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# Prediction of the Yield Based on the BP Neural Network and Fitting

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ABSTRACT

Deoxidizing alloying is an important process in steel smelting. In this paper, a prediction model for the yield of carbon and manganese elements is established, and the control space theorem is defined to judge the prediction accuracy of the model. Using BP neural network and the fitting of two kinds of methods, respectively, set up the deoxidation alloying process of alloying elements yield prediction model, shorten training time, improve the model prediction accuracy, it is concluded that the BP neural network predictive value are above 85%, fitting prediction were over 82%, the BP neural network forecasting model is more conform to the requirements of the production.



## 1. Introduction

With the development of computer technology, the automatic ingredient model with alloy yield prediction and cost optimization algorithm has been studied to achieve the purpose of automatic deoxyalloy. At present, some workshops in China introduce this technology and are successfully applied to production, but in general, there is still a big gap compared with the international advanced countries.

For different kinds of steel at the end of melting, different quantities of alloys should be added to make the alloy elements meet the standard, and finally enable the finished steel to meet certain specific requirements in certain physical properties. With the continuous improvement of the production of high value - added steel, how to optimize the production type and quantity, ensure the quality of steel water and minimize the production cost of alloy steel is an important problem to improve their competitiveness. One or more elements larger with oxygen affinity than iron are added to the steel, and capturing the excess oxygen in the steel is anaerobic. Deoxyalloy refers to the operation of adding different quantities and different kinds of alloys to the steel after the melting of different steel to meet the alloy elements, and finally makes the finished steel meet the regulation requirements in some physical properties. The loss of alloy elements in the process of deoxyalloy are: mainly the oxidation of the elements by the oxides in the steel water and the elements remaining in the steel slag without entering the steel water. There are many factors affecting the oxidation degree of alloy. In the process of alloying, the most important factors are: steel liquid oxygen activity, unstable oxide activity in slag, steel slag alkali degree, blowing argon mixing strength, steel water temperature and steel water quality.

The divided deoxygen elements are deoxygen reaction between C and Si,Mn and oxygen, mainly divided into three reactions

$$[Si]+2[O]=SiO_2(s) \qquad \Delta G=-576440+218.2T \quad (1)$$

$$lgK=lg\left(a_{Si}a_O^2\right)=-\frac{30410}{T}+11.58 \quad (2)$$

$$[Mn]+[O]=(MnO) \qquad \Delta G=-244300+108.83T \quad (3)$$

$$lgK=lg\frac{a_{(MnO)}}{a_{[Mn]}\bullet a_{[O]}}=-\frac{14450}{T}+6.43 \quad (4)$$

$$[C]+[O]=\{CO\} \qquad \Delta G=-22200-38.34T \quad (5)$$

$$lgK_{CO}=lg\left(\frac{P_{CO}}{a_C\bullet a_O}\right)=-\frac{1168}{T}-2.07 \quad (6)$$

Due to a large collection of historical steelmaking data, prediction methods such as BP neural network and fitting can be used to predict the yield and bring the content of C,Mn and other elements to the national standard.

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## 2.Calculation of the historical C、Mn element yield

The resulting alloy yield refers to the ratio of the weight of the alloy element absorbed by steel water during deoxyallozation to the total weight of the element. Therefore, the formula for calculating the element yield is as follows:

$$y_i = \frac{T_i \times G_i - (G_i + \sum_{j=1}^{17} M_j) \times Q_i}{\sum_{j=1}^{17} M_j \times \omega_i} \tag{6}$$

Where in the formula, $y_i$ is the yield corresponding to the $i$ element, $i = C, Mn$, $G_i$ is the net weight of the molten steel, $T_i$ is the continuous casting, $M_j$ is the mass of an alloy, the $j$ represents the alloy, and the proportion of the element containing the element $\omega_i$.

