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Temperature and key element content prediction based on optical information data Abstract

In the process of metal smelting, the precise control of temperature and key element content has important significance in improving the performance of metal smelting, reducing the production cost and achieving energy saving and emission reduction.

For problem one, firstly the wavelength –light intensity map of the original data is analyzed, and the optical information is found to be very obvious in a certain range. Then, through screening and seeking overlapping over the full waveband, three wavebands with monotonic variation f_700-f_1200 , f_1400-f_1550 , f_1700-f_1900 are selected. Secondly, the polynomial fitting equations is established to fit three wavebands, and the parameters of the waveband information can be obtained. Finally, with time t, the cumulative consumption of combustion gas Q, combustion

gas cumulative consumption ratio P, and the Kelvin temperature T and the content of key element C, the parameters $(t,Q,P,a_1,b_1,c_1,a_2,b_2,c_2,a_3,b_3,c_3,T,C)$ of optical data feature which can describe data samples can be obtained.

For problem two, establishing the prediction model based on the BP neural network. The parameters $(t,Q,P,a_1,b_1,c_1,a_2,b_2,c_2,a_3,b_3,c_3)$ which can describe the characteristics of optical data are selected as the input parameters of the model. The Kelvin temperature T and the content C of key elements are as the output parameter. Training device $< net_key, net_T >$ which can describe the relationship of each data sample set is obtained through training, and the key element content and the Kelvin temperature T were predicted. The mean square error between the predicted value and the actual value was respectively 0.00032564 and 0.00045701, which shows that it has a higher accuracy.

Finally, the genetic algorithm is used to optimize the input nodes, the number of hidden nodes and the MSE target value of the BP neural network, and the key element content C and Kelvin temperature T of each sample set are predicted by using the optimized neural network. The results show that the neural network prediction accuracy is improved by 10.62% and 16.58%, which shows that the neural network

prediction Performance has been significantly improved.

Keywords: Polynomial fitting; BP neural network; Cross experiment; genetic algorithm

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1 Restatement of the problem

1.1 Problem Background

As one of the effective means to obtain target metal, the efficiency and pollution of metal smelting is receiving more and more people's attention. Its working principle is mainly that through putting the metal material in the specific furnace and melting according to the certain temperature, the harmful elements can be controlled or eliminated and the useful elements can be retained or increased, so that the target metal with the best performance can be obtained. The final smelting effect is mainly affected by temperature and the content of key elements.

1.2 Our work

- According to the data provided, a mathematical model or algorithm model is established to find the characteristics of optical information data, and then these features will be extracted and output to the Excel table.
- In order to probe the relationship between Kelvin temperature T and key element content C, based on the optical information feature data extracted in Problem One and existing time data, the cumulative consumption of combustion gas, the mathematical model or algorithm model can be established.
- Based on the above research, designing the cross experiment scheme, and testing the error produced by forecast target, and then on the basis of error analysis, the scheme of error control will be provided.

2 Assumptions

- Assuming that the photodetector is able to detect all of the optical information emitted by the flame.
- Assuming that the external environment will not interfere with the photoelectric detection system.

3 Symbols and Definitions

Symbol	Definitions	
$\lambda_1, \lambda_2, \cdots \lambda_{12}$	Extracted feature of optical information	
Φ	Function classes that are not more than n of all times	
p_{j}	Input measure	
$\omega_{_{j}}$	Weight measure	
$f(\cdot)$	Activated function	
norm(errij)	Error mode of predictive value and actual value	
length(errij)	Dimension of predictive value and actual value	

4 Model establishment and solution

4.1 Feature extraction of optical information data based on polynomial fitting

4.1.1 Analysis of spectral information data

The amount of data received by the photodetector every 0.5 seconds is 2048, in order to use the values of 2048 light intensities to predict the temperature of the flame and the content of key elements in the real-time feedstock, if the data of 2048 light intensity values at a certain time are taken as input, the flame temperature and the key element content of the key element are taken as the output, there will be a large error in the structure of the mathematical model because of the relatively large input quantity. In order to improve the applicability of the prediction model, the characteristic values of one or more light intensity data are extracted to reduce the input data^[1].

