



Research Progress in the Application of Artificial Neural Networks in Catalyst Optimization

Zhiqiang Liu^{1*} and Wentao Zhou¹

¹East China University of Science and Technology, 200237 Shanghai, China.

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

The catalyst can speed up the chemical reaction and increase the selectivity of the target product, playing an important role in the chemical industry. By improving the performance of the catalyst, the economic benefits can be greatly improved. Artificial Neural Network (ANN), as one of the most popular machine learning algorithms, has parallel processing and self-learning capabilities as well as good fault tolerance, and has been widely used in various fields. By optimizing the catalyst through ANN, time and resource consumption can be greatly reduced, and greater economic benefits can be obtained. This article reviews how CNN technology can help people solve highly complex problems and accelerate progress in the catalytic world.

Keywords: Artificial neural network (ANN); catalyst; catalysis.

1. INTRODUCTION

In recent decades, Artificial neural network (ANN), as a non-linear fitting algorithm, has become one of the most popular machine learning techniques due to its advantages of easy-training, adaptive

structure, and tunable training parameters [1,2]. With the development of algorithms, there are currently a large number of ANN methods, such as the back-propagation neural network (BPNN) [3,4], general regression neural network (GRNN) [5], and extreme learning machine (ELM) [6].

*Corresponding author: E-mail: y30210002@mail.ecust.edu.cn;

More recently, the deep neural network (DNN) has raised broad interests due to its strong learning capacity and the popular concept of deep learning techniques. Previous studies have shown that different neural network algorithms have different advantages for practical applications.

However, as far as we know, few review studies have summarized the application of neural networks in catalysis research. Therefore, it is necessary to discuss in detail the potential applications of neural networks in experimental and theoretical catalysis. This article summarizes the application progress of neural networks in catalysis in recent years from an experimental point of view.

2. ARTIFICIAL NEURAL NETWORKS

2.1 Overview of Artificial Neural Networks

Artificial Neural Network, which is abbreviated as Neural Network, is an abstraction and simulation of the human brain. It is an interdisciplinary discipline involving biology, computer science, and mathematics. It is widely used in artificial intelligence and machine learning. It abstracts the neural network of human brain from the perspective of information processing, establishes some simple model, and forms different networks according to different connection modes. Artificial neural network is a parallel interconnected network with self-adaptive self-learning adjustment function composed of the most basic unit group neurons. Artificial neural networks can simulate the response of the biological nervous system to specific objects through training and learning. The basic unit neuron is a simplification and simulation of biological neurons. Artificial neural network is based on the simplification and simulation of these biological neurons [7].

The network system of artificial neural network is very complex, it is composed of many and single basic neurons, the neurons simulate the human brain to process information, and connect with each other, carrying on the nonlinear change to process information [8]. By training the information sample, the artificial neural network information processing information is input into the neural network, so that it has the memory and recognition function of human brain, and all kinds of information processing is completed. Artificial neural network has good non-linear transformation ability, parallel processing ability,

self-learning and self-adaptation ability and good associative memory ability, but also avoid complex mathematical derivation, to ensure that the sample defect and parameter drift can ensure stable output [9].

As an important part of artificial intelligence, artificial neural network has the advantages of super robustness, fault tolerance, full approximation of any complex nonlinear relationship, parallel processing, learning and self-adaptation. There is a broad space for development in many fields involving the processing of nonlinear and complex problems. The main application areas are auxiliary assembly system [10,11], intelligent driving [12,13], Chemical product development [14-16], auxiliary medical diagnosis [17-19], image processing [20-22], automatic control of power systems [23-25], signal processing [26-28], process control and optimization [29-31], troubleshooting [32,33], game theory [34,35], etc.

2.2 Classification

Artificial neural network can be divided into feedback network and forward network in terms of structure, and can be divided into random network or deterministic network in terms of performance, which can also be called discrete network and continuous network. It can also be divided into management network and free network according to the method of learning. According to the nature of connection, it can be divided into first order linear correlation network and high order nonlinear correlation network. This paper focuses on the analysis of the topology of artificial neural network [36].