The yield distribution of the C、Mn element can be calculated separately according to the historical data, as shown in the following figure;

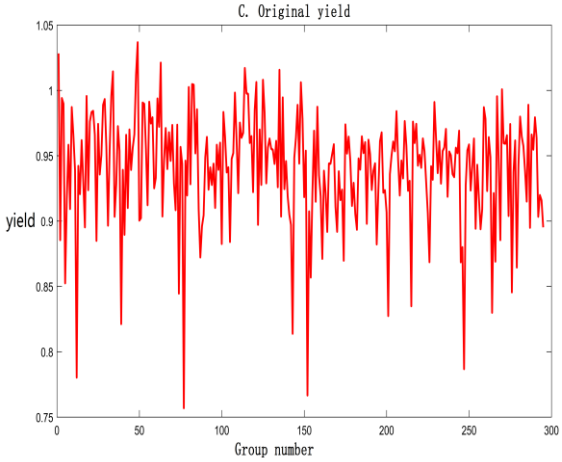


**Fig. 1.** Historical yield of C

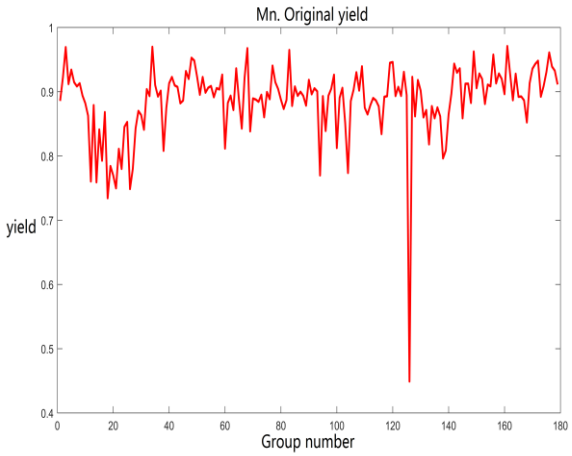


**Fig. 2.** Historical yield of Mn

## 3.Correlation analysis

Grey relational analysis refers to the method of quantitative description and comparison of a system development and change situation. The basic idea is to determine whether the connection is tight by determining the geometric similarity of the reference data column and several comparison data columns. It reflects the degree of correlation between curves. This method can usually be used to analyze the degree of influence of various factors on the results. It can also be used to solve the comprehensive evaluation problem with time. The core of the problem is to establish a reference sequence that changes with time according to certain rules, and to evaluate each object over time. The change is used as a comparison sequence, and the degree of correlation between each comparison sequence and the reference sequence is obtained, and the conclusion is drawn according to the correlation size.

The specific calculation steps of the grey correlation analysis are as follows:

***Step1:*** Determining the analysis series

Determine the reference sequence that reflects the characteristics of system behavior and the comparison sequence that affects system behavior. Reflect the behavior characteristics of the system. Data sequence, called the reference sequence. A sequence of data composed of factors that affect the behavior of a system, called a comparative sequence.

Reference number is

$$Y = \frac{Y(k)}{k} = 1, 2 \ldots n \tag{7}$$

Comparison number is

$$X_i = \frac{X_i(k)}{k} = 1, 2 \ldots n; i = 1, 2 \ldots m \tag{8}$$

***Step2:*** Dimensionless of variables

Because the data in each factor column of the system may be different due to the dimension, it is not convenient to compare or it is difficult to get positive when comparing. Therefore, the dimensionless processing of data is generally required in the grey relational analysis. There are two main methods:

Initialization processing:

$$x_i(k) = \frac{x_i(k)}{x_i(1)}, k = 1, 2 \ldots n; i = 0, 1, 2 \ldots m \tag{9}$$

Meanization processing:

$$x_i(k) = \frac{x_i(k)}{\overline{x_i}}, k = 1, 2 \ldots n; i = 0, 1, 2 \ldots m \tag{10}$$

Where $k$ corresponds to the time period and $i$ corresponds to one of the comparison series.

***Step3:*** Calculate the correlation coefficient

$$\begin{aligned} \xi_i(k) &= \frac{M + N}{G + T} \\ M &= min_i min_k \left| y(k) - x_i(k) \right| \\ N &= \rho max_i max_k \left| y(k) - x_i(k) \right| \\ G &= y(k) - x_i(k) \\ T &= \rho max_i max_k \left| y(k) - x_i(k) \right| \end{aligned} \tag{11}$$

Where $\rho$ is called the resolution coefficient, the smaller $\rho$ is, the larger the resolution is. The value range of $\rho$ is generally determined by the specific value of $(0,1)$. When $\rho \le 0.5463$, the resolution is best, usually take $\rho = 0.5$