To extract the characteristic value of light intensity data, the original data is processed and analyzed firstly, without considering the time factor, and the wavelength intensity relation diagram is made by using MATLAB, as shown in Figure 1.

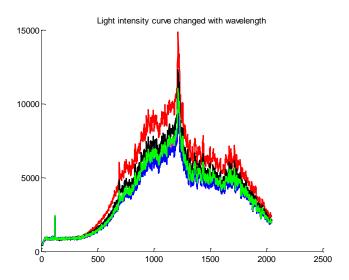


Fig. 1 The relation of light intensity and wavelength

It can be seen from Figure 1, the variation of light intensity with wavelength is fluctuating, there is no monotone, and there is a peak and invalid data. (That is, the data value is too large, and the trend is not in conformity with the surrounding data), but in a certain range of wave band, it has a very obvious monotony^[2], and the whole graph of Figure 1 can be replaced by a smooth curve. And on the data processing, the data which is consistent with the curve of the data has a good regularity, can get a very good fitting results.

In order to characterize the spectral characteristics better, this paper selects the full band, selects 3 lights^[3]($f_-700 - f_-1200$, $f_-1400 - f_-1550$, $f_-1700 - f_-1900$) intensities with the change of the wavelength of the band, and then the curve of each

monotone band is fitted^[4].

4.1.2 The establishment of polynomial fitting equation

In the polynomial fitting of the data, assuming a given data point (x_i, y_i) $(i = 0, 1, \dots, m)$, Φ is a class of functions that are not more than $n(n \le m)$ of the number of times. Now solving $p_n(x) = \sum_{k=0}^n a_k x^k \in \Phi$ to make:

$$I = \sum_{i=0}^{m} [p_n(x_i) - y_i]^2 = \sum_{i=0}^{m} (\sum_{i=0}^{m} a_k x_i^k - y_i)^2 = \min$$
 (1)

When the fitting function is polynomial, it is called the polynomial fitting, and if satisfying the formula of 1. It is called the least square fitting polynomial. In particular, when n = 1, it is called a linear fitting or a straight line fitting.

Obviously,
$$I = \sum_{i=0}^{k} (\sum_{k=0}^{k} a_k x_i^k - y_i)^2$$
 is the multivariate function of $a_0, a_1, \dots a_n$, so

the above question is the same to search extremum problem of $I = I(a_0, a_1, \dots a_n)$.

According to the necessary condition for the extremum of multivariate function, this

According to the necessary condition for the extremum of multivariate function, this paper can get:

$$\frac{\partial I}{\partial a_{i}} = 2\sum_{i=0}^{m} \left(\sum_{k=0}^{n} a_{k} x_{i}^{k} - y_{i}\right) x_{i}^{j} = 0, \qquad j = 0, 1, \dots, n$$
(2)

That is:

$$\sum_{k=0}^{\infty} (\sum_{i=0}^{\infty} x_i^{j+k}) a_k = \sum_{i=0}^{\infty} x_i^{j} y_i, \qquad j = 0, 1, \dots, n$$
(3)

The above formula is the linear equations about $a_0, a_1, \dots a_n$, which can be shown in matrix:

$$\begin{bmatrix} m+1 & \sum_{i=0}^{m} x_{i} & \cdots & \sum_{i=0}^{m} x_{i}^{n} \\ \sum_{i=0}^{m} x_{i} & \sum_{i=0}^{m} x_{i}^{2} & \cdots & \sum_{i=0}^{m} x_{i}^{n+1} \\ \vdots & \vdots & & \vdots \\ \sum_{i=0}^{m} x_{i}^{n} & \sum_{i=0}^{m} x_{i}^{n+1} & \cdots & \sum_{i=0}^{m} x_{i}^{2n} \end{bmatrix} \begin{bmatrix} a_{0} \\ a_{1} \\ \vdots \\ a_{n} \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^{m} y_{i} \\ \sum_{i=0}^{m} x_{i} y_{i} \\ \vdots \\ \sum_{i=0}^{m} x_{i}^{n} y_{i} \end{bmatrix}$$

$$(4)$$

Formula (3) or formula (4) is called the normal equations or method equations. It can be proved that the coefficient matrix of the equation group (4) is a positive definite matrix, so there is a unique solution. $a_k(k=0,1,\dots,n)$ can be obtained from the formula (4), and the polynomial can be obtained.