(1) Feedback network: Feedback network mainly includes BAM, Hamming, Hopfield, etc. Feedback networks with feedback between neurons can be represented by an undirected complete graph. The state of the neural network in the aspect of information processing is transformative and can be processed by using the dynamic system theory. The associative skill function of the system is closely related to the stability of the system, and Boltzmann machine and Hopfield network belong to this type.

(2) Forward network includes BP, multi-layer perceptron, single-layer perceptron, adaptive linear network, etc. In a forward network, each neuron in the network receives input from the previous level and outputs it to the next level. The network can be represented by a directed

acyclic graph, which has no feedback. The network converts signals from the input space to the output space, and the multiple combinations of its information processing capabilities are derived from simple nonlinear functions. The network structure is easy to implement and relatively simple. Back propagation network is a typical forward network [37].

2.3 Artificial Neural Network Learning Rules

The learning rules of artificial neural networks are actually a network training method. The purpose is to modify the weight of the neural network and adjust the threshold of the neural network so that the neural network can better complete certain specific tasks. Currently, neural networks have two different learning methods: tutored learning (also called supervised learning) and unsupervised learning (also called autonomous learning) [9].

2.3.1 Supervised learning

The so-called supervised learning refers to the process in which the neural network needs to supervise the training data during the training process. This process is the process of continuously adjusting the weights under the influence of the expected output, that is, when the training data is input to the neural network after training [38]. After learning the output, the network compares the output with the expected output. If the error of the output of the neural network relative to the expected output is within the allowable range, it can be considered that the neural network learning has been completed. If it is not an error within the allowable range, the weight of the neural network must be continuously adjusted to reduce the error, so that the output of the neural network is close to the expected output, until the error is within the allowable error range, and the training ends. It can be seen that the learning process with a tutor is a process of weight adjustment under supervision and expectations. In this process, the changes in the weights of the neural network reflect the learning process of the entire network. The last adjusted weight is this nerve. In this way, after continuous supervised learning, a neural network model with preliminary intelligence is basically established [7,39].

2.3.2 Unsupervised learning

Unsupervised learning is also called autonomous learning and supervised learning. The difference

is that unsupervised learning has no external supervision mechanism. It has no expected output. After the training data is input to the network through the input layer, it is not included in the output. The entire neural network checks the characteristics and rules of the training input data, and formulates judgment criteria. The network adjusts the weight according to this standard. This kind of unsupervised learning can be regarded as a kind of self-organized learning. The discrimination standards established before training are also pre-set rules, such as competition rules. Through the collaboration between neurons, the weights of the network are constantly adjusted to respond to the excitation of the input pattern until the entire neural network forms an orderly state [39].

2.4 Schematic Structure of an ANN

A complete traditional ANN algorithm structure consists of at least three different layers: input layer, hidden layer and output layer (Fig. 1) [1]. Each layer is composed of a certain number of neurons. Each neuron is connected to all neurons in the next layer. Each connection represents a weight that contributes to the accessory. Under the appropriate activation function, the optimized combination of weights can generate predictions for the dependent variable:

$$NET = \sum_{i,j}^n w_{i,j} x_i + b \quad (1)$$

Where $w_{i,j}$ represents the weight value of a connection, x_i represents an inputted independent variable, and b represents a bias. For the activation function ($f(NET)$), the sigmoid function is one of the most popular forms that can introduce a smooth non-linear fitting to the training of an ANN (Equation (2)). The training of ANN is essentially based on the optimization of each weight contribution based on the data set in the training set. The most commonly used weight optimization method is the backpropagation algorithm, which iteratively analyzes the error and optimizes each weight based on the error generated by the next layer. As we mentioned above, there are some other types of networks, such as GRNN and ELM. Although there are some differences in weight training and algorithm structure, the basic principles, as well as the

training and testing process are very similar. More details about their principles can be found in the references [38].