***Step4:*** Calculate the degree of relevance

Because the correlation coefficient is the degree of correlation between the comparison sequence and the reference sequence at each moment (that is, each point in the curve), it has more than one number, and the information is too scattered to make a global comparison. Therefore, it is necessary to concentrate the correlation coefficient of each moment (that is, each point in the curve) into one value, that is, calculate its average value, and represent it as the number of correlation degree between the comparison sequence and the reference sequence. The correlation degree formula of $r_i$ is as follows,

$$r_i = \frac{1}{n}\sum_{k=1}^{n}\xi_i(k), k = 1,2\ldots n \tag{12}$$

***Step5:*** Sorting degree of relevance

The degree of association is sorted by size. If $r_1 < r_2$, the reference sequence $y$ is more similar to the comparison sequence $x_2$. After calculating the correlation coefficient between the $X_i(k)$ and the $Y(k)$, the average value of each type of correlation coefficient is calculated, and the average value $r_i$ is called the correlation degree between $X_i(k)$ and $Y(k)$.

***Step6:*** Normalized processing

Because the different variables are heterogeneous, the numerical differences are also different. It is not appropriate to directly weight them, and it has no practical significance. In order to reflect the actual situation as much as possible and avoid unreasonable phenomena, firstly normalize the data of each variable.

$$z = \frac{x_i - \bar{x}}{s} \tag{13}$$

Where $x_i$ represents the specific value of the selected variable, $\bar{x}$ represents the mean of the variable, and $s$ represents the standard deviation of the variable.

## 4.Grey correlation solution

Firstly, based on the calculation of the element yield rate, based on the previous data screening, the data of the alloy yield greater than 1 or less than 0.8 is removed, and the data are classified according to the steel number, and a total of 151 sets of data are obtained.

According to the above method of grey correlation analysis, this paper classifies different steel number data in effective data. Taking low alloy HRB400B steel as an example, the yield of *C* element is set as reference series $Y_C = \frac{Y(k)}{k} = 1,2\ldots n, n = 128$, and the yield of *Mn* element is set as reference series.

$$Y_{Mn} = \frac{Y(k)}{k} = 1,2\ldots n, n = 128 \tag{14}$$

the possible influencing factors are set to compare series

$$X_i = \frac{X_i(k)}{k} = 1,2\ldots 128; i = 1,2\ldots 14, i_1 \sim i_{14} \tag{15}$$

respectively representing the converter end temperature, converter end point C, converter end point Mn, converter end point S, converter end point P, converter end point Si, molten steel net weight, vanadium nitrogen alloy (import) , ferrovanadium (FeV50-B), silicoalumino, silicon manganese surface, petroleum coke recarburizer, manganese silicon alloy FeMn68Si18 (qualified block), silicon carbide (55%), etc.

Gray correlation analysis was performed on C and Mn for 14 factors. The results are shown in the following table:

**Tab.** 1.Gray correlation degree between various factors and yield of steel number HRB400B

| | r(C Yield) | r(Mn Yield) |
|---|---|---|
| Converter end temperature | 0.97585 | 0.97084 |
| Converter end point C | 0.94826 | 0.95470 |
| Converter end point S | 0.88452 | 0.80042 |
| Converter end point Si | 0.87316 | 0.86942 |
| Molten steel net weight | 0.89809 | 0.87423 |
| Ferrovanadium | 0.82803 | 0.81761 |
| Recarburizer | 0.89044 | 0.88405 |
| Manganese silicon alloy | 0.88110 | 0.87351 |
| Silicon carbide | 0.74187 | 0.73007 |
| Converter end point Mn | 0.77249 | 0.76351 |
| Converter end point P | 0.58871 | 0.58326 |
| Vanadium-nitrogen alloy | 0.72016 | 0.73264 |
| Silicon aluminum calcium | 0.72386 | 0.71616 |
| Silicon manganese surface | 0.73523 | 0.73498 |

You can see from the table above: the temperature of converter, converter end point C, steel net, manganese silicon alloy FeMn68Si18, end S of converter, converter end Si, vanadium iron (FeV50 - B), oil carbon agent, such as the eight factors impact on the yield strength is very big, the terminal temperature of converter, converter end C influence on the yield is the largest, this phenomenon reflects directly the two variables at the same time had the greatest influence of C and Mn yield, thus it can be concluded that influence the main factors that influence the rate of C and Mn for converter of endpoint temperature and converter C.

## 5.The Establishment of the BP Neural Network

BP neural network is a nonlinear dynamical system containing three layers of input layer, implicit layer and output layer. Set the input vector to be $X = (x_1, x_2, \cdots, x_n)^T$ ,The implied - layer output vector is $Y = (y_1, y_2, \cdots, y_m)^T$ ,Output layer output vector is $G = (g_1, g_2, \cdots, g_k)^T$ ,The expected output vector is $D = (d_1, d_2, \cdots, d_l)^T$ The weight matrix between output and implied layers $V$ , $V = (v_1, v_2, \cdots, v_m)$.

