Team Number :	1016

Problem Chosen :	B

Research of Properties of Deformed Steel Bar Based on Multiple Stepwise Regression and BP Neural Network

Abstract

With the continuous development of steel smelting technology in China, technicians have not only already known the exact proportion of elements compounded in metallurgical products, but are also able to gain exact control of the proportion of alloy elements. In 2015, steel plants in China produced eleven billion tons of iron and steel products, which ranked the first throughout the world. For Chinese steel plants, one of the most important missions is to improve the strength of steel while to cut costs simultaneously. Since elements mixed in steel will influence its performance to some extent, it is essential to research composition proportions of elements, which is the solution of the questions above.

First, the paper selects production data of a certain enterprise from Attachment 1 as statistical object. According to the actual performance of the material and production data, discard extraordinary data which is detrimental to a correct conclusion. Then in order to find out the principal elements influencing the performance of steel materials , stepwise regression is used based on Statistical Product and Service Solutions (SPSS) , considering elements C, Mn, S, P, Si, Cr, Mo, Cu, Ni, Alt, V as determining variable and considering tensile strength, yield strength and percentage elongation as dependent variable.

Second, excluding secondary factors and reserving decisive factors of steel properties, relationship between the properties of deformed steel bar and chemical elements is analyzed by applying stepwise multiple linear regressions. The scatter diagram is drafted with SPSS; possible fitted curves of various categories are established (e.g., exponential model, logarithmic model, logistic model, linear model) .Then the quantitative curve relationship is determined. Research shows that the influence added by chemical elements is neither a simple linear relationship nor a nonlinear one, but belongs to a complex multivariable coupled system. B.P. (abbr. for Backpropagation) neural network, a feedforward network formed of non - linear transformation units, is able to realize adjustment of multi-layer feedforward neural weight and handle highly-nonlinear problems intelligently. Therefore, the paper utilized MATLAB to design and modify B.P. neural network model. Reflection between steel properties and chemical elements are trained by the model repeatedly.

According to the requirements of problem, the mathematics model of is obtained on condition that the error of training is extremely small. The modified model is inspected with systematic-sampling extracted data from attachment 1. The high degree of fit of the modified model is proved with the comparison between the predictor and practical value.

Finally, change tendency of properties of deformed steel bars is analyzed and an optimization program on composition proportion of chemical elements and cost of production is provided by MATLAB using control variables method.

Keywords：stepwise regression, B.P. neural network, chemical composition, property, deformed steel bar

Contents

1. Introduction

1.1Background and significance of the research

Hot-rolled ribbed bar is commonly known as deformed steel bar, it's mainly used for skeleton of reinforced concrete component and it requires certain mechanical strength, bending and deformation properties, fabrication weldability in use. The chemical composition in steel is the basic element that influences the final structure property of hot rolled steel. Most deformed steel bar adopts micro alloying method, that is to add expensive microelement (such as Mn alloy material, V alloy material, etc.) into steel, adjust the composition proportion and improve structure property.

Tensile strength is a measurement of the force required to pull something such as rope, wire, or a structural beam to the point where it breaks. The tensile strength of a material is the maximum amount of tensile stress that it can take before failure, for example breaking. It reflects the fracture resistance of the material. The yield strength is the limit of the yield behavior of metal materials, that is, resistance to micro-plastic deformation. If the part is subjected to external force greater than this strength, the part will be permanently disabled and cannot be restored. Percentage elongation after fracture is the ratio of the elongation of the material to the original length after the tensile fracture of the metal material. It reflects the plastic deformation capacity of the indicators.

Experiments shows that adding some expensive microelement in the smelting process can significantly increase tensile strength, yield strength and percentage elongation after fracture, which are major mechanics performance indexes of steel materials. China is one of the biggest steel material producers around the world, therefore cutting the average production cost of still will be much good for environment protection and development of the country. In this respect, giant steel producers like Anshan Steel Plant and Wuhan Steel Plant organized a large number of researchers to study and examine performance indexes of steel materials, meaning to achieve the highest return with the lowest cost. It can be seen that research of composition proportion of elements is significant to steel and other relevant industries.

The element Cr in steel can significantly increase the strength, hardness and wear resistance. When the plant uses mine rich in Cr, the Cr content in liquid iron will significantly increase. Therefore, if it is possible to reduce expensive alloy materials contents like Mn and V in allowance range when Cr content increases, the plants would get the cost control successfully. This paper will establish mathematical model to analysis and process production data provided by a certain enterprise and work out these problems：

1) Finding out the main elements that influence properties of deformed steel bar like yield strength, tensile strength and percentage elongation after fracture and analyze the correlation between these factors.

2) Modelling the influence rule between deformed steel bar properties and chemical elements like C, Mn, Cr, V, and N.

3) Researching the reduction of alloy material like Mn and V in allowance range of deformed steel bar properties by Cr content increase and present the content modification scope of main elements and design composition optimization scheme.

1.2 Problem Analysis

The properties of the deformed steel bars are related to the microstructure, and the microstructure is related to the kinds of elements and the processing technology. Therefore, the influence of element type and content on the properties of deformed bars is a statistical regression problem of multivariate variables, that is, there is a mapping relationship between multiple independent variables and multiple dependent variables. By analyzing the mapping relationship, we can predict the value of the dependent variable from the known independent variables to establish the model of the element type and content of the alloy on the performance of the deformed bar.

Problem 1: Large amounts of data in Attachment 1 are sorted and filtered, and dead pixels are removed. The influence of each element on the properties of deformed steel bars and the correlation between these elements are analyzed by SPSS stepwise linear regression analysis. Then the main factors affecting the properties of the steel are obtained.

Problem 2: This part studies the correlation of single variable to the performance of deformed bars. According to surveys, the influence added by chemical elements is neither a simple linear relationship nor a nonlinear one, but belongs to a complex multivariable coupled system. So modifying of algorithm and model is essential. A neural network model containing an input layer of principal factors, a hidden layer with 10 intersections and an output layer of tensile strength, yield strength and percentage elongation after fracture is obtained by BP neural network and MATLAB programming. The control variables are used to analyze the variables one by one to obtain the correlation, which is fitted with higher confidence after 50,000 times of training.

Problem 3: This problem has a strong practical value and significance. On the basis of the answers to the first two questions, add the program, use the loop statement, and control the strength of the deformation of steel within the allowable range. Then increase the Cr content to minimize the amount of expensive metals like Mn and V to balance performance and cost and save energy.

2. Assumptions

1) Assume that equipment and technology of product 1 and product 2 processing does not change significantly.

2) Ignore the impact of other factors on the mechanical properties of steel except composition proportion of chemical elements.

3) Assume that the shape, size and length of the tested samples of the same kind are same during experiments of measurements of tensile strength, yield strength and percentage elongation.

4) Assume that the chemical composition of the steel does not change over time.

5) Ignore the influence of materials mechanical properties (Fatigue properties, corrosion resistance, and high temperature resistance) on tensile strength, yield strength and percentage elongation.

3. Symbol Description

Symbol	Symbol Description
X_C	Composition proportion of C
X_{Mn}	Composition proportion of Mn
X_S	Composition proportion of S
X_P	Composition proportion of P
X_{Si}	Composition proportion of Si
$X_{C_{eq}}$	Composition proportion of Ceq
X_V	Composition proportion of V
X_{Cr}	Composition proportion of Cr

Symbol	Symbol Description
X_{Ni}	Composition proportion of Ni
X_{Cu}	Composition proportion of Cu
X_{Mo}	Composition proportion of Mo
X_{Al_t}	Composition proportion of Al_t
Y_{ts_1}	Tensile strength of product 1
Y_{ts_2}	Tensile strength of product 2
Y_{ys_1}	Yield strength of product 1
Y_{ys_2}	Yield strength of product 2
Y_{pef_1}	Percentage elongation after fracture of product 1
Y_{pef_2}	Percentage elongation after fracture of product 2

4. Model establishment

4.1 Discard extraordinary data

According to statistics, preliminary inferring that the chemical composition of steel and low alloy high strength steel properties are generally linear correlation. Divide data of attachment 1 into two charts according to the specification of product.

