



Optimization of Extraction Process 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.

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ABSTRACT

Liquid-liquid extraction is a chemical unit operation that utilizes the difference in solubility or distribution ratio of target components in two immiscible solvents to achieve separation, extraction or purification. There are many factors that affect the extraction efficiency, and it is difficult to quickly optimize the process using traditional methods. Artificial neural network is a system structure composed of multiple artificial neuron models, with functions such as self-learning, associative storage and fault tolerance. It can be used for optimization or control of multi-variable complex systems, and has been successfully applied to the extraction process of various products. optimization. This paper discusses the basic situation of artificial neural network, and analyzes the research progress of extraction process optimization based on neural network.

Keywords: Artificial neural network; model; extraction; application research.

1. INTRODUCTION

Artificial neural networks have the four basic characteristics of non-linearity, non-limitation, very qualitative and non-convexity [1]. They are mainly used to solve the two types of problems of regression and classification.

Artificial neural networks have been widely used in the fields of pattern recognition, intelligent robots, automatic control, predictive estimation, etc., and have helped solve many practical problems. For example, in the field of intelligent control, artificial neural networks can be used to control smart cars. Combine it with open CV for

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3D perception and object detection in unmanned driving technology. It can also make intelligent garbage classification more accurate in the field of garbage classification.

As the core technology of artificial intelligence, the importance of artificial neural networks has gradually emerged, and has been widely used in many fields such as chemistry and chemical engineering [2-4], and it is worthy of in-depth study. This article mainly introduces the application status and research progress of artificial neural networks in the chemical field of extraction.

2. OVERVIEW OF ARTIFICIAL NEURAL NETWORKS

2.1 The Origin and Development of Artificial Neural Network

Artificial neural network (ANN) is an operation model composed of a large number of interconnected neurons. It simulates the processing method of the human brain from the perspective of information transmission. Its main function is to receive signals, process signals and output signals. This model originated from the MP model [5] established by psychologist McCulloch and mathematical logician Pitts in the 1940s. Since then, the era of artificial neural network research has arrived. In the 1960s, although the advent of perceptrons and adaptive linear components further improved the neural network model, which promoted the development of artificial neural networks, under the influence of Minsky and others, as well as the background of the era when the development of new types of computers and new ways of artificial intelligence was unnecessary and urgent, the research of artificial neural networks fell into a low ebb. Until the 1980s, the physicist Hopfield proposed the Hopfield neural grid model and the continuous-time Hopfield neural network model, which strongly promoted the research of neural networks, and then Boltzmann model, BP algorithm [6] and parallel distributed processing theory, new self-organization theory, etc., all of which promoted the development of artificial neural networks [7]. Since the 21st century, the concept of deep network and deep learning has triggered an upsurge in artificial neural network research, which has led to its rapid development.

The many advantages of artificial neural network make it attract much attention in various fields. For example, Gao et al. [8] proposed a three-

layer WPP Model considering historical power measurement data and Numerical Weather Prediction (NWP) systems which can be used to predict the power variation law of wind turbines. In the field of construction engineering, artificial neural networks are used to predict concrete strength and find the nonlinear input-output relationship between concrete strength and its influencing factors [9,10]. In addition, artificial neural networks are used in the field of plant diseases control [11-13], process control and optimization [14-16], troubleshooting [17-19], intelligent control of industrial product assembly line [20-22], robotic surgery [23-25], intelligent driving [26-28], chemical product development [29-31], signal processing [32-34], and so on.

2.2 BP Neural Network Model

The BP neural network model is one of the most widely used neural network models [35]. It is a multi-layer network trained according to the error back propagation algorithm [36]. BP neural network is a typical multi-layer forward network, that is, each neuron in the network accepts the input of the previous level and outputs to the next level, and there is no feedback between the layers. The biggest feature of this kind of neural network is that it can learn and store a large number of highly nonlinear mappings without having to establish a mathematical equation describing the mapping relationship in advance.