$$p_n(x) = \sum_{k=0}^n a_k x^k \tag{5}$$

It can be proved that $p_n(x)$ in formula (5) is satisfied with the formula (1),

which is to say that $p_n(x)$ is the polynomial fitting. The $\sum_{i=0}^{m} [p_n(x_i) - y_i]^2$ is known

as the square error^[5] of the least square fitting polynomial $p_n(x)$, recorded as:

$$||r||_2^2 = \sum_{i=0}^m [p_n(x_i) - y_i]^2$$
 (6)

By the formula (6), the result can be obtained:

$$||r||_{2}^{2} = \sum_{i=0}^{m} y_{i}^{2} - \sum_{k=0}^{n} a_{k} \left(\sum_{i=0}^{m} x_{i}^{k} y_{i} \right)$$
 (7)

The rough scatter diagram of the function can be drawn according to the data given by each waveband, such as $f_{-}700 - f_{-}1200$, which is shown is Figure 3. The data in this waveband is in line with the two degree polynomial fitting. Therefore, the value of the above polynomial principle k is 2, and the two degree polynomial can be expressed as:

$$p_2(x) = ax^2 + bx + c \tag{8}$$

Among them, a,b,c are respectively the undetermined coefficients of the independent variable light intensity of different power.

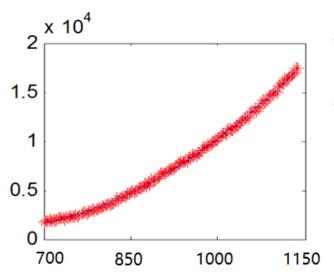


Fig. 2 Scatter diagram of initial data

The function expression obtained after fitting contains all the data information in the corresponding waveband, so each data sample set is divided into three wavebands, which can get a set of value a,b,c, and it is recorded as: $a_1,b_1,c_1,a_2,b_2,c_2,a_3,b_3,c_3$.

With time t, the cumulative consumption of combustion gas Q, combustion gas cumulative consumption ratio P, and the Kelvin temperature T and the content element C. optical data feature a set of parameters $(t,Q,P,a_1,b_1,c_1,a_2,b_2,c_2,a_3,b_3,c_3,T,C)$ which can be representative of data samples can be obtained. Do the same processing of each data sample set, and finally the characteristics of optical data λ can be got. The resulting optical data characteristics are output to an Excel table, and partial optical data feature can be seen in the following table, the whole data can be seen in the attached table (feature_output1-3).

Table 1 Partial optical data feature

Time		Wave band 1					
t (s)	Q	p	a_1	b_1	c_1	key	T
0.00	2579.22	70.03%	-0.0120298	33.358285	-12743.875	128.98	1755.1148
0.50	2583.97	70.16%	-0.0078641	23.025196	-9059.353	128.80	1755.8772
1.00	2583.97	70.16%	-0.0084672	25.161242	-9663.4688	128.80	1755.8772
1.50	2588.75	70.29%	-0.0079245	22.611262	-8784.7809	128.60	1756.6444
2.00	2593.44	70.42%	-0.0081156	24.073987	-9546.7988	128.40	1757.3971
2.50	2593.44	70.42%	-0.0061126	20.515824	-8155.9169	128.40	1757.3971
3.00	2598.2	70.55%	-0.0115617	31.39541	-11749.725	128.17	1758.1611
3. 50	2598.2	70.55%	-0.007359	21.173535	-8219.0153	128.17	1758.1611

4.2 Kelvin temperature and key element prediction based on artificial neural network

The contents of Kelvin temperature T and key element C both will have an important impact on the performance of metal smelting, so accurate prediction of temperature and content of C are very important to improve the efficiency and quality of smelting. Metal smelting process is complex, involving a number of components, and it is a complex nonlinear system, it is difficult to accurately predict the content of T and key elements C in general mathematical model. Neural network has strong nonlinear, self-organization, self-learning ability, can handle non-linear information. Using BP neural network method, the sample data can be fast and effectively locked.