Under the theorem in Materials Mechanics, the value of yield strength is less than the value of tensile strength, which is determined by their definition. The difference between tensile strength and yield strength is used as a measure of whether the data is valid. Input the data to excel and draft the scattered plot.

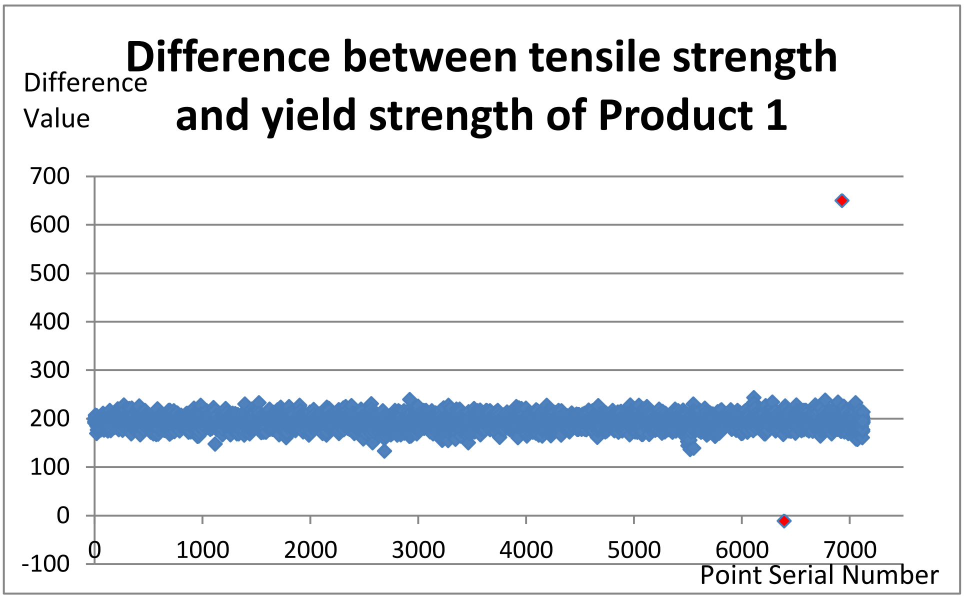

Figure 1. Difference between tensile strength and yield strength of Product 1

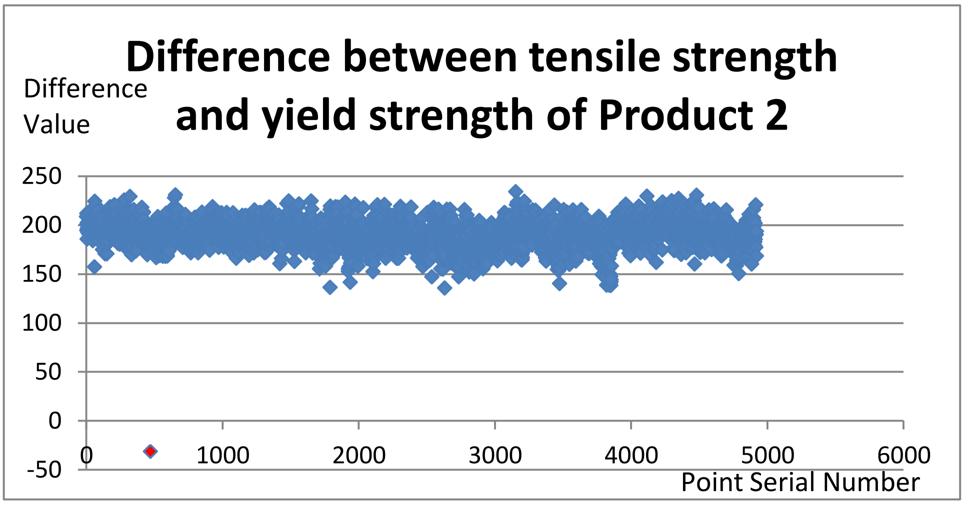

Figure 2. Difference between tensile strength and yield strength of Product 2

Because the red points in the figure deviate greatly from the mean difference, the data contained in them did not meet the calculation requirements of the topic, which will cause interference to the calculation. Discard these three red dots as shown in Figure 1 and Figure 2.

4.2 Multiple stepwise regression analysis

Multiple regression analysis is suitable for circumstances when there is a dependency relationship between several determining variables and one dependent variable and there are difficulties confirming the primary and secondary variables. In the study of this problem, the change of steel strength is affected by the content of several elements, and then multiple regression analysis is needed.

The relationship between dependent variable and determining variable fits the function below under this circumstance.

$$y = b_0 + b_1 x + b_2 x \ldots \ldots + b_n x + \varepsilon \quad (1)$$

*y refers to interpreted variable, x refers to explanatory variables, b_i refers to parameters to be estimated, and ε refers to random interference term.

The random error term ε has zero mean, covariance and sequence non-correlation.

In the next step, launch the multiple regression analysis process on the verified and classified charts and establish a regression equation with the assist of SPSS.

4.2.1 Group 1(Product 1)

Firstly, regard tensile strength as dependent variable, output the determining variables in order of SI, C, Cr,Al_t and consider them as principal factors .

The results are shown in Chart 1.

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	654.092	2.912		224.582	.000
	Si	64.748	5.451	.139	11.879	.000
2	(Constant)	627.977	4.806		130.665	.000
	Si	63.053	5.439	.136	11.592	.000
	C	125.828	18.454	.080	6.819	.000
3	(Constant)	636.809	5.003		127.273	.000
	Si	50.106	5.818	.108	8.612	.000
	C	136.632	18.489	.087	7.390	.000
	Cr	-193.075	31.345	-.077	-6.160	.000
4	(Constant)	635.899	5.004		127.085	.000
	Si	49.701	5.813	.107	8.550	.000
	C	139.580	18.486	.089	7.551	.000
	Cr	-190.839	31.318	-.076	-6.094	.000
	Alt	60.379	15.331	.046	3.938	.000
5	(Constant)	653.070	7.675		85.095	.000
	Si	58.807	6.579	.127	8.938	.000
	C	152.216	18.966	.097	8.026	.000
	Cr	-174.707	31.776	-.070	-5.498	.000
	Alt	60.422	15.323	.046	3.943	.000
	Mn	-17.571	5.957	-.040	-2.950	.003

a. Dependent Variable: tensile_strength

Chart 1 multiple regression analysis on relationship between tensile strength and elements

According to regulations, when the calculated values of significance test are lower than 0.05, we could refuse null hypothesis. All the calculated values of significance test in the chart are lower than 0.05.

A linear equation is obtained below.

$$\mathrm{Y}_{\mathrm{ts}_1} = 653.070 + 58.807\mathrm{X}_{\mathrm{Si}} + 152.216\mathrm{X}_{\mathrm{C}} - 174.707\mathrm{X}_{\mathrm{Cr}} + 60.422\mathrm{X}_{\mathrm{Al}_\mathrm{t}} - 17.571\mathrm{X}_{\mathrm{Mn}} \quad (2)$$

$*\ \mathrm{Y}_{ts_1}$ Refers to tensile strength of product 1

Due to the influence of random factors lying in the linear equation, it is important to perform residual analysis on the constant number ε .