As shown in Fig. 1, the structure of the BP neural network model includes an input layer, an output layer and a hidden layer [37]. The hidden layer can be multiple layers, and each layer can have multiple nodes. The process of BP neural network operation is to input the information from the input layer and then process the hidden layer and transmit it to the output layer. If the expected output is not reached, the error signal is returned in the original way, and then the weight and threshold of the network are continuously adjusted. Minimize the sum of squared errors of the network. It can be seen that the learning process of the BP algorithm uses the steepest descent method, through the forward propagation of information and the back propagation of errors to continuously modify the connection weights between neurons in each layer, so as to minimize the error signal. The neuron transformation function adopts the Sigmoid function, which realizes any non-linear mapping from input to output. Although the BP neural network has some shortcomings such as slow learning convergence speed and easy to fall

into local minimums, many studies have proposed corresponding improvement measures for these shortcomings [38].

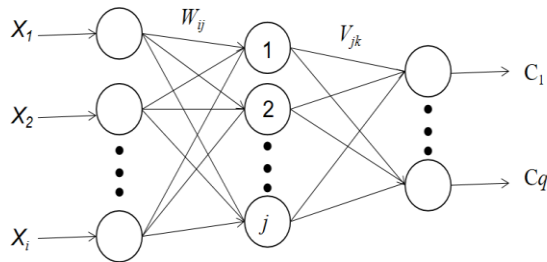


Fig. 1. The structure of the BP neural network

In recent years, the BP neural network model has been widely used in various fields. For example, in the flight test binocular vision measurement engineering application, there are many non-linear influencing factors in the calibration link of the airborne camera, and it is difficult to establish a strict and accurate mathematical calibration model. Some researchers apply the BP neural network to the calibration of airborne camera, it was found that the camera calibration accuracy based on the BP network is high, which can meet the mission requirements of the flight test. Before applying the BP network algorithm to dual-camera calibration, it is necessary to prepare input and output samples. The entire BP network construction and training process is completed through the matlab neural network toolbox. In order to speed up the convergence of the training network, unify the data collection unit and adapt to the transfer function between the hidden layer and the output layer, the linear function conversion is used to normalize the sample data, which is also beneficial to the output data conversion after using the network. The actual evaluation results also show that the camera calibration based on BP network has high accuracy and can meet the requirements of flight test tasks. The application of BP neural network in airborne camera calibration is feasible [39]. In addition, the BP network is also introduced into the star map recognition algorithm to improve the poor robustness of the grid algorithm and increase the recognition speed. This is the use of the BP network itself to quickly recognize the characteristics, and it matches the star database. Parallel processing is selected between the navigation star database and the characteristic star database, which shortens the matching time [40]. In the field of information security, some researchers have proposed a method for judging

the credibility of node information based on the BP network for the problem of the credibility of node information in wireless sensor networks. The traditional node security communication scheme is to use symmetric encryption method to encrypt the information transmitted by the node, and use asymmetric encryption method to authenticate the identity of the node. This scheme requires a huge amount of calculations. Due to the limited computing power of sensor nodes, it is inconvenient to perform a large number of encryption/decryption operations, and security issues cannot be well protected after the key is cracked. In order to reduce the amount of node calculations, extend the life cycle of wireless sensor networks, and improve system security performance, when the data collected by sensor nodes arrive at the border router after being routed in the area, the BP neural network judgment method can be set in the border router to determine the node data. This method can accurately determine the interference of illegal data and clear the interference data. This method can also be combined with traditional security assurance methods to further enhance system security [41].

2.3 RBF Neural Network Model

The radial basis function network model is an artificial neural network model that uses the radial basis function as the activation function. The RBF network [42] is based on the function approximation theory and is also a forward network. However, compared with the BP network as a typical global approximation network, the RBF network is a local approximation network, which only exists in a certain local area of the input space. A small number of neurons are used to determine the output of the network. For this reason, compared with the BP network, the RBF network is usually larger in size and faster in learning speed, and the function approximation ability, pattern recognition and classification ability of the network are better.