2.5 Model Development

The rational development of knowledge-based artificial neural network model includes two parts : (I) training and (II) testing. The training process is a so-called "learning" process from the database, while the testing process is the validation of the training model using data sets that have not previously participated in the training process. See sections 2.5.1 and 2.5.2 for a detailed discussion. It should be noted that the training and testing process applies not only to the topics discussed in this review, but also to ANN model development in many other areas.

2.5.1 Model training

The training of the ANN includes the preparation of the database and the selection of variables. The size of the database should be large enough to avoid overfitting. For each variable (especially the dependent variable), the data range should be wide enough to ensure good training. If the

data range is too narrow, the trained model may only have good predictive ability in very local areas. In numerical prediction, the dependent variable is usually a property that is difficult to obtain in conventional measurement or calculation. On the other hand, the independent variable should be easy to measure and have a potential relationship with the selected dependent variable. More details about the training standards can be found in the references [40].

2.5.2 Model testing

In order to verify the trained ANN, a testing process is necessary. The test of the model should use the data set not used in the training process. With the input of the test set, the output data can be compared with the actual data of the test set, and the root mean square error (RMSE) can be calculated by Equation (3):

$$f(NE\text{T}) = \frac{1}{1 + e^{-NE\text{T}}} \tag{2}$$

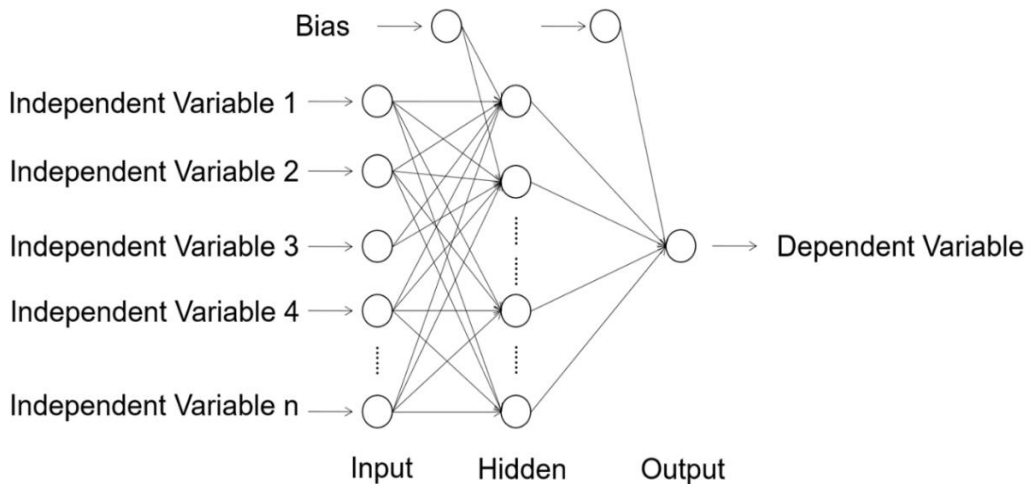


Fig. 1. Algorithmic structure of a typical artificial neural network (ANN)

$$RMSE = \sqrt{\frac{\sum_i^n (P_i - A_i)^2}{n}} \tag{3}$$

where P_i represents the predicted value outputted by the ANN, A_i is the actual value, and n represents the total number of samples. If the calculated RMSE from the testing set is relatively small, it means that the ANN is well-trained. It should be noted that for the training and testing of an ANN, a cross-validation process should be performed using different components of the training and testing datasets. If the database is relatively large, a sensitivity test can be performed to replace the cross-validation, in order to avoid a high computational cost [41].

It should be noted that for typical ANN algorithms (such as BPNN), the entire neural network structure needs to be optimized before determining the final number of hidden layers and hidden nodes. Use different ANN structures for repeated training and testing. On the one hand, if the number of hidden layers and/or hidden neurons is too high, there is a risk of overfitting; on the other hand, if their number is too small, it will cause inappropriateness. Generally, the best ANN algorithm configuration can be defined by comparing the average RMSEs of the test set during cross-validation or sensitivity testing [42].