The calculating formula is shown below.

$$e_i = y_i - \hat{y}_i (i = 1,2,3 \dots \dots \mathrm{n}) \quad (3)$$

$*\ e_i$ refers to residual; y_i refers to value of observation; $\hat{y}_i$ refers to value of prediction.

If the results of the residual analysis follow a normal distribution, then the linear equations generated by the regression analysis are in accordance with the requirements.

The result of residual analysis is shown in the figure below.

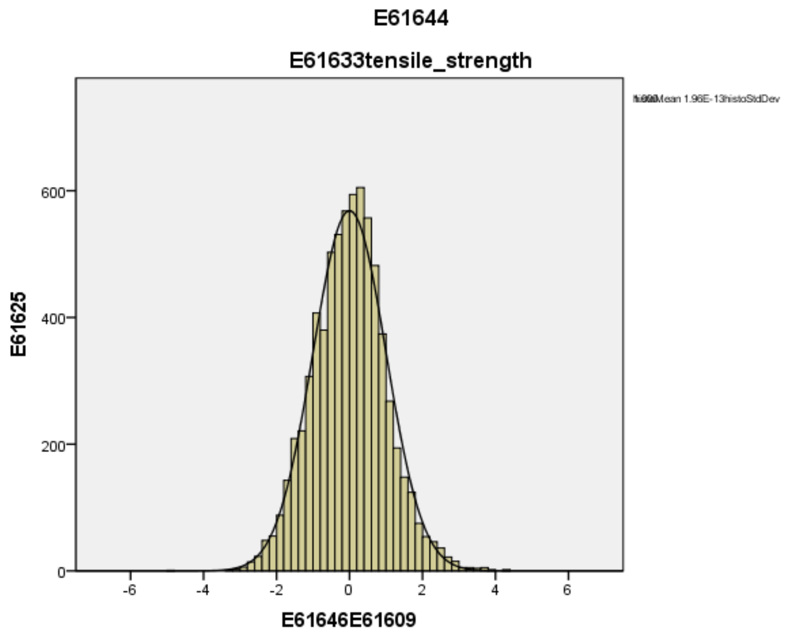

Figure 3 residual analysis on ε of tensile strength linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

Secondly, regard yield strength as dependent variable, output the determining variables in order of SI, Cr, C, Alt, Mn and V and consider them as principal factors. The results are displayed in Chart 2.

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	466.975	2.437		191.644	.000
	Si	53.235	4.560	.137	11.673	.000
2	(Constant)	474.527	2.860		165.934	.000
	Si	44.506	4.873	.115	9.133	.000
	Cr	-131.640	26.212	-.063	-5.022	.000
3	(Constant)	458.055	4.195		109.189	.000
	Si	42.502	4.878	.109	8.713	.000
	Cr	-144.996	26.280	-.069	-5.517	.000
	C	83.054	15.502	.063	5.358	.000
4	(Constant)	457.329	4.196		109.000	.000
	Si	42.179	4.874	.109	8.653	.000
	Cr	-143.213	26.260	-.069	-5.454	.000
	C	85.405	15.500	.065	5.510	.000
	Alt	48.169	12.855	.044	3.747	.000
5	(Constant)	472.655	6.435		73.456	.000
	Si	50.307	5.516	.129	9.120	.000
	Cr	-128.814	26.641	-.062	-4.835	.000
	C	96.683	15.902	.073	6.080	.000
	Alt	48.206	12.847	.044	3.752	.000
	Mn	-15.684	4.995	-.043	-3.140	.002
6	(Constant)	469.349	6.573		71.404	.000
	Si	49.921	5.517	.128	9.049	.000
	Cr	-126.332	26.651	-.060	-4.740	.000
	C	92.886	15.972	.070	5.816	.000
	Alt	47.856	12.844	.044	3.726	.000
	Mn	-17.854	5.071	-.049	-3.521	.000
	V	247.428	101.285	.030	2.443	.015
7	(Constant)	472.569	6.722		70.299	.000
	Si	46.612	5.704	.120	8.172	.000
	Cr	-103.156	28.530	-.049	-3.616	.000
	C	95.527	16.009	.072	5.967	.000
	Alt	49.040	12.850	.045	3.816	.000
	Mn	-17.918	5.070	-.049	-3.534	.000
	V	240.466	101.302	.029	2.374	.018
	Cu	-155.079	68.259	-.031	-2.272	.023

a. Dependent Variable: yield_strength

Chart 2 multiple regression analysis on relationship between yield strength and elements

A linear equation is obtained from Chart 2：

$$
\begin{aligned}
Y_{ys_1} = 472.569 + 46.612X_{Si} - 103.156X_C + 95.527X_{Cr} + 49.040X_{Al_t} \\
- 17.571X_{Mn} + 240.466X_V - 155.079X_{Cu} \qquad (4)
\end{aligned}
$$

$*\ Y_{ys_1}$ Refers to yield strength of product 1

The result of residual analysis is shown in the figure below.

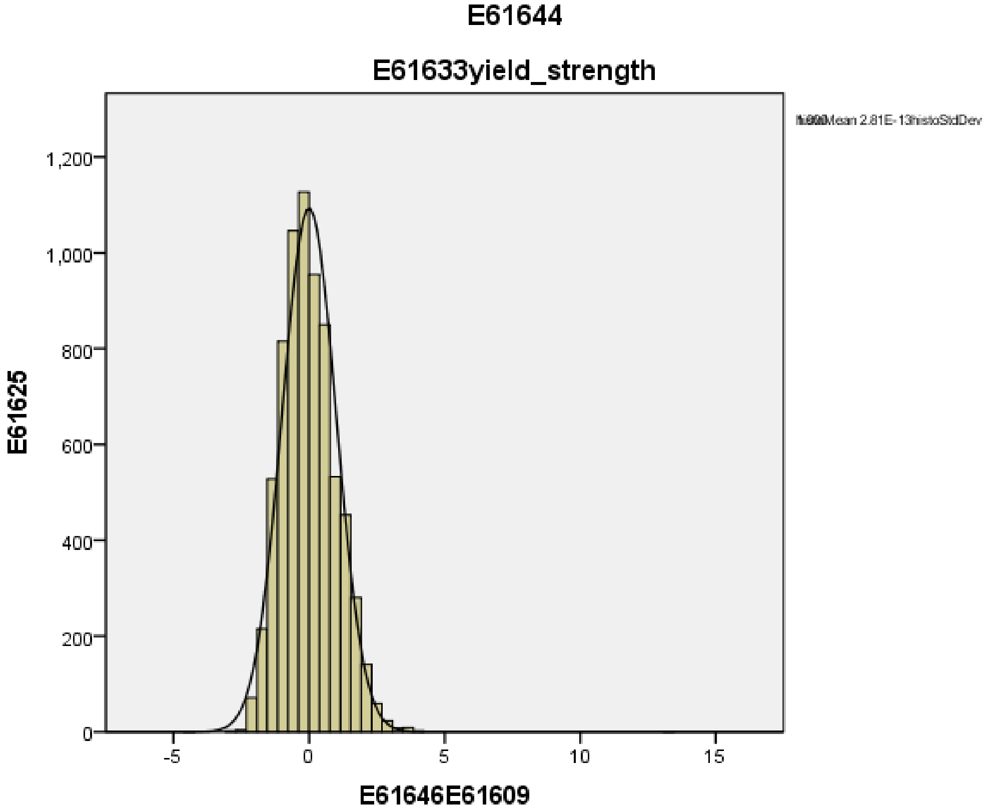

Figure 4 residual analysis on ε of yield strength linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

Thirdly, regard percentage elongation after fracture as dependent variable, output the determining variables in order of V, Alt, Ni, S, Mo, P and Cr. and consider them as principal factors.

The results are shown in Chart 3.

