambient temperature, surrounding population density, distance from fire facilities and rescue capabilities. 20-30 groups of valid sample data are formed, and each group of data is input into the network for calculation, respectively, to obtain the risk level of each indicator, and gradually increase the sample self-learning frequency and reduce the sample error. After the learning, 10 groups of training results were selected for correlation testing, and the model was determined to be reasonable and effective. At the same time, the risk warning results of safe production of hazardous chemicals are divided into four levels, as shown in Table 1.
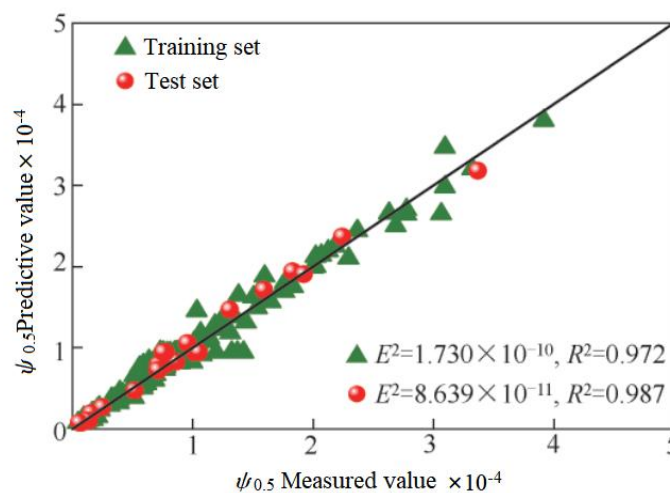

Fig. 10. Comparison between the predicted value and the measured value of the BR-BPNN segmentation particle size model [52]

Table 1. Risk warning level of hazardous chemical production safety 56

Number	Risk warning level	Risk description	expected output value
1	low risk	represented in blue	[1 0 0 0]
2	general risk	represented in yellow	[0 1 0 0]
3	medium risk	represented in orange	[0 0 1 0]
4	high risk	represented in red	[0 0 0 1]

4.3.2 Artificial neural network structure design

In the BP neural network topology, the input layer and output layer are single layers, and the hidden layer is single layer or multi-layer [57]. The model uses samples composed of multiple indicators for each set of data as input, and takes the early warning value of hazardous chemical safety production risk as output data, so the number of nodes in the input layer corresponds to the number of sample indicators, and the number of nodes in the output layer is 1. The hidden layer nodes are the most complex in the entire network. The number of hidden layer nodes directly affects the computing scale of the network space. The appropriate number of nodes can not only ensure the accuracy of the calculation results, but also ensure the calculation efficiency. The data dimension directly affects the transmission of sample data from the input layer to the hidden layer, so it is necessary to use the conversion function to convert the input data. The sigmoid tangent function tansig is used as the excitation function of the hidden layer neurons in the network construction of the dangerous chemical safety production risk early warning model.

4.3.3 Implementation of risk early warning model

The neural network toolbox in MATLAB is used to train the BP network on the sample data 56. Before inputting the sample data, the transformation function is used to normalize it, the method is the (0,1) normalization method. The calculation method is shown in Equation (6).

$$Y_i = \frac{x_i - x_{min}}{x_{max} - x_{min}} \tag{6}$$

Among them, Y_i is the normalized result of data i; x_i is the actual value of data i; x_{max} and x_{min} are the maximum and minimum values of the data group, respectively. The experimental results show that after 300 sets of training sets are input to the neural network training, the test results of 60 sets of test samples show that only 2 sets of data do not match the expected output. The neural network has a 97% recognition rate for chemical categories. Since the training sample set is limited, theoretically a certain number of training sample sets can make the combination of the weight coefficient and the threshold value in the neural network to make the actual output of the test sample closer to the expected output.
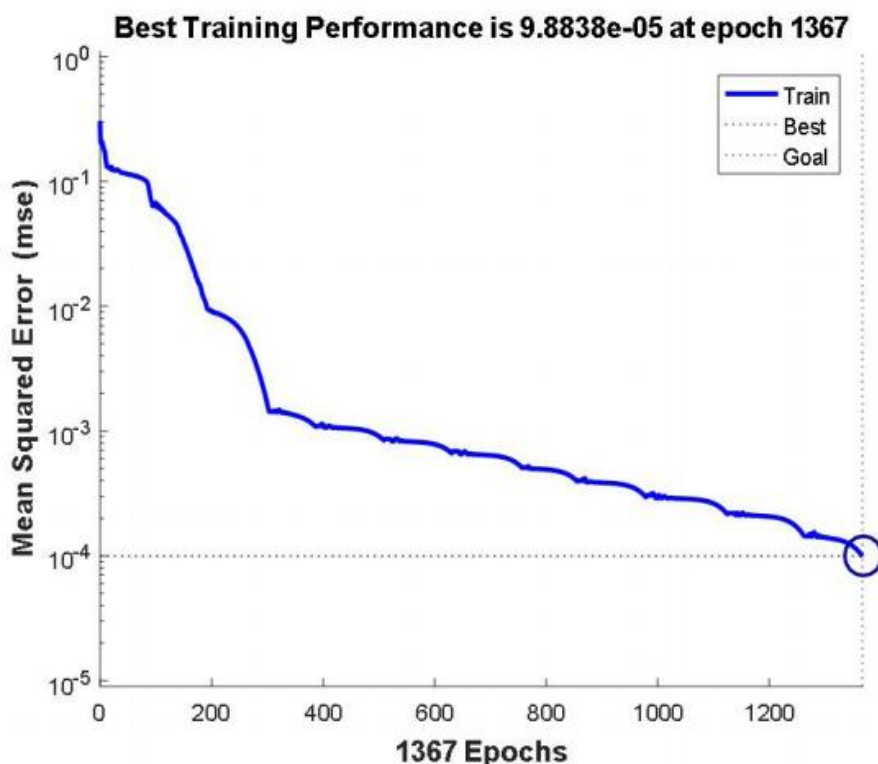

Fig. 11. Convergence of mean square error under the algorithm 57

5. CONCLUSION

In recent years, new breakthroughs have been made in the research of artificial intelligence technology, and data feature description models have been established in aspects such as quality control [58], physical property estimation [59], expert system [60], and cluster analysis [61]. The prediction accuracy of technologies including BP neural network, recurrent neural network, support vector machine, and convolutional neural network can meet the application requirements. However, the application of ANN in the field of chemistry and chemical industry still has a long way to go, and further theoretical and technical improvement is needed. In particular, how to effectively combine programming language with a complete set of chemical compound description symbols, reaction kinetics, molecular simulation, etc. in order to achieve the goal of intelligence and autonomous learning. This requires continuous optimization of the neural network model and further improvement of the corresponding database to ensure the accuracy of prediction. In the face of the system with complex structure of reactants and unclear reaction mechanism, using neural network to simulate small-scale experimental data for black-box analysis can greatly reduce the time and energy invested in research. To sum up, ANN has broad development prospects, and the continuous innovation and application will surely provide a powerful tool for chemical and chemical research.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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