4.2.1 The basic principle of artificial neural network

Artificial neural network is an information processing system that imitates the function and structure of the biological nervous system. Neuron is the basic unit of artificial neural network^[6], and it is generally a nonlinear element with multiple input and single output[1]. A neuron with r multiple input components is shown in Figure 3, among it, the input components are connected with the weight components which multiplies with it. And after the sum, the input of activation function can be formed.

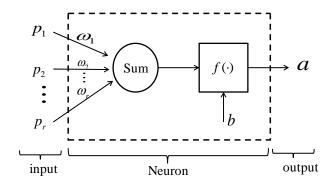


Fig. 3 Neuron model diagram

In addition to the effect of the input signal, the neuron output a is affected by other factors. Therefore, there is often an additional input signal b, called the deviation, also known as the threshold. The neural network is trained by the sample to learn and to change the internal connection weights and thresholds, so that the error of output value and the target value can be minimum^[7]. The BP neural network model includes input layer, middle layer and output layer. The structure of neural network model is shown in Figure 4.

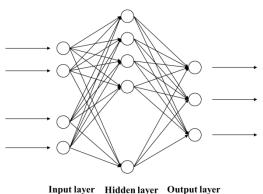


Fig. 4 Sketch of BP neural network

4.2.2 Neural network training and prediction

(1)The determination of each parameter

a. Determination of input and output layers

Input layer is the role of the buffer. The number of nodes selected in the input layer is too many, which makes the network too large. On the contrary, it cannot guarantee the effectiveness of the output results. In the input layer selection process, based on the feature information extracted from the optical data, 12 characteristic parameters of input layer are selected, which called , the corresponding output layer node number is 2, and the content of T and key elements in the Kelvin temperature, respectively.

b. Determination of the number of hidden layers

The number of hidden layers is the same important. Increase the hidden layer of the neural network, the ability of the network to extract input features will be increased accordingly, reducing the output error^[8] and improve the training accuracy[3]. Unfortunately, that will greatly increase the time required for training, so the selected number of hidden layers of the network is two. According to the

following empirical formula, select the number of hidden layer neurons.

$$h = 2m+1$$

$$h = \sqrt{m+n} + a * 1 < a^* < 10$$

$$0.02m < h < 4m$$

$$h = \log_2^n$$

Where: h is the number of hidden layers; m is the number of input layers; n is the number of output layers. The structure of BP neural network predicting the relationship between Kelvin temperature T and key element C is (10,21,2), the neuron activation function of the hidden layer and the output layer of the network are respectively selected by tansing and logsing.

c. Selecting the Initial Value of the Network

The connection weights of neurons are particularly important. If the initial value is too large, the network will be in the beginning of training into the saturation region of S type function, resulting in local optimal, on the contrary, it cannot guarantee the effectiveness of the learning efficiency. To avoid this, using random weight method of randomly selected double^[9] type on the real [-1,1].

d. Selecting the Learning Rate and Expected Error

The learning rate will directly affect the length of training time. The choice of learning rate is too large, the stability of the system will be affected, on the contrary, it cannot guarantee the effectiveness. On the basis of this, a smaller value 0.05 is chosen when choosing the learning rate.