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	27.040	.297		91.091	.000
	V	-65.690	9.940	-.078	-6.609	.000
2	(Constant)	27.005	.296		91.108	.000
	V	-66.136	9.923	-.079	-6.665	.000
	Alt	6.707	1.302	.061	5.153	.000
3	(Constant)	26.754	.300		89.144	.000
	V	-65.899	9.906	-.078	-6.652	.000
	Alt	6.800	1.300	.062	5.232	.000
	Ni	21.013	4.199	.059	5.004	.000
4	(Constant)	27.190	.313		86.992	.000
	V	-63.744	9.900	-.076	-6.439	.000
	Alt	6.756	1.298	.061	5.207	.000
	Ni	20.662	4.193	.058	4.928	.000
	S	-19.852	4.049	-.058	-4.903	.000
5	(Constant)	27.208	.312		87.176	.000
	V	-64.766	9.887	-.077	-6.550	.000
	Alt	6.587	1.296	.060	5.083	.000
	Ni	20.595	4.186	.058	4.919	.000
	S	-20.218	4.043	-.059	-5.000	.000
	Mo	35.516	7.471	.056	4.754	.000
6	(Constant)	26.982	.321		84.162	.000
	V	-65.792	9.887	-.078	-6.654	.000
	Alt	6.504	1.296	.059	5.020	.000
	Ni	20.114	4.187	.056	4.804	.000
	S	-19.993	4.042	-.058	-4.947	.000
	Mo	35.267	7.467	.055	4.723	.000
	P	9.617	3.148	.036	3.056	.002
7	(Constant)	27.071	.322		83.955	.000
	V	-67.164	9.899	-.080	-6.785	.000
	Alt	6.422	1.296	.058	4.957	.000
	Ni	27.787	5.190	.078	5.354	.000
	S	-20.103	4.040	-.058	-4.975	.000
	Mo	31.477	7.617	.049	4.133	.000
	P	11.200	3.209	.042	3.490	.000
	Cr	-7.870	3.148	-.037	-2.500	.012

a. Dependent Variable: percentage_elongation_after_fracture

Chart 3 multiple regression analysis on relationship between percentage elongation after fracture and elements

A linear equation is obtained from Chart 3：

$$Y_{pef_1} = 27.071 - 67.164X_V + 6.422X_{Al_t} + 27.787X_{Ni} - 20.103X_S + 31.477X_{Mo} + 11.200X_P - 7.870X_{Cr} \quad (5)$$

$*\ Y_{pef_1}$ Refers to percentage elongation after fracture of product 1

The result of residual analysis is shown in the figure below.

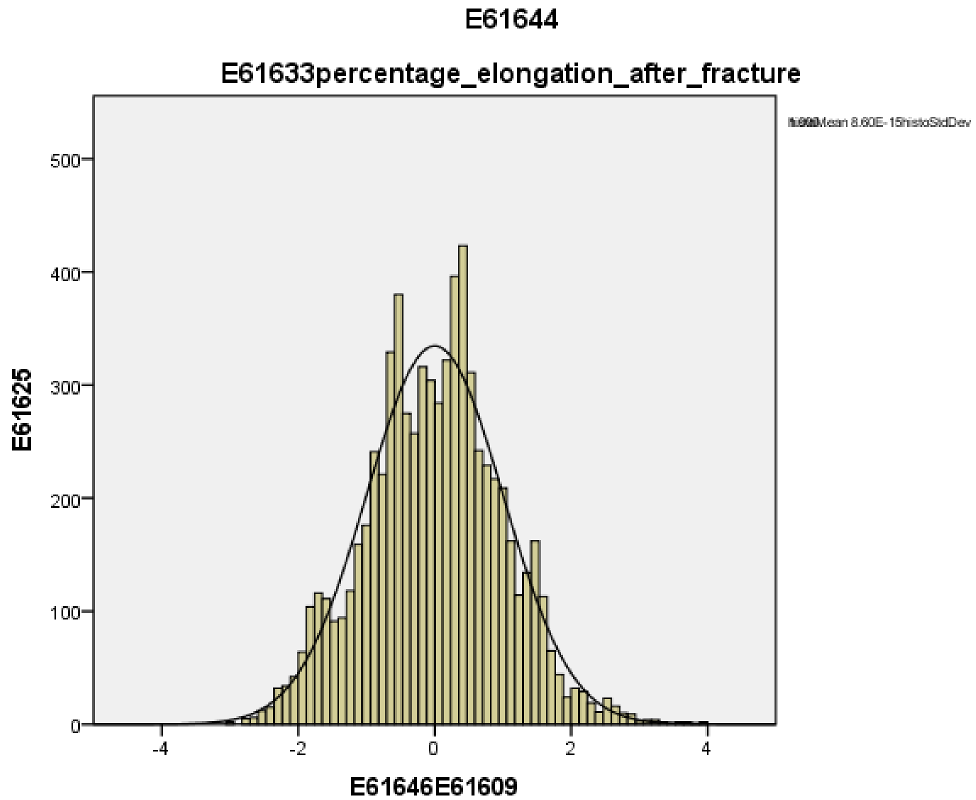

Figure 5 residual analysis on ε of percentage elongation after fracture linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

4.2.2 Group 2(Product 2)

As for group two, the analysis method is exactly the same, so there is no need to repeat again.

Firstly, regard tensile strength as dependent variable, output the determining variables in order of Si, C, S, Cu, Mo, and Mn and consider them as principal factors.

The results are shown in Chart4.

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	655.861	3.689		177.767	.000
	Si	52.899	6.860	.109	7.712	.000
2	(Constant)	628.327	5.906		106.391	.000
	Si	51.502	6.840	.106	7.530	.000
	C	132.122	22.178	.084	5.957	.000
3	(Constant)	633.398	6.082		104.148	.000
	Si	50.372	6.840	.104	7.364	.000
	C	132.575	22.155	.084	5.984	.000
	S	-179.700	52.382	-.048	-3.431	.001
4	(Constant)	638.503	6.357		100.442	.000
	Si	44.906	7.121	.093	6.306	.000
	C	137.136	22.202	.087	6.177	.000
	S	-175.943	52.365	-.047	-3.360	.001
	CU	-227.336	82.980	-.040	-2.740	.006
5	(Constant)	638.430	6.354		100.480	.000
	Si	45.245	7.119	.093	6.356	.000
	C	134.784	22.212	.086	6.068	.000
	S	-174.634	52.342	-.047	-3.336	.001
	CU	-225.616	82.942	-.040	-2.720	.007
	MO	342.406	140.950	.034	2.429	.015
6	(Constant)	652.977	9.599		68.027	.000
	Si	52.054	7.873	.108	6.611	.000
	C	143.511	22.621	.091	6.344	.000
	S	-184.314	52.544	-.050	-3.508	.000
	CU	-207.398	83.404	-.037	-2.487	.013
	MO	352.412	140.992	.035	2.500	.012
	MN	-14.084	6.967	-.032	-2.021	.043

a. Dependent Variable: tensile strength

Chart 4 multiple regression analysis on relationship between tensile strength and elements

Linear equation obtained from Chart 4:

$$\mathrm{Y}_{ts_2} = 652.977 + 52.054\mathrm{X}_{\mathrm{Si}} + 143.511\mathrm{X}_{\mathrm{C}} - 184.314\mathrm{X}_{\mathrm{S}} - 207.398\mathrm{X}_{Cu} + 352.412\mathrm{X}_{Mo} - 14.084\mathrm{X}_{Mn} \tag{6}$$

$*\ \mathrm{Y}_{ts_2}$ Refers to tensile strength of product 2

The result of residual analysis is shown in the figure below.