As shown in Fig. 2, the RBF network model is also composed of input layer, hidden layer and output layer [37]. On the whole, the transformation of the network from the input layer to the hidden layer is nonlinear, and the transformation from the hidden layer to the output layer is linear. That is, the mapping of the network from input to output is non-linear, while the output of the network is linear for the adjustable parameters, which greatly speeds up

the learning speed, and can avoid falling into local minima, and has good versatility [43].

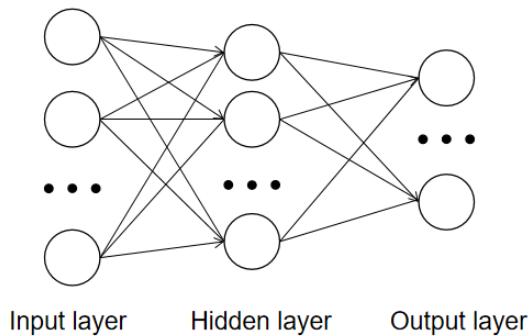


Fig. 2. The structure of the RBF neural network

In recent years, the application of RBF neural network has become more and more extensive. For example, in terms of gesture recognition, applying the RBF network to the gesture recognition device can improve the problem of low accuracy and slow response speed of the gesture recognition system. This is because the current gesture recognition is mainly realized through cameras and various sensors. When processing gesture data, the collected gesture capacitance data has a large difference, and cannot be represented by an accurate linear relationship. RBF network is a non-linear dynamic system. For some problems with unclear rules, complex test conditions, incomplete or sudden samples, RBF networks can provide reliable analysis results through the analysis and training of samples. The experimental results also show that the gesture recognition device based on the RBF network has a high recognition accuracy and a fast response speed. Compared with the camera-based gesture recognition device, gesture recognition devices using RBF networks have the advantages of low power consumption, low cost, and easy operation. While being easy to implement, it satisfies the accuracy and real-time requirements of gesture recognition technology in human-computer interaction, and can be widely used in gesture recognition systems of human-computer interaction devices such as smart homes [44]. In addition, the RBF network also plays an important role in the defect image recognition and processing technology. Defective image refers to the part that is difficult to identify in the image, which has a high degree of difficulty for the defect image recognition and processing technology itself. In our country, the traditional

defect image recognition and processing technology generally has the problem that the application effect cannot reach the expected effect in the actual application process. There are also certain limitations in the research of defect image recognition and processing technology. The recognition of the defect image is mainly realized by establishing the defect image feature recognition matrix and obtaining the defect image feature recognition projection. Applying the RBF network to the research of defect image recognition and processing technology, using the RBF network to process local feature descriptors can directly reflect the subtle component information in the defect image, and greatly improve the resolution of the defect image recognition and processing. Helped to complete tasks that cannot be achieved by traditional recognition and processing technologies. Firstly, RBF network is used to divide information space, physical space and human cognitive space. High-frequency information is divided into information space and physical space, and low-frequency information is divided into human cognitive space. The best fitting plane of training data is found in the multi-dimensional space. Then, the original defect image and the processed defect image were set as two groups of channels. Finally, defect image output processing is carried out according to the vector of feature descriptors, so that the defect image can be directly input or output processing. Through the above steps, the experiment successfully achieved good results [45].

3. APPLICATION STATUS OF ARTIFICIAL NEURAL NETWORK IN EXTRACTION

3.1 Extraction

Extraction is a unit operation that uses the different solubility of the components in the solvent to separate the mixture. It is mainly based on the law of distribution. Compared with other separation methods, the extraction can be carried out at room temperature, and the operation is simple and convenient, so the extraction operation is still being researched and developed continuously.