The column vector $v_m$ is the weight vector corresponding to the implied layer $m$ and the weight matrix between the implied layer

and the output layer is expressed by $W$, $W=(w_1,w_2,\cdots,w_i)$, where the column vector $w_i$ is the weight vector corresponding to the $i$ neuron of the output layer. neurons,

$$\begin{cases} G_j = f(net_j), j=1,2,\cdots,k, The\ input\ layer \\ net_j = \sum_{i=0}^{m} \omega_{ij} g_i, j=1,2,\cdots,k, \ Hidden\ layer \\ f(x) = \dfrac{1}{1+e^{-x}}, \ Transfer\ function \\ f'(x) = f(x)[1-f(x)] \end{cases} \tag{16}$$

Among them, the transfer function $f(x)$ is a unipolar *Sigmoid* function, and the $f(x)$ has continuity derivability.

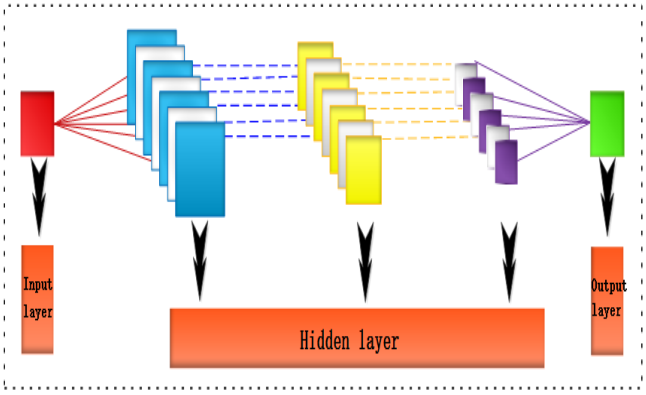


**Fig. 3.**BP Neural Network Structure Map

Definition of network error and weights update. When the network output is different from the expected output, there is an output error, defined as follows:

$$E = \frac{1}{2}(D-G)^2 = \frac{1}{2}\sum_{i=1}^{k}(d_i - g_i)^2 \tag{17}$$

Expand the above error definitions to the implied layer has:

$$\begin{aligned} E &= \frac{1}{2}\sum_{i=1}^{k}[d_i - f(net_i)]^2 \\ &= \frac{1}{2}\sum_{i=1}^{k}[d_i - f\left(net_i = \sum_{i=0}^{m} w_{ij} g_i\right)]^2 \end{aligned} \tag{18}$$

Expand further to the input layer, with:

$$\begin{aligned} E &= \frac{1}{2}\sum_{i=1}^{k}\left\{d_i - f[\sum_{i=0}^{m} w_{ij} f(net_i)]\right\}^2 \\ &= \frac{1}{2}\sum_{i=1}^{k}\left\{d_i - f[\sum_{i=0}^{m} w_{ij} f\left(\sum_{i=0}^{n} v_{ij} g_i\right)]\right\}^2 \end{aligned} \tag{19}$$

A s can be obtained from the above formula, the network error is a function of each layer weight $w_{ij}, v_{im}$, so adjusting the weight can change the error $E$ ,Obviously, the principle of adjusting the weights is to continuously reduce the error, so that the adjustment amount of the weights should be made proportional to the error gradient reduction, namely:

$$\begin{aligned} \Delta w_{ij} &= -\eta \frac{\partial E}{\partial w_{ij}} \quad i=0,1,2,\cdots,n; \ j=1,2,\cdots,k \\ \Delta v_{mi} &= -\eta \frac{\partial E}{\partial v_{mi}} \quad m=0,1,2,\cdots,l; \ i=1,2,\cdots,n \end{aligned} \tag{20}$$

In formula, the negative sign the gradient descent and the constant $\eta \in (0,1)$ the proportional coefficient, reflecting the learning rate [4] in training.

## 6.Prediction of C、Mn element yield by BP Neural Network

Seek the data group of C,Mn yield, divide the data group into 90% training set and build three - layer network layer; input vector is $X=(x_1,x_2,\cdots,x_n)^T$, implied layer output vector is $Y=(y_1,y_2,\cdots,y_m)^T$, output layer output vector is $G=(g_1,g_2,\cdots,g_k)^T$.