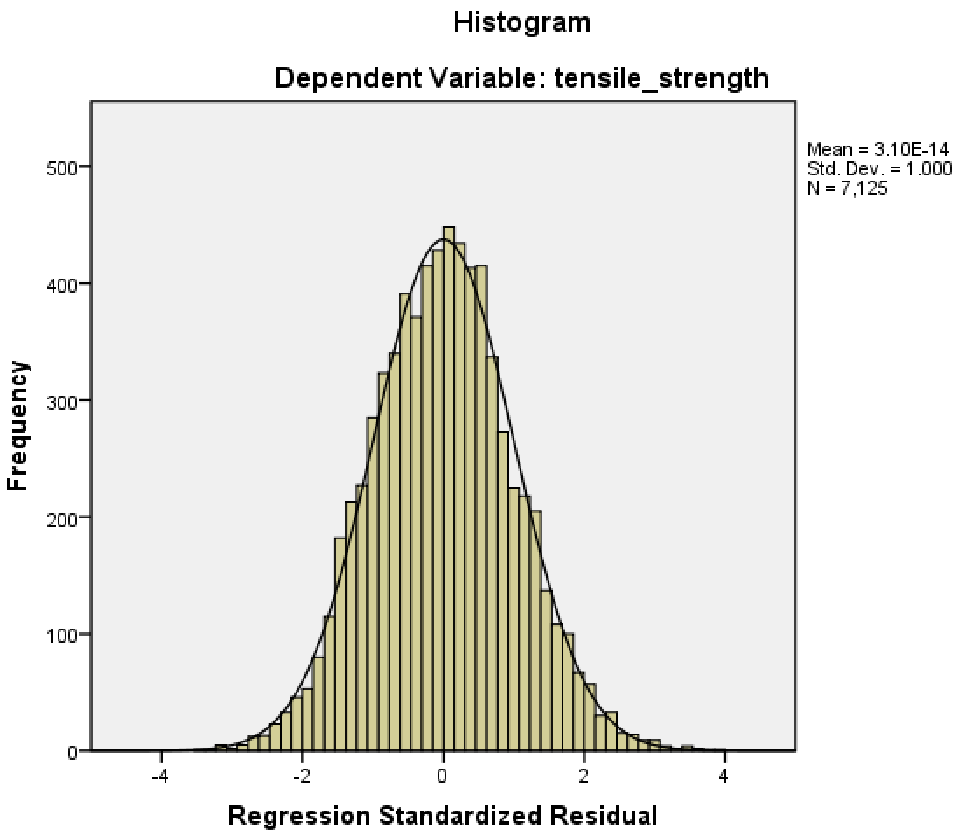

Figure 6 residual analysis on ε of tensile strength linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

Secondly, regard yield strength as dependent variable, output the determining variables in order of Si, Cr, C, S, Cu, C and Mn and consider them as principal factors.

The results are shown in Chart 5.

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	461.900	3.213		143.775	.000
	Si	58.826	5.973	.139	9.849	.000
2	(Constant)	474.655	3.696		128.439	.000
	Si	44.242	6.311	.105	7.010	.000
	Cr	-231.471	33.623	-.103	-6.884	.000
3	(Constant)	459.144	4.866		94.361	.000
	Si	38.999	6.387	.092	6.106	.000
	Cr	-223.732	33.583	-.099	-6.662	.000
	V	607.445	124.349	.070	4.885	.000
4	(Constant)	454.209	5.078		89.443	.000
	Si	40.876	6.405	.097	6.382	.000
	Cr	-210.500	33.778	-.093	-6.232	.000
	V	598.921	124.245	.069	4.820	.000
	S	153.686	45.782	.047	3.357	.001
5	(Constant)	457.952	5.293		86.522	.000
	Si	38.011	6.504	.090	5.844	.000
	Cr	-187.164	35.034	-.083	-5.342	.000
	V	591.353	124.216	.068	4.761	.000
	S	160.609	45.842	.050	3.504	.000
	CU	-185.913	74.569	-.038	-2.493	.013
6	(Constant)	450.042	6.276		71.704	.000
	Si	37.329	6.508	.088	5.736	.000
	Cr	-192.221	35.084	-.085	-5.479	.000
	V	551.026	125.348	.063	4.396	.000
	S	159.722	45.822	.049	3.486	.000
	CU	-196.635	74.675	-.040	-2.633	.008
	C	45.616	19.475	.033	2.342	.019
7	(Constant)	461.967	8.502		54.338	.000
	Si	43.599	7.171	.103	6.080	.000
	Cr	-182.857	35.361	-.081	-5.171	.000
	V	599.034	127.416	.069	4.701	.000
	S	151.973	45.958	.047	3.307	.001
	CU	-184.044	74.896	-.037	-2.457	.014
	C	52.354	19.736	.038	2.653	.008
	MN	-12.862	6.188	-.034	-2.079	.038

a. Dependent Variable: yield strength

Chart 5 multiple regression analysis on relationship between yield strength and elements

Linear equation obtained from Chart 5:

$$\mathrm{Y}_{ys_2} = 461.997 + 43.599\mathrm{X}_{\mathrm{Si}} - 182.857\mathrm{X}_{\mathrm{Cr}} + 599.034\mathrm{X}_{\mathrm{V}} + 151.973\mathrm{X}_{S} - 184.044\mathrm{X}_{Cu} + 52.354\mathrm{X}_{C} - 12.862\mathrm{X}_{\mathrm{Mn}} \quad (7)$$

$*\ \mathrm{Y}_{ys_2}$ refers to yield strength of product 2.

The result of residual analysis is shown in the figure below.

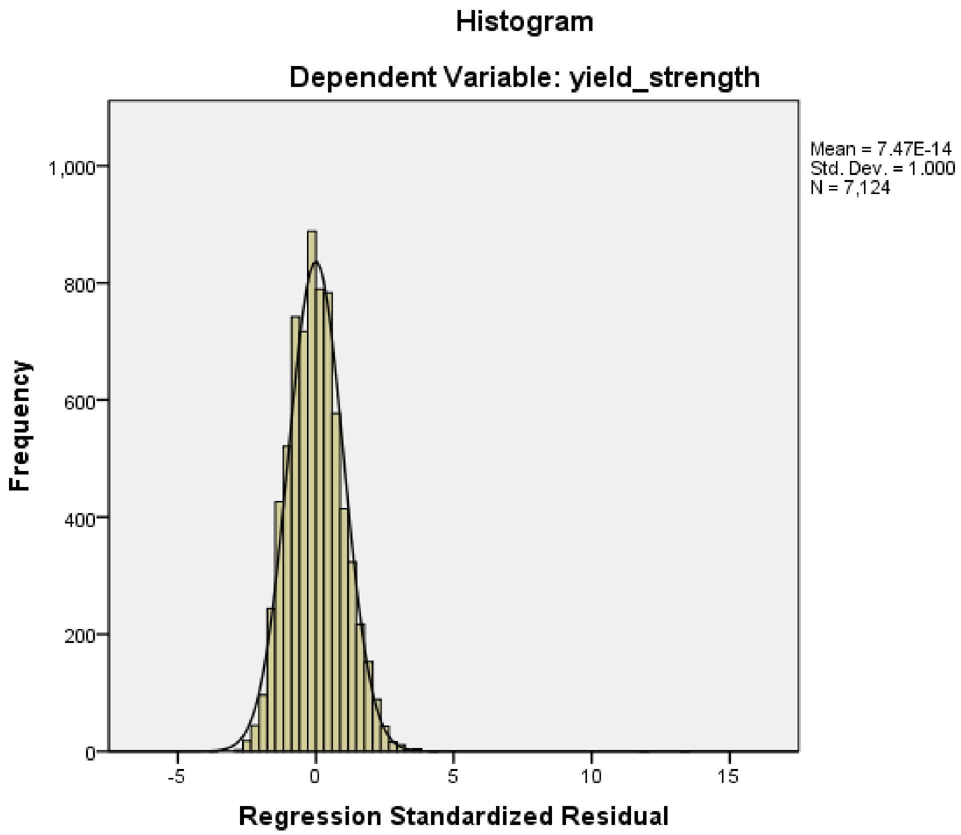

Figure 7 residual analysis on ε of yield strength linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

Thirdly, regard percentage elongation after fracture as dependent variable, output the determining variables in order of V, Al_t, P, Mo, Mn, Si, Cr, Ni and S and consider them as principal factors.