(2) Training and prediction

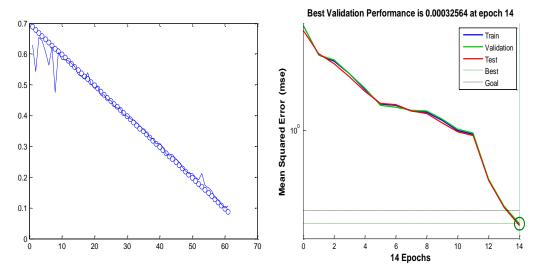


Fig. 5 Training effect chart of key element

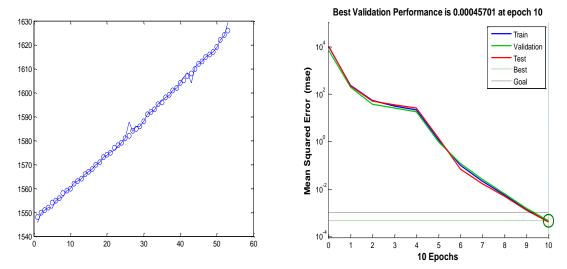


Fig. 6 Training effect chart of Kalvin temperature

Through the prediction curve fitting analysis of predicted value and actual value in Fig.5-6, it can be found in the use of BP neural network to predict the content of key elements that there is a large error in the early prediction, and the later predicted value is in agreement with the actual value. When the number of training reached fourteenth times, it can achieve the best prediction performance^[10], and the mean square error is 0.00032564. When the BP neural network is used to predict the Kelvin temperature, the predicted Kelvin temperature is in agreement with the actual temperature, only a small amount of points have occurred fluctuations. In the determination of the training accuracy of 0.001, the temperature of the best verification performance appears in the tenth training, the mean square error is 0.00045701.

Generally speaking, the BP neural network is used to predict the temperature and the key element content of Kelvin, and the prediction accuracy is high.

4.3 The design of cross experimental

In the second problem, the Kelvins temperature T and the content of key elements were predicted by BP neural network^[11]. And the training device net(k)_key and net(k)_T (k = 1, 2, 3) is obtained by training the relationship of each data sample set.

In order to verify the universality of generated net(k)_key and net(k)_T, the design is as follows:

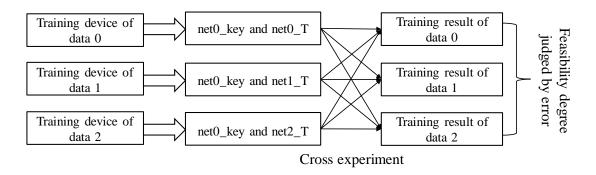


Fig. 7 Cross experiment

4.3.1 Cross experimental design of key element

Three training devices about key element data sample set can be obtained by the training of neural network^[12]. Then the training device $net(k)_k$ is used to train the sample set 1, 2, 3, so that the contrast and error diagrams of predictive value and actual value of key element of each sample set can be got, which are shown in Figure 8.

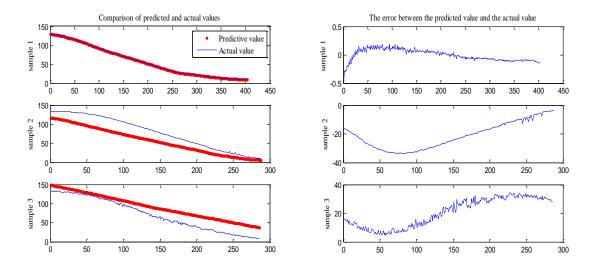


Fig. 8 Effect chart of training device net(0)_key

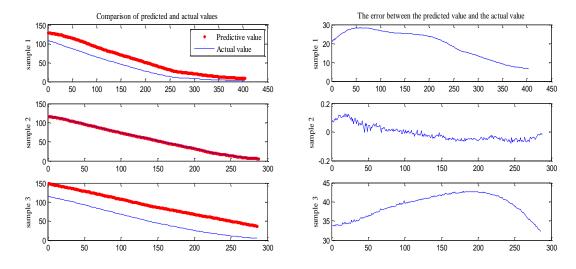


Fig. 9 Effect chart of training device net(1)_key

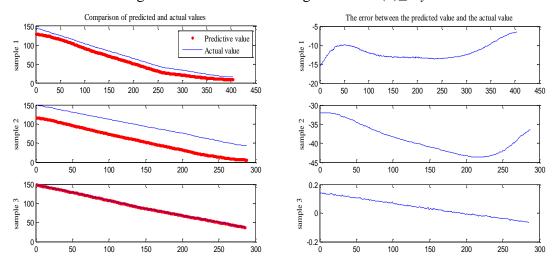


Fig. 10 Effect chart of training device net(3) key

By analyzing the contrast and error diagrams of predictive value and actual value of *key* element of each sample set which are trained by net(k)_*key*, the result can be got:

- By training the sample set, the predictive value of the key content of the sample set is basically consistent with the actual value, and the error of the actual value and the predicted value is close to 0 with the increase of the number of training.
- By using the training of net (0) _key as the training device, it can be obtained that the predicted value of the key content of the sample set 1 is close to the actual value with the increase of the training times, while training of sample set 2, when the training time is small, the error between the predicted value and the actual value is small.
- By using the training of net (1) _key as the training device, it can be obtained that the predicted value of the key content of the sample set 0 is close to the actual value with the increase of the training times, while there is a large error between the predicted value and the actual value in sample 2.
- Similarly, by using the training of net (1) _key as the training device, it can be

obtained that the prediction value of key content of sample set 0 is consistent with the actual value, while the prediction value of sample set 1 has a large error with the actual value, as the number of training increases.

In summary, Net (0) _key can be used to get the sample set of 0 and sample set 2 of the key content prediction, however, there is a large error when net (0) _key and net (2) _key were used to predict the content of key in the sample set 1. So in the actual metal smelting process, in order to achieve the prediction of the key element content in the three sets of samples, only net (0) _key (or net (2) _key) and net (1) _key need to be generated to accurately predict the content of key elements.

4.3.2 The design of temperature cross experiment

According to the above cross experimental process of *key* element, the contrast and error diagrams of predictive value and actual value of temperature T of each sample set can be got^[13], which is shown in appendix.

By analyzing the contrast and error diagrams of predictive value and actual value of *key* element of each sample set which are trained by net(k)_*key*, the result can be got:

Net (2) _T can be used to get 3 sets of T content prediction. While with net (0) _key and net (2) _T for prediction of T content, there is a big error. Therefore in the actual metal smelting process, to achieve the T content prediction of 3 sets of samples, just generating the training device net(2)_T [14] to achieve the temperature prediction of 3 sample sets.

4.3.3 Error analysis of cross experiment

In order to test the prediction effect of the BP neural network model established by Problem 2, the key element content and the association error^[15] between the temperature prediction value and the actual value were calculated by the formula (9). The results are shown in Table 1-2.

$$a_{ij} = \frac{norm(errij)}{length(errij)} \tag{9}$$

Trainers Test sample set	0	1	2
0	0.005	1.3691	1.3459
1	1.0489	0.0031	2.3127
2	0.5918	2.3044	0.0042

Table 2 Covariance matrix of key element prediction

Through the analysis of the covariance matrix of key element prediction, the minimum error between the predicted value and the actual value of the key content can be get by using the trained trainers, and net (2) _key also can be used as the training device to predict the content of the key element in the sample set 0.

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Table 3	Covariance	matrix	\cap t	temperature	nrediction
I auto I C	Covariance	mania	$\mathbf{o}_{\mathbf{I}}$	terriperature	production

Trainers			
Test	0	1	2
sample set			
0	0.0021	2.3425	3.3881
1	1.8873	0.0058	2.0406
2	0.7118	1.6996	0.0048

Through the analysis of the covariance matrix of temperature prediction, the training device can be obtained by training the sample set, use it to train its own set of samples, and the covariance error between the predicted temperature and the actual value is minimum^[16]. In a certain error threshold, to achieve the 3 sets of samples of the T element content prediction, only need to generate net (2) _T this trainer can achieve three sample set temperature forecast.

In summary, by calculating the *key* element content and the covariance of temperature predicted value and actual value, the forecast effect is basically consistent with the conclusion of the problem^[17]. So it can be considered that the model is reasonable and effective in problem two.