Research on the use of artificial neural networks for simulation and prediction in the extraction process has gradually attracted attention. Among them, the BP artificial neural network has been widely used because of its strong function approximation ability. In 2007, Li et al. [46] used

a BP neural network model to simulate the process of CO₂ high-pressure extraction of solanesol. The artificial neural network model in the research is established by preprocessing the orthogonal test data of CO₂ high-pressure extraction of solanesol in tobacco leaves, and then determining the number of hidden nodes, and then performing model training and model testing. The BP network structure in this study has 3 nodes in the input layer, 6 nodes in the hidden layer, and 2 nodes in the output layer, where the input parameters are extraction pressure, extraction temperature and entrainer flow rate, and the output parameters are extraction mass yield and extraction selectivity. Compared with the experimental value, the test result of this model has very little error. Research shows that the artificial neural network model can be applied to the process design and optimization of CO₂ high-pressure extraction of solanesol. In 2009, in order to predict the yield of larch oligomeric proanthocyanidins during the extraction process of oligomeric proanthocyanidins with ethyl acetate, Guo et al. [47] analyzed the extraction process of oligoproanthocyanidin with ethyl acetate from the perspective of extraction kinetics, and obtained several important external factors affecting the yield, and then simulated the prediction by using BP neural network model. The input parameters of the BP network model established in this study were material quantity, extraction dose, extraction temperature and oscillation time, and output parameter was the yield of oligomeric proanthocyanidins. The prediction accuracy of this model is high, and the difference between the predicted value and the actual value is not significant, and the error is much lower than that of the conventional quadratic polynomial regression model [48]. The research shows that artificial neural network technology is largely due to conventional methods, which can be further amplified to provide help for industrial design.

3.2 Complexation Extraction

Complex extraction is to make the solute to be separated contact with the complexing agent in the extractant to form a complex and transfer to the extraction phase to achieve the purpose of separation. This method not only has the advantages of good extraction effect and high selectivity, but also overcomes the shortcomings of poor reversibility of chemical extraction, can be recycled, and has simple operation and low cost. Therefore, complex extraction technology is an important direction for the research and

development of chemical separation processes [49].

At present, many studies have applied artificial neural networks to complex extraction. In 2004, Guan et al. [50] applied BP artificial neural network to the study of complex extraction of butyric acid. The extractant is composed of tributyl ester and n-octanol. The equilibrium distribution coefficient of extraction and the volume fraction of tributyl phosphate, the initial concentration of butyric acid and temperature are related to establish a neural network model for complex extraction equilibrium distribution coefficient. The predicted data of the model is compared with the measured data. It is found that the model not only has a high degree of calculation accuracy, but also The prediction deviation is not large, and it can be used to solve the actual problems in the complexation extraction process. In 2014, Zhou Yu et al. [51] also applied BP artificial neural network to the experiment of tributyl phosphate complexation extraction of Np (IV, VI). In this experiment, two different systems were designed, both of which use tributyl phosphate as the extractant and kerosene as the diluent. The difference lies in whether the medium HNO₃ contains uranium. Therefore, the equilibrium distribution ratio is correlated with the initial concentration of nitric acid, the initial concentration of Np(IV, VI), the initial concentration of U(VI), and the temperature, etc., to establish BP artificial neural network models under two different systems. The experimental value and the predicted value of the model are compared, and the error is not large. Thus, the artificial neural network model has fast calculation speed and calculation speed. The advantages of high accuracy can be applied to the conclusions of the analysis of the actual complexation extraction process.

3.3 Supercritical Extraction

Supercritical fluid extraction, also known as supercritical extraction. Usually a high-pressure, high-density supercritical fluid is used as a solvent. Among them, CO₂ is a common extractant for supercritical extraction due to its advantages of chemical stability, non-flammable and explosive, non-toxic and harmless, non-corrosive and easy to reach supercritical state. The basic process of supercritical extraction is mainly divided into extraction section and analysis section, and there are four typical processes of temperature and pressure changes in the extraction kettle and separation kettle,

namely isothermal pressure change, isothermal temperature change, isothermal temperature change and isothermal temperature change. Because supercritical extraction has multiple advantages that traditional ordinary fluid extraction methods do not have, this method has attracted widespread attention at home and abroad [52].