The results are shown in Chart 6.

Coefficients[a]

Model		Unstandardized Coefficients B	Unstandardized Coefficients Std. Error	Standardized Coefficients Beta	t	Sig.
1	(Constant)	24.448	.023		1083.435	.000
	ALT	7.249	1.385	.074	5.233	.000
2	(Constant)	23.920	.106		225.567	.000
	ALT	7.098	1.382	.073	5.136	.000
	P	19.876	3.902	.072	5.093	.000
3	(Constant)	23.877	.106		224.682	.000
	ALT	6.848	1.380	.070	4.961	.000
	P	19.774	3.895	.072	5.077	.000
	MO	49.146	10.809	.064	4.547	.000
4	(Constant)	26.133	.672		38.873	.000
	ALT	6.890	1.379	.071	4.997	.000
	P	21.990	3.945	.080	5.574	.000
	MO	50.283	10.803	.066	4.655	.000
	MN	-1.624	.478	-.049	-3.398	.001
5	(Constant)	26.139	.671		38.927	.000
	ALT	6.793	1.378	.070	4.931	.000
	P	25.053	4.036	.091	6.207	.000
	MO	51.554	10.797	.068	4.775	.000
	MN	-2.462	.534	-.074	-4.613	.000
	Si	2.064	.589	.056	3.507	.000
6	(Constant)	25.866	.674		38.398	.000
	ALT	6.809	1.375	.070	4.951	.000
	P	23.026	4.059	.084	5.673	.000
	MO	55.377	10.818	.073	5.119	.000
	MN	-2.759	.538	-.083	-5.131	.000
	Si	2.959	.626	.080	4.726	.000
	Cr	12.516	3.020	.064	4.145	.000
7	(Constant)	25.780	.673		38.300	.000
	ALT	6.583	1.375	.068	4.788	.000
	P	23.070	4.053	.084	5.692	.000
	MO	59.711	10.865	.078	5.496	.000
	MN	-2.912	.538	-.087	-5.407	.000
	Si	3.630	.650	.098	5.583	.000
	Cr	20.881	3.745	.106	5.576	.000
	Ni	-21.090	5.597	-.066	-3.768	.000
8	(Constant)	26.288	.695		37.818	.000
	ALT	6.632	1.374	.068	4.827	.000
	P	23.760	4.057	.086	5.856	.000
	MO	59.292	10.858	.078	5.461	.000
	MN	-3.037	.540	-.091	-5.626	.000
	Si	3.577	.650	.097	5.504	.000
	Cr	20.086	3.752	.102	5.353	.000
	Ni	-21.588	5.596	-.068	-3.858	.000
	S	-11.680	4.037	-.041	-2.893	.004

a. Dependent Variable: percentage elongation after fracture

Chart 6 multiple regression analysis on relationship between percentage elongation after fracture and elements

Linear equation obtained from Chart 6:

$$Y_{pef_2} = 26.288 - 6.632X_{Al_t} + 23.760X_P + 59.292X_{MO} - 3.037X_{Mn} + 3.577X_{Si} + 20.086X_{Cr} - 21.588X_{Ni} - 11.680X_S \quad (8)$$

$*\ Y_{pef_2}$ refers to percentage elongation after fracture of product 2.

The result of residual analysis is shown in the figure below.

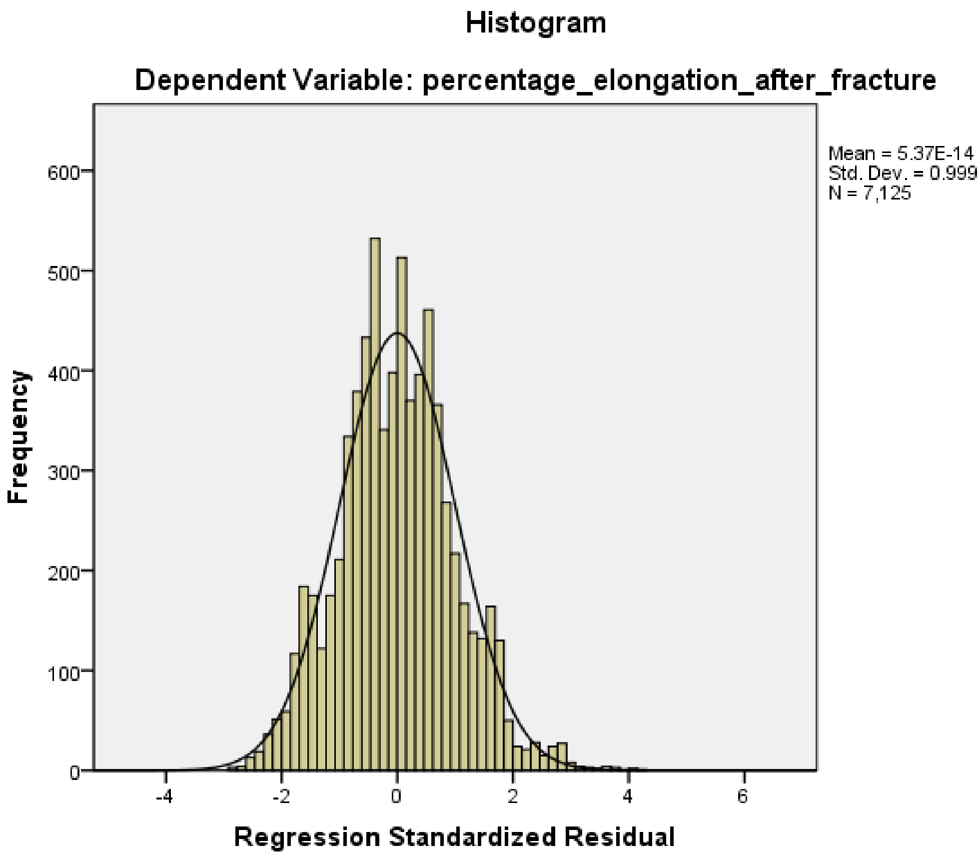

Figure 8 residual analysis on ε of percentage elongation after fracture linear equation

As can be seen from the figure, the residual analysis of ε follows a normal distribution. So the linear equation is correct.

The stepwise regression analysis of relationship between each component in the data table and tensile strength, yield strength and percentage elongation after fracture is carried out by using stepwise regression and residual analysis methods.

According to the frequency of the various elements in No. 1 and No. 2 steel and the value of the parameters estimated, the paper concludes that elements C, Mn, Cr, V and S have significant impact on the material properties.

The table is displayed below.

	C	Mn	Cr	V	Ni	S	P
ts1	152.216	-17.571	-174.707				
ys1	95.527	-17.918	-103.156	240.466			
pef1			-7.870	-67.164	27.787	-20.103	11.200
ts2	143.511	-14.084				-184.314	
ys2	52.354	-12.862	-182.857	599.034		151.973	
pef2		-3.037	20.086		-21.588	-11.680	23.760

Chart 8 Estimating parameter of element

Through the study of the steel treatment technology, in the heat treatment process of steel, the metal Ni can improve the tensile strength and yield strength of the steel; the metal P can improve the atmospheric corrosion resistance of the steel, and improve the yield strength of the steel; Ceq, the carbon equivalent, determines the material strength and weldability.