3. APPLICATIONS OF ANN FOR CATALYSIS

Generally speaking, the comprehensive evaluation indexes of industrial catalysts are activity, selectivity and service life, and the catalyst for specific reaction may also have good heat resistance, mechanical strength and anti-carbon properties, so the development cycle is often very long. When it comes to specific reactions, the preparation methods and operating conditions of catalysts depend more on practical experience. In order to further study the micro-reaction mechanism of catalysts, there are often multiple mechanism models for the same reaction, but these models often have their limitations. However, there are many factors affecting the properties of the catalyst. On the one hand, there is interaction between its own properties, such as active metal, preparation method, preparation conditions and activation conditions, and on the other hand, reaction conditions will also affect its activity. If all the experimental verification will consume huge energy. The nonlinear mapping ability of BP neural network can achieve certain precision

prediction with less data in a short period of time, which is particularly efficient.

3.1 Prediction of Catalytic Activity

In 1994, Kito et al. [43] did one of the earliest catalytic applications. They predicted the distribution of ethylbenzene oxidative hydrogenation products. The product components were styrene, benzaldehyde, benzene + toluene, CO and CO₂ as the network Output. In terms of the input of the neural network, they used 9 different independent variables, which are potentially related to the productivity and selectivity of the catalytic reaction, including: abnormal valence, catalyst surface area, catalyst dosage, typical valence, ionic radius, coordination Number, electronegativity, partial charge of oxygen ions, standard heat generation of oxides. Their results found that in a good experimental database, a single hidden layer neural network can perform accurate predictions of product selectivity. Sasaki et al. [44] first proposed that ANN can be used to predict catalytic activity and optimize experimental conditions. The experimental results show that a well-trained neural network can accurately predict the yield and by-products of the Cu/ZSM-5 molecular sieve catalyst decomposing NO. For other more complex reactions, such as polymer-supported Mo (VI) complexes catalyzed by the 1-hexene epoxidation reaction, Mohammed et al. [45] showed that neural networks have a strong ability to predict its catalytic activity. The experimental conclusions are very consistent. For photocatalysis, neural networks also show strong predictive capabilities. Frontistis et al. [46] studied the photocatalytic degradation of 17-ethinyl estradiol (EE2) with different concentrations of TiO₂ catalyst. Taking the reaction time, TiO₂ concentration, EE2 initial concentration, matrix dissolved organic carbon (DOC), and matrix conductivity as inputs, they found that the average RMSE of a single hidden layer ANN was the smallest during the test. In terms of biotechnology catalysis, Rahman et al. [47] also found that with temperature, reaction time, substrate molar ratio, and enzyme amount as input, the optimized ANN structure can be used for lipase-catalyzed synthesis of dioctyl adipate. Yield prediction. In recent years, with the development of data mining concepts, Gunay and Yildirim [48] successfully used 1,337 data points from 20 studies on selective CO oxidation on copper-based catalysts. They concluded that ANN modeling can be used to extract valuable

experimental results from previous literature data and provide strong guidance for future experimental design. In addition to catalysis, Raccuglia et al. [49] further discovered that similar concepts can even help discover materials from failed experimental data. It can be seen from these typical studies that for different types of reaction systems, catalysis and data sets, the optimal ANN prediction structure is significantly different. We can see that different response types have very different input variables and output indicators. This means that each prediction task should be predicted by a specific model with optimal weight contribution and network structure.

This article is based on the modeling of Fe₃O₄ composite oxide catalyst formulation based on artificial neural network. In this article, the selection of two auxiliary elements, the ratio of elements, and the drying temperature and roasting temperature in the preparation of the catalyst are the keys to the final catalyst service life and hydrogen generation rate. Factors, the auxiliary element M1, the auxiliary element M2, the ratio of the auxiliary element M1 and Fe M/Fe, the ratio of the auxiliary element M2 and Fe M2/Fe, the drying temperature T1 and the roasting temperature T2 are selected as the input units of the artificial neural network, and the output units are catalyst life (CL) and hydrogen generation rate (formation rate of hydrogen, FRH).

Based on the above analysis, the orthogonal design method is used to design a six-factor, five-level orthogonal experiment table, and the obtained samples are tested in the micro-reaction system using the experimental method described above. The experimental results are shown in Table 1.