At present, there are many mathematical models that can describe the extraction mechanism to a certain extent, but they are not enough to guide engineering design. Since Fullana [53] et al. first applied artificial neural networks to the study of supercritical extraction kinetics, more and more researchers began to apply artificial neural network technology to the supercritical extraction process.

In 2001, Yin [54] used a three-layer BP network to establish a kinetic model for simulation research in the study of supercritical CO₂ fluid extraction of sea buckthorn oil for the first time. This experiment uses isothermal pressure reduction method to achieve supercritical extraction. The extraction process is clearly divided into three stages: equilibrium extraction section, transition section and slow extraction section. The input parameters of the BP network are extraction pressure, extraction temperature and extraction time, and the output parameter is the amount of oil extracted, and the original data is normalized and preprocessed. From the experimental results and simulation results, the prediction error of the 3-layer BP network model established by the research is small. Compared with the previous mathematical model, it overcomes the problem of solving the problem. The error caused by the quality rate.

In 2007, Yang et al. [55] used a typical 3-layer BP network model for simulation and prediction in the ultrasonic enhanced supercritical extraction of flavonoids from *Toona sinensis* leaves, including 7 nodes in the input layer, 10 nodes in the hidden layer, and 1 node in the output layer. The experiment simulates the effects of extraction temperature, extraction pressure, fluid flow, amount of entrainer, extraction time, and ultrasonic power on the extraction rate of total flavonoids. The simulation results have small errors. Research shows that artificial neural network technology can affect the extraction results. Amplification prediction can provide a basis for the selection of process conditions in the actual production process and the extraction of similar substances. In the same

year, Li et al. [56] also used a three-layer BP network model for simulation and prediction in the process of supercritical CO₂ fluid extraction of essential oil from Michao. The structure of the BP network is 4 nodes in the input layer, 6 nodes in the hidden layer, and 1 node in the output layer, the input parameters are extraction temperature, extraction pressure, supercritical CO₂ fluid flow rate and the average particle size of the raw materials, and the output parameter is the yield of Michao essential oil. In the study, the predicted value of the BP network model is compared with the measured value of the experiment. Although the deviation in the initial stage of extraction is slightly larger, the relative deviation after 20 minutes of extraction is small, so the artificial neural network model can be used for super Simulation and prediction of the critical CO₂ fluid extraction process of Mica essential oil.

In 2009, Miao Cunqian et al. [57] used a BP neural network model for simulation in a study comparing the extraction of lotus leaf volatile oil by supercritical CO₂ extraction and steam distillation. The input layer of the BP network consists of 4 nodes, the hidden layer of 4 nodes, and the output layer of 1 node. In the extraction methods of two different processes, the error of the simulated value obtained by the BP neural network model compared with the measured value is very small, indicating that the prediction accuracy of the model is high. In this study, orthogonal experiment and artificial neural network simulation were combined to determine the optimal extraction conditions of the two different extraction processes, which provided a new method for the extraction of active components from plants.

4. CONCLUSION

After decades of development, artificial neural networks have been widely used and perfected in many chemical fields, and their applications in extraction have gradually matured. Artificial neural networks are not only easy to operate, but also save a lot of manpower and material resources. In dealing with non-linear problems, the accuracy of simulation prediction is high. The BP neural network is mainly used to describe the relationship between the extraction process operating conditions and the equilibrium distribution ratio, which provides a great help for the simulation prediction of the extraction operation. However, the application of artificial neural networks in extraction needs to be

improved at present, and there are still problems such as large initial prediction deviations, so the research on artificial neural networks still needs to be more in-depth. With the development of science and technology, the application of artificial neural networks will become more common. This is an indispensable force for the development of the extraction field, and it will also play an extremely important role in the future development of the chemical industry.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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