The calculation formula of Ceq is shown below.

$$\mathrm{Ceq} = \mathrm{C} + \frac{1}{6}\mathrm{Mn} + \frac{1}{5}(\mathrm{Cr} + \mathrm{V} + \mathrm{Mo}) + \frac{1}{15}(\mathrm{Cu} + \mathrm{Ni}) \tag{9}$$

It is concluded that C, Mn, Cr, V, Ni, S, P, Ceq are the main elements affecting the properties of steel, while other elements play a minor role in changing the mechanical properties of steel or not directly related to the mechanical properties of steel.

4.3 Mathematical Model of Relationship between Properties of Steel and Components of Main Elements

According to the above analysis process, several key elements that affect the mechanical strength index of steel have been selected. Then, using these elements as independent variables, multiple linear regression analysis process is started with tensile strength, yield strength, and percentage elongation after fracture as dependent variables.

The calculating formula is shown below.

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST} = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{10}$$

*SST refers to total sum of squares; SSR refers to regression sum of squares, SSE refers to error sum of squares; R^2 refers to variance, $\bar{y}$ refers to average value.

Use the previously imported data to continue the test in SPSS, draft the scatter plot of the element and the performance index, and plotting the regression plots that are likely to be consistent.

The figures are shown below.

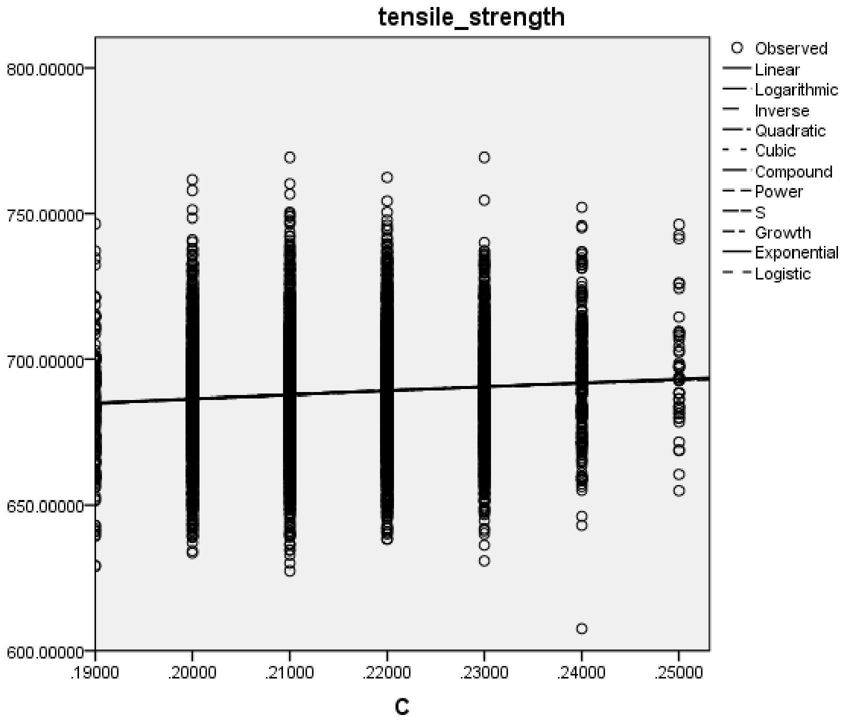

Figure 9 The scattered plot and fitted curve between element C and tensile strength

According to the scattered plot and fitted curve between element C and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

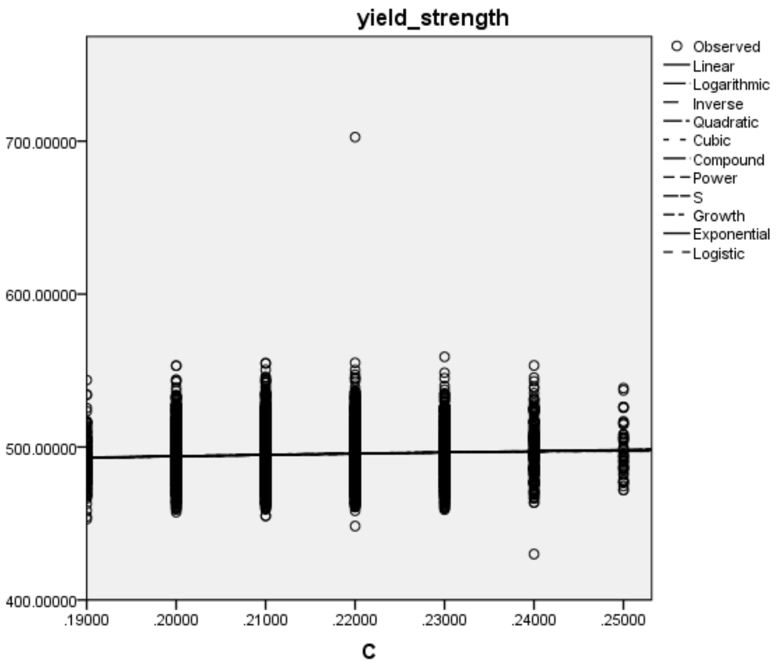

Figure 10 The scattered plot and fitted curve between element C and yield strength

According to the scattered plot and fitted curve between element C and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

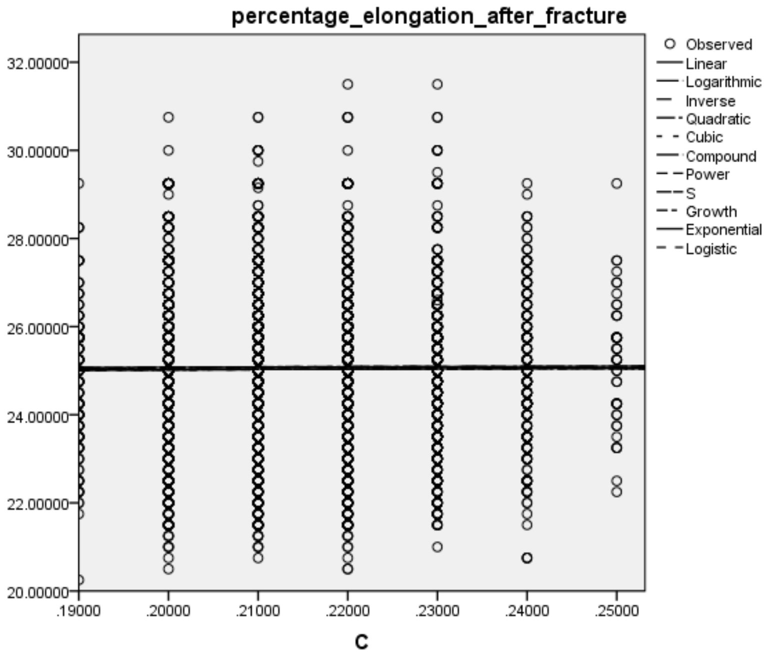

Figure 10.1.The scattered plot and fitted curve between element C and percentage elongation after fracture

According to the scattered plot and fitted curve between element C and percentage elongation after fracture, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