From the experimental results of the initial sample, it can be seen that the life of the prepared Fe₃O₄ composite oxide is generally poor, and the hydrogen generation rate obtained is also uneven. Therefore, a suitable method must be used to obtain a better formula. For the system studied in this paper, the catalyst life of the output layer can be converted into a relative life (divided by 100), and the hydrogen generation rate is divided by 1.20, so that the data obtained are all between 0 and 1. Choose a relatively simple Sigmoid function as the activation function of each layer is conducive to the convergence of the learning algorithm.

In order to choose a faster learning algorithm, use the initial catalyst formulation sample set obtained in Section 2.1 to test several learning algorithms, and select the most appropriate method from them. As shown in Table 1, the traditional BP algorithm, moment method. The convergence performance of the improved BP algorithm and the improved BP algorithm of the Levenberg-Marquardt method are investigated. The networks used in Fig. 1(a)~(c) are all 6-12-4-2 type BP networks, and the training samples used are all 25 catalyst formulations and their evaluation results in Table 1. The difference is the training method. Among them, the learning rate (step size) of the traditional BP algorithm is 0.01; in the BP algorithm improved by the moment method, the learning rate (step size) is 0.01, the learning rate is increased by 1.05, the reduction is 0.7, and the moment is 0.9; In the training process of BP algorithm improved by Levenberg-Marquardt method, the initial input value is 0.001, the input increase rate is 10, and the decrease rate is 0.1. Since the convergence speed of the traditional BP algorithm and the improved BP algorithm of the moment method is slow, the criterion of whether the network has been trained (that is, the root means square error that can be allowed by training) is set to 0.01; while the Levenberg-Marquardt method, The method converges quickly, so the criterion is adjusted to 0.000001.

From the comparison of Fig. 1 (a) and (b), it can be seen that the Levenberg Marquardt method only needs 141 times to converge to 10⁻⁷; the traditional BP algorithm requires about 200,000 iterations to converge to 0.01; the moment method requires 2 About ten thousand iterations converge to 0.01. From the time required for each iteration, the Levenberg-Marquardt method is longer than the traditional BP algorithm and the moment method, which is caused by a large number of matrix operations in the calculation. At the same time, as the number of input samples (input mode) increases, the number of iterations of the Levenberg-Marquardt method will increase accordingly. The time required for each iteration will also become longer. Error) should also be appropriately relaxed (but the highest cannot be greater than 0.001), which is related to the increase in the amount of calculation caused by the increase in the number of input samples (input mode). But it should be noted that even when the number of input samples (input mode) increases, the convergence speed of the Levenberg-Marquardt method is still much faster than that of the traditional BP algorithm.

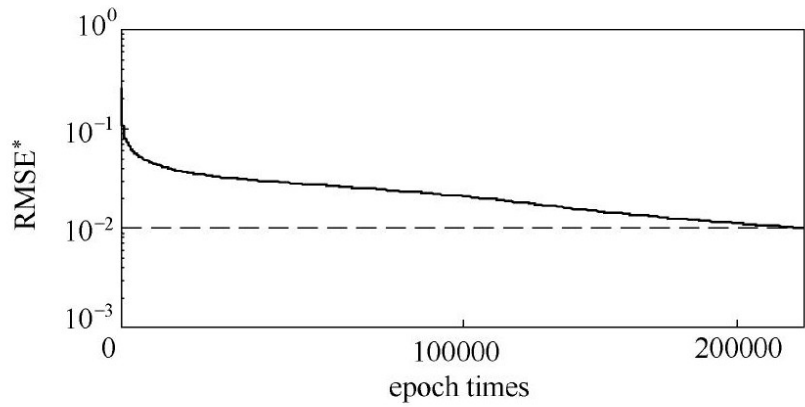
Therefore, the Levenberg-Marquardt method is used for modeling.