Layer 1 network layer, weight matrix dimension (3, 5), coefficient matrix:

$$\begin{pmatrix} -1.437e-01 & -6.769e+03 & -8.658e-01 & -3.423e-01 & -6.118e-01 \\ -7.061e-01 & -5.459e-01 & -2.675e-01 & -1.788e-01 & 6.723e-02 \\ -1.400e-01 & 3.167e-01 & -5.119e-01 & 6.549e-01 & -8.186e-01 \end{pmatrix}$$

Layer 2 network layer, weight matrix dimension (5, 3), coefficient matrix:

$$\begin{pmatrix} 5.209e-01 & 8.111e-01 & -3.232e-01 \\ 3.695e+03 & -1.918e+03 & -3.749e+03 \\ -7.187e-01 & -7.984e-01 & -5.719e-01 \\ 6.550e-01 & -6.957e-01 & -1.366e-01 \\ 7.931e-01 & 5.744e-02 & 3.323e-01 \end{pmatrix}$$

Layer 3 network layer, weight matrix dimension (3, 1), coefficient matrix:

$$\begin{pmatrix} 1041.223 \\ 2042.366 \\ 2141.848 \end{pmatrix}$$

The true and predicted values of Mn yield in any 100 furnace are shown below:

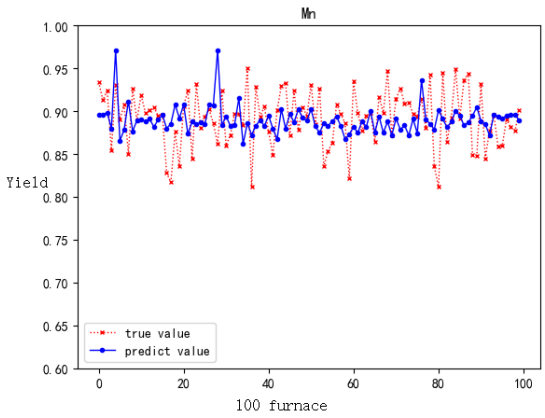


**Fig. 4.** Predicted and true values of Mn

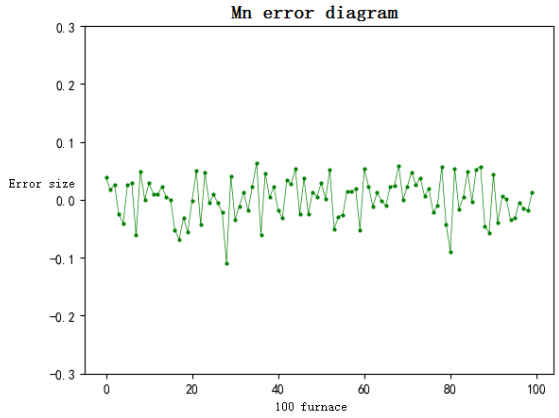


**Fig. 5**. The error of Mn

The predicted value of the 100 furnace end Mn is above 85% , partly exceeding 95% or even 100% , the error value of Mn, the partial error is zero, and the error range above 95% does not exceed the interval [-0.1,0.1].

The true and predicted values of C yield in any 100 furnace are shown below:

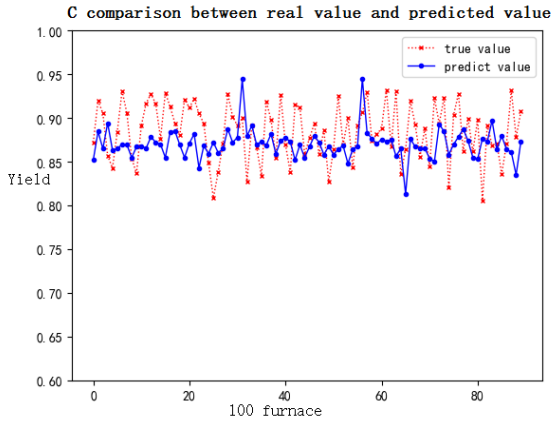


**Fig. 6**. Predicted and true values of C

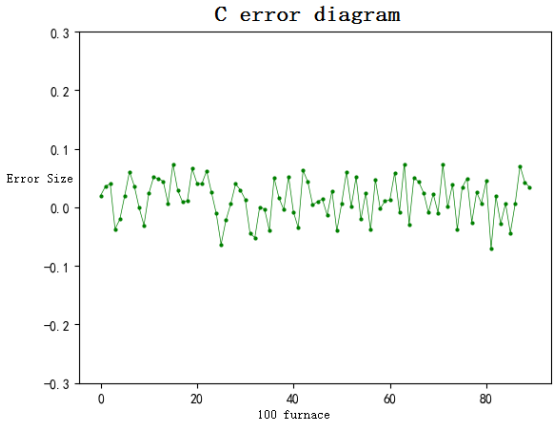


**Fig. 7**. The error of C

Most of the prediction value of the 100 furnace end component C reaching above 85% , a few prediction values exceeding 87% , and also, the 100 group error value of C, most of the error value tends to zero, all error range does not exceed the interval [-0.1,0.1]

## 7. Proposed legal yield prediction of C、Mn elements

Random draw of 10 sets of data from the historical yield for fitting analysis:

**Tab**. 2. 10 Group Year and Rate.

| The temperature | yield |
|---|---|
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |
| 1678 | 0.865 |

Let the curve fitting function be the

$$y = a_1 + a_2 x + \cdots + a_m x^{m-1} \tag{21}$$

Three fitting curves can be obtained:

$$\begin{cases} y = 1.9455 - 0.0006x \\ y = 88.180 - 0.104x + 0.00003x^2 \\ y = 180658 - 441.676x + 0.404x^2 - 0.00016x^3 + 2.517x^4 \end{cases}$$

The above three fitting curves are shown as follows:

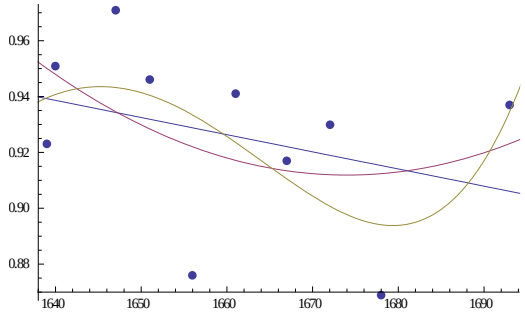

**Fig. 8**. The fitting curve diagram

When the $m \to \infty$ , the fitting effect greatly increases .

First, the partial historical yield is described as a series of irregularly discrete points $y_i$ , on the right - angle coordinate system can set the approximation to $y_i^*$ , so $\delta_i = y_i - y_i^*$ can be called the residual, the smaller the residual reflects the better the fit of the approximation function.

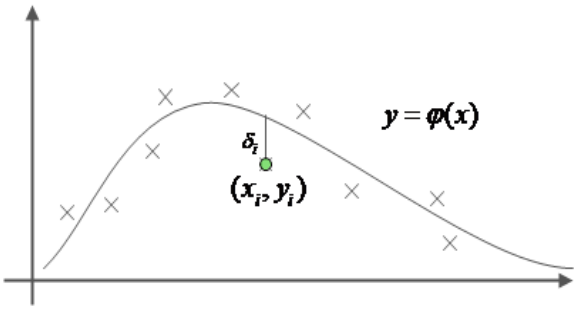


**Fig. 9**. Residual Schematic

Let the curve fitting function be:

$$y = a_1 + a_2 x + \cdots + a_n x^{n-1} \tag{22}$$

If the square and sum of the residual is minimized, the approximation is close to the real value, therefore:

$$\sum_i^n \delta_i^2 = min \tag{23}$$

You can select a set of functions

$r_1(x), r_2(x), \cdots, r_m(x) \quad m < n$ first, in particular,

$$\{r_1(x), r_2(x), \cdots, r_m(x)\} = \{1, x, x^2, \ldots, x^{m-1}\} \tag{24}$$

make

$$\varphi(x) = a_1 r_1(x) + a_2 r_2(x) + \cdots + a_m r_m(x) \tag{25}$$

Determine $a_1, a_2, \cdots, a_m$ so that

$$\begin{aligned} J(a_1, a_2, \cdots, a_m) &= \sum_i^n \delta_i^2 = \sum_i^n \left[\varphi(x_i) - y_i\right]^2 \\ &= \sum_i^n \left[\sum_{k=1}^m a_k r_k(x_i) - y_i\right]^2 \end{aligned} \tag{26}$$