5 Model evaluation and improvement

5.1 Error analysis of model

In the prediction model of BP neural network, the number of input layer nodes hidden layer and hidden layer nodes is the most important parameter in the BP network prediction model. And for the prediction of the BP neural network, only three layers are needed, and the number of output nodes can be determined according to the function of prediction. So the parameters that affect the ability of BP network prediction are only the number of input nodes and the number of hidden nodes, which is topological structure of neural network. Besides, the training error of MSE (Mean of Squared Error) allowed by neural network also affects its prediction. Experiments show that the optimal network model is corresponding to a certain topological structure, and converges to an optimal position which is determined by the MSE target value. The convergence position is not the global optimal point of the network. In order to improve the accuracy of neural network prediction, this paper uses genetic algorithm to optimize the number of input nodes, the number of hidden layer nodes and the MSE target value.

5.2 Optimization design based on genetic algorithm

In this paper, the genetic algorithm parameters are designed as the following: population number n = 30, gene string (chromosome) uses binary encoding, the crossover rate and mutation rate were respectively 0.50 and 0.05, and evolutionary algebra is 100 generation. N, M and MSE are 5 bit binary code. In order to avoid the number of nodes is 0, after decoding, the number of nodes in the input layer and 5 to get N, while the number of hidden layer nodes plus 10 to get M. The content of *key* element and the covariance matrix of temperature of predicted value and actual value,

which is shown in Table 4-5:

Table 4 Predicted covariance matrix of *key* element (After optimization)

Training device Test sample set	0	1	2
0	0.0012	1.2901	1.0261
1	0.9818	0.003	2.2579
2	0.6662	1.8044	0.0017

Comparing the data of Table 2 and 4, adding all error, the sum of covariance in Table 2 is 8.951; the sum of covariance in Table 4 is 7.8324, and the optimized neural network has improved the accuracy of key element content prediction by 10.62%.

Table 5 Predicted covariance matrix of temperature(After optimization)

Training device			
Test sample	0	1	2
set			
0	0.0011	2.9410	0.8143
1	1.9993	0.0008	1.0507
2	0.6252	2.6465	0.0019

Comparing the data in Tables 3 and 5, and summing all the errors, the total error of covariance in Table 2 is 12.0826, and the total error of covariance in Table 4 is 7.9639, the predicted accuracy of the optimized neural network is improved by 16.58%.

In summary, the prediction performance of the neural network optimized by genetic algorithm is improved obviously, and the prediction ability of the model has achieved better effect.

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Appendix

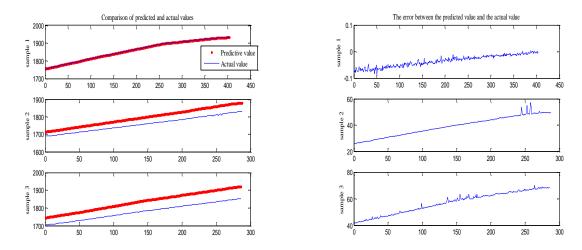


Fig. 10 Training effect chart of training device net(0)_T

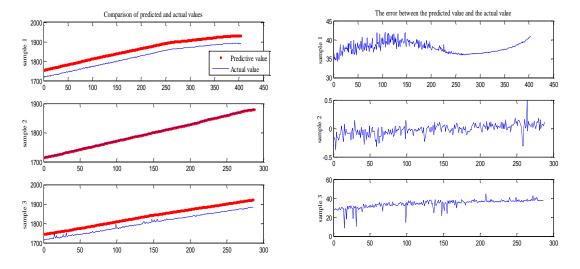


Fig. 11 Training effect chart of training device net(1)_T

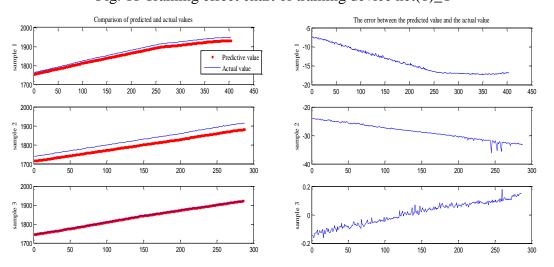


Fig.12 Training effect chart of training device net(2)_T