In order to determine the number of nodes in the hidden layer of the network, the aforementioned 25 catalysts are used as training samples (training set), and networks of different structures are tested to find the best structure. The evaluation index mainly depends on the generalization ability of the network. For this reason, 12 catalysts are prepared and evaluated by a random method, and their formula and experimental results are used as the sample (test set) to test the generalization ability of the network. Due to the small number of samples in the training set, the generalization ability of the trained network is generally unsatisfactory. The structure with relatively good generalization ability can be selected as the modeling network. The test results are shown in Fig. 2.

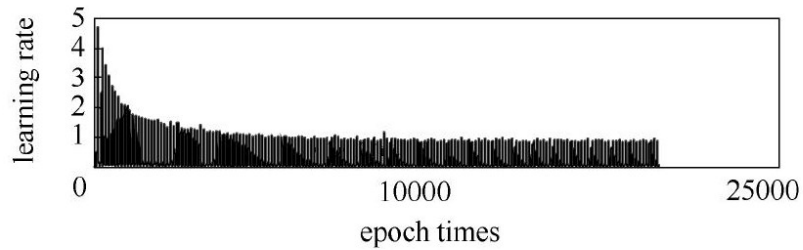
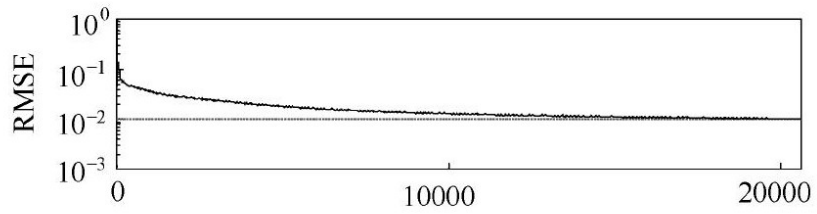
From the results in Fig. 2, it can be seen that due to the small number of hidden layer nodes in Net 1, the simulation of the relationship between influencing factors and response results is not accurate enough; the number of hidden layer nodes in Net 2 reaches 40, and the experimental data is Overfitting, the test results reflect its poor generalization ability; although the total number of hidden layer nodes of Net 3 is the same as that of Net 4, one hidden layer is added, and the test results are not Obtained too much improvement, but increased the amount of calculation; Net 4 meets the requirements both from the test results and the number of hidden layer nodes, and is similar to the conclusion drawn by the selection method of previous studies. According to the above analysis, Net 4 was selected to model the formula of the methane hydrogen production reaction system based on Fe₃O₄ composite oxide.