To minimize $J(a_1, a_2, \cdots, a_m)$, you need to derive partial derivatives for it:

$$\frac{\partial J}{\partial a_k} = 0 \quad (k = 1, \cdots m) \tag{27}$$

The matrix form is:

$$\begin{pmatrix} (r_1, r_1) & (r_1, r_2) & \cdots & (r_1, r_m) \\ (r_2, r_1) & (r_2, r_2) & \cdots & (r_2, r_m) \\ \cdots & \cdots & \cdots & \cdots \\ (r_m, r_1) & (r_m, r_2) & \cdots & (r_m, r_m) \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix} = \begin{pmatrix} (y, r_1) \\ (y, r_2) \\ \vdots \\ (y, r_m) \end{pmatrix}$$

If you remember

$$Q = \begin{bmatrix} r_1(x_1) & \cdots & r_m(x_1) \\ \cdots & \cdots & \cdots \\ r_1(x_n) & \cdots & r_m(x_n) \end{bmatrix} \quad a = \begin{bmatrix} a_1 \\ \vdots \\ a_2 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

The regular equations at this point are: $(Q^T Q)a = Q^T y$

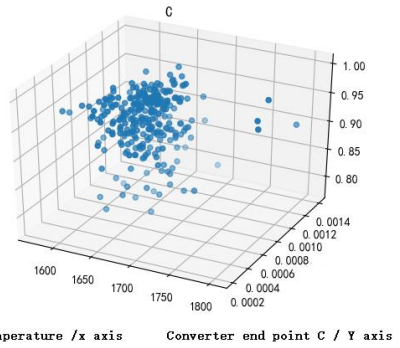


**Fig.10** Schematic of 3 - D Relations between Impact Factors and C Rate

Therefore, the predicted yield is obtained, and the analysis of the predicted values of any ten groups of C is taken, and the following table is given:

Tab. 3. Forecast value of C element fitting

| The temperature | yield |
|---|---|
| 1678 | 0.829 |
| 1640 | 0.951 |
| 1651 | 0.946 |
| 1656 | 0.876 |
| 1661 | 0.941 |
| 1667 | 0.917 |
| 1693 | 0.937 |
| 1681 | 0.926 |
| 1672 | 0.930 |
| 1647 | 0.971 |

Conclusion: The lowest carbon yield in the ten groups of prediction data is 0.829377, the highest value is 0.971045, and the prediction rate is above 82%, so the prediction effect of interpolation fitting is worse than BP neural network prediction [11].

According to the two factors affecting the yield of Mn, the converter end temperature and the converter end point C, the temperature is $x$ axis, the converter end point C is $y$ axis, and the yield is $z$ axis, and the three-dimensional spatial relationship diagram is as follows:

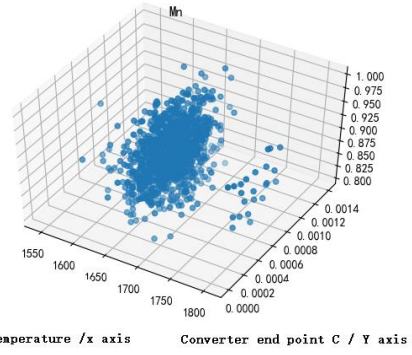


**Fig.11** Diagram of 3 D Relations between Two Factors and Mn Rate

Therefore, the predicted yield can be obtained, and any ten groups of Mn yield analysis can be taken out, and the following table is given:

**Tab**. 4. Forecast value of Mn element fitting

| The temperature | yield |
|---|---|
| 1684 | 0.937 |
| 1663 | 0.943 |
| 1705 | 0.950 |
| 1639 | 0.894 |
| 1571 | 0.846 |
| 1710 | 0.912 |
| 1692 | 0.920 |
| 1645 | 0.931 |
| 1668 | 0.941 |
| 1655 | 0.951 |

Conclusion: The lowest yield of manganese in the ten groups of prediction data is 0.845525, the highest value is 0.951274, and the prediction rate is above 82%, so the prediction effect of interpolation fitting is worse than BP neural network prediction.

## 8. Summary

With the continuous increase of high value - added steel production in the steel industry, establish mathematical model of deoxyalloy link through historical data to realize online prediction and optimize the type and quantity of input alloys, and reduce the production cost of alloy steel to the premise of ensuring steel water quality, which is the decisive guarantee to enhance the competitiveness of major steel enterprises and obtain long - term development interests.

Combining big data thinking, analyzing the influence of each variable on the charging rate of alloy elements, extracting actual production data, ensuring the reliability of the model, BP neural network prediction value is above 85% meets the production requirements.

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