Table 1. All experiments were performed on the same reaction conditions

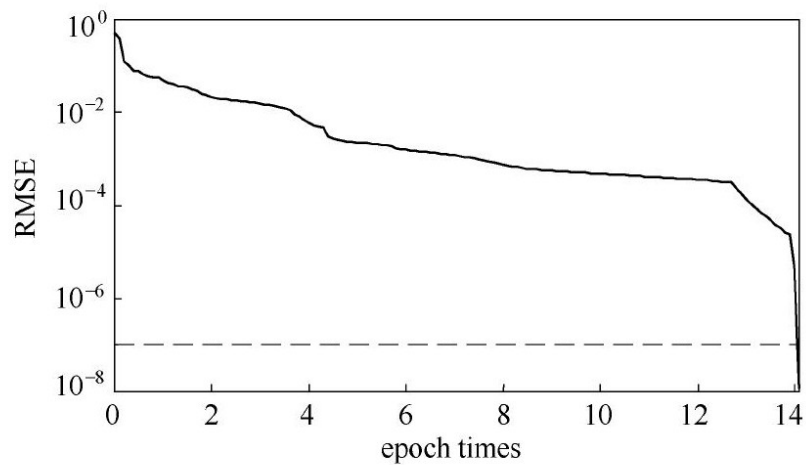
Catalyst	Influencing factors					Experimental results		
	M ₁	M ₂	M ₁ /Fe	M ₂ /Fe	T ₁ /°C	T ₁ /°C	CL/h	FRH/mmol·min ⁻¹ ·(g Fe) ⁻¹
MH1-1	Cu	Cr	2	2	120	500	1.59	0.23
MH1-2	Cu	W	6	6	135	540	1.58	1.07
MH1-3	Cu	Al	10	10	150	580	0.41	0.97
MH1-4	Cu	V	14	14	165	620	0.29	1.13
MH1-5	Cu	Ti	18	18	180	660	0.14	0.83
MH1-6	Ni	Cr	6	10	165	660	0.44	0.99
MH1-7	Ni	W	10	14	180	500	1.77	1.12
MH1-8	Ni	Al	14	18	120	540	1.41	1.13
MH1-9	Ni	V	18	2	135	580	1.04	0.65
MH1-10	Ni	Ti	2	6	150	620	1.12	0.68
MH1-11	Zr	Cr	10	18	135	620	2.12	0.96
MH1-12	Zr	W	14	2	150	660	0.18	0.75
MH1-13	Zr	Al	18	6	165	500	0.57	0.48
MH1-14	Zr	V	2	10	180	540	2.23	0.34
MH1-15	Zr	Ti	6	14	120	580	2.15	0.26
MH1-16	Pd	Cr	14	6	180	580	0.13	0.49
MH1-17	Pd	W	18	10	120	620	2.51	0.18
MH1-18	Pd	Al	2	14	135	660	2.72	0.55
MH1-19	Pd	V	6	18	150	500	2.05	0.46
MH1-20	Pd	Ti	10	2	165	580	0.36	0.29
MH1-21	Co	Cr	18	14	150	540	2.51	0.85
MH1-22	Co	w	2	18	165	580	2.91	1.04
MH1-23	Co	Al	6	2	180	620	0.02	0.12
MH1-24	Co	V	10	6	120	660	1.81	1.03
MH1-25	Co	Ti	14	10	135	500	1.83	0.35



(a) trained by gradient method (training for 200441 epochs)



(b) trained by method of moment (training for 20622 epochs)



(c) trained by Levenberg-Marquardt method (training for 141 epochs)

Fig. 2. Comparison of three training methods

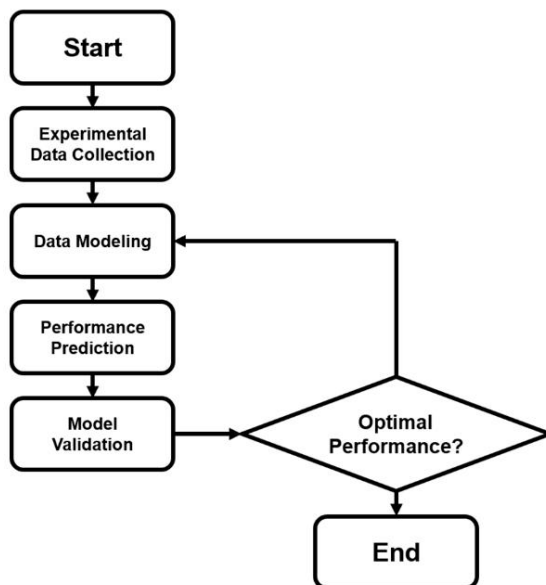


Fig. 3. Optimization modeling that combines both experimental and computational steps

3.2 Optimization of Catalysis

In addition to activity prediction, more importantly, how can we use the predictive power of neural networks to design new catalysts? Because we know that artificial neural networks can accurately predict the catalytic performance of various catalytic systems, we can set new inputs and perform practical simulations with well-trained neural networks to obtain their catalytic performance and optimization methods. A general algorithmic flow chart of catalyst optimization summarized by Maldonado and Rothenberg is reconstructed in Figure.

Optimization is more challenging than catalyst prediction. Corma et al. [50], who first applied ANNs for the optimization of potential catalyst compositions for the oxidative dehydrogenation of ethane (ODHE). It should be noted that in this catalysis optimization, a genetic algorithm (GA) was introduced as the promoter of design generation. Omata and Yamada [51] developed an ANN to predict an effective additive for Ni/Activated carbon (AC) catalysts for methanol gas phase carbonylation by using a trained network and discovering that tin is an effective element that improves catalyst performance. Hou et al. [52] first proposed a computer-aided framework for catalyst design based on ANN. They found that this method can effectively design promising propane ammoxidation catalysts. In addition, in a

similar catalytic system for propane ammoxidation, Cundari et al. [53] combined neural networks with genetic algorithms to achieve rapid catalyst selection. Using genetic algorithms, the catalyst can be designed more reasonably by optimizing the input of the artificial neural network. Similarly, Umegaki et al. [54] combined GA and ANN with parallel activity testing to optimize the Cu-Zn-Al-Sc oxide catalyst for methanol synthesis. Rodemerck et al. [55] promoted the ga-assisted neural network method and proposed a general framework for the screening of new solid catalytic materials, which is in good agreement with their experimental data. Baumes et al. [56] further developed an "ANN filter" for high-throughput screening (HTS) for heterogeneous catalysis discovery based on the previous ga-assisted ANN method. Taking the water vapor shift (WGS) reaction as an example, they showed that although the optimization method developed by Corma et al. is successful for ODHE (as described at the beginning of this section), it cannot accurately estimate the activity of the WGS reaction. However, using a well-trained neural network classifier as a filter to help define "good" and "bad" catalysts, WGS catalysts can be rationally designed, and ga-assisted HTS methods can be used.

Based on the BP neural network, Baroi et al. [57] established a correlation model for the structural properties of the supported H-Y zeolite catalyst,

such as the micropore area, mesopore area, pore size and loading amount, and the esterification reaction activity. Only 8 models were simulated and the reliable results were obtained. Wu et al. used momentum factor-adaptive learning rate to improve BP neural network model and orthogonal design to adjust the process parameters of high-energy ball milling WC-MgO to control its grain size., BP model through item by item, intensive scanning techniques, diameter of grinding ball, ball mill speed and ball material ratio in the operating range value, ensure the comprehensive forecast samples. The experimental verification results show that the optimal catalyst particle size training times designed by the BP improved model with the optimal structure is only 38 times, and the prediction accuracy is also better than that of the orthogonal design. Huang Kai et al. improved BP neural network by using L-M algorithm and matrix algorithm respectively, and proposed a hybrid model based on improved BP and genetic algorithm to optimize Fe₃O₄ composite oxide catalyst to improve methane hydrogen production performance. In this model, the catalyst life and hydrogen generation rate are composed of target parameters, and GA algorithm is used for global optimization, which improves the convergence rate, accuracy and generalization ability of the network. The hydrogen generation rate of catalyst with auxiliary element ratio and preparation conditions is higher than that of the same experimental conditions, and its lifetime is extended by up to 150%. Similarly, Abbasi et al. also designed nan-modified perovskite catalysts using a mixture model of GA and BP (Ann-GA), and predicted the reaction performance of CH₄-CO₂ with only 20 groups of experimental data for the metal molar ratio of the catalyst. The predicted value of catalyst designed by the global optimization of genetic algorithm is in good agreement. Hadi et al. [58] used AN-GA model and RSM to design bimetallic catalyst for MTP reaction, the propylene selectivity of the catalyst prepared by the former is higher than that of the latter in terms of the Ce load, calcination temperature and calcination time, and the prediction accuracy is also satisfactory.

4. CONCLUSION AND PROSPECTS

Since the establishment of artificial neural network in the 1930s, neural network theory has achieved extensive success in many research fields such as pattern recognition, automatic control, signal processing, assisted decision

making and artificial intelligence. In the past two decades, artificial neural networks have been widely used in chemical fields, especially in the field of catalysis. As we all know, in the field of catalysis, the design and optimization of catalyst is the most important research direction. Artificial neural network (ANN) has become a hot topic in catalytic field because of its good nonlinear and easy training.

Although artificial neural networks have achieved great success and can facilitate the development of catalytic systems, there are some common challenges that need to be addressed in future research. For example, a large number of relevant researches are completed by BP neural network. We hope to apply the most advanced network model to the field of catalysis. Compared with other research fields, the application of neural network in the field of catalysis is not popular and the research is not in-depth enough.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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