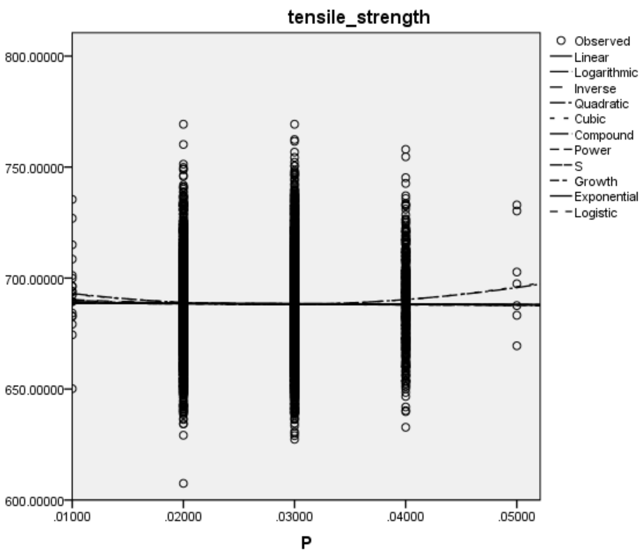

Figure 11.The scattered plot and fitted curve between element P and tensile strength

According to the scattered plot and fitted curve between element P and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

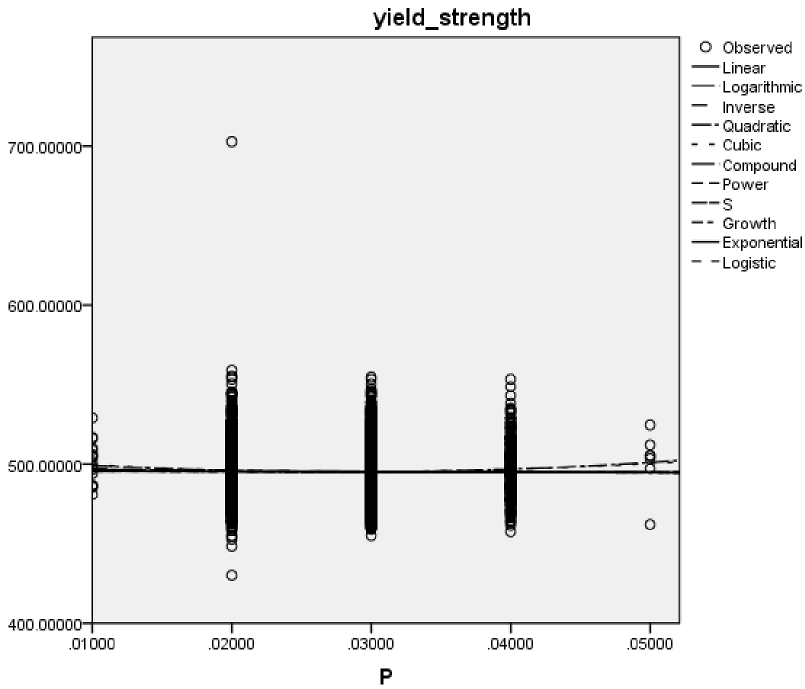

Figure 12.The scattered plot and fitted curve between element P and yield strength

According to the scattered plot and fitted curve between element P and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

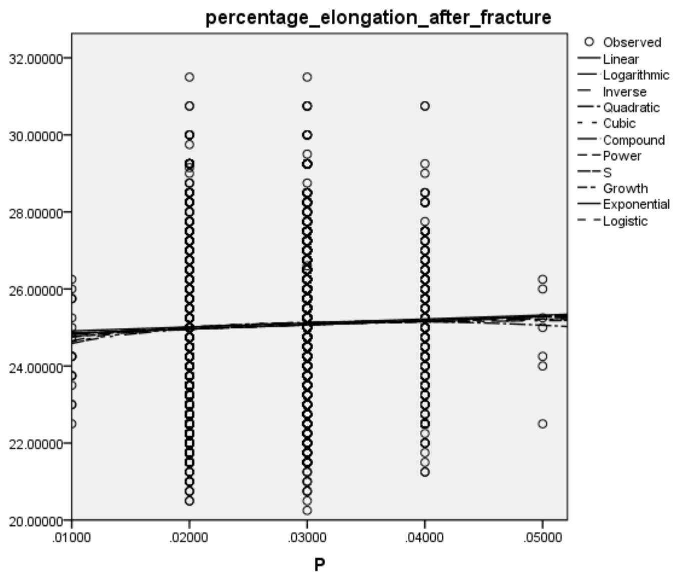

Figure 13.The scattered plot and fitted curve between element P and percentage elongation after fracture

According to the scattered plot and fitted curve between element P and percentage elongation after fracture, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

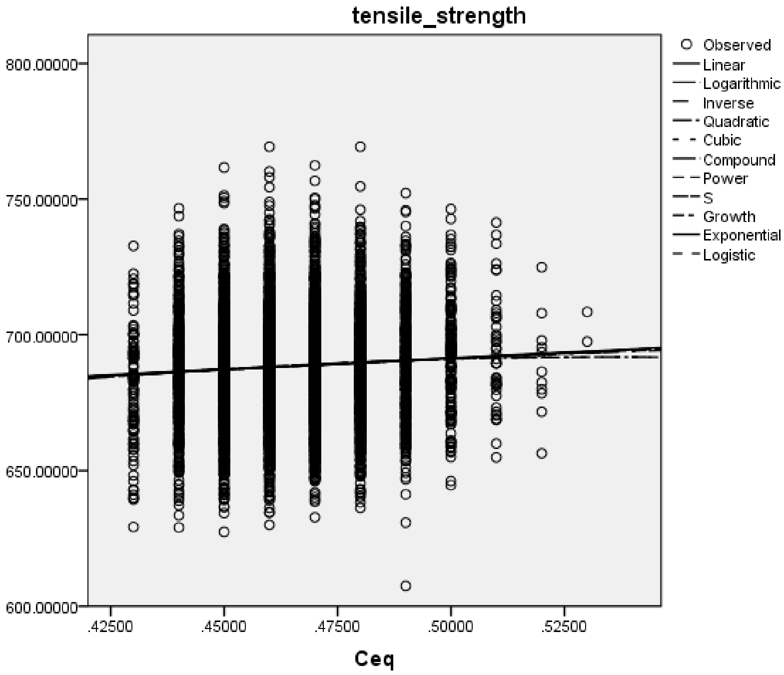

Figure 14.The scattered plot and fitted curve between element Ce_q and tensile strength

According to the scattered plot and fitted curve between element Ce_q and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

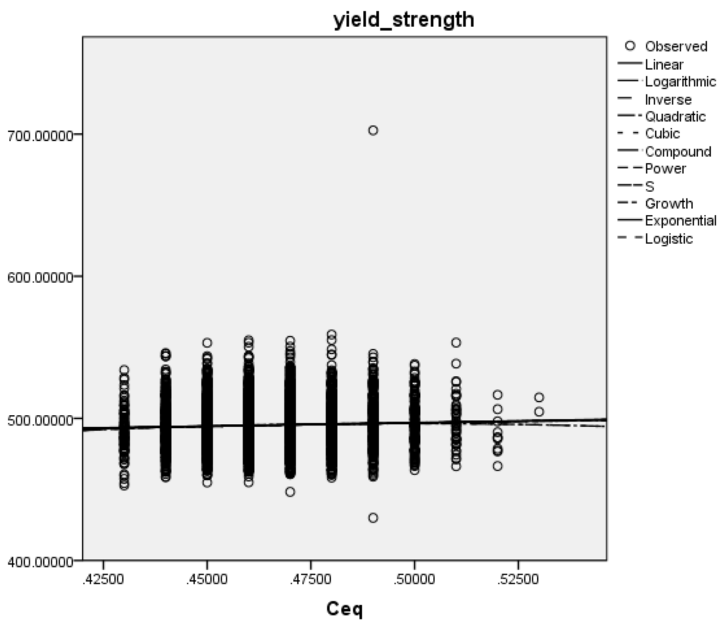

Figure 15.The scattered plot and fitted curve between element Ce_q and yield strength

According to the scattered plot and fitted curve between element Ce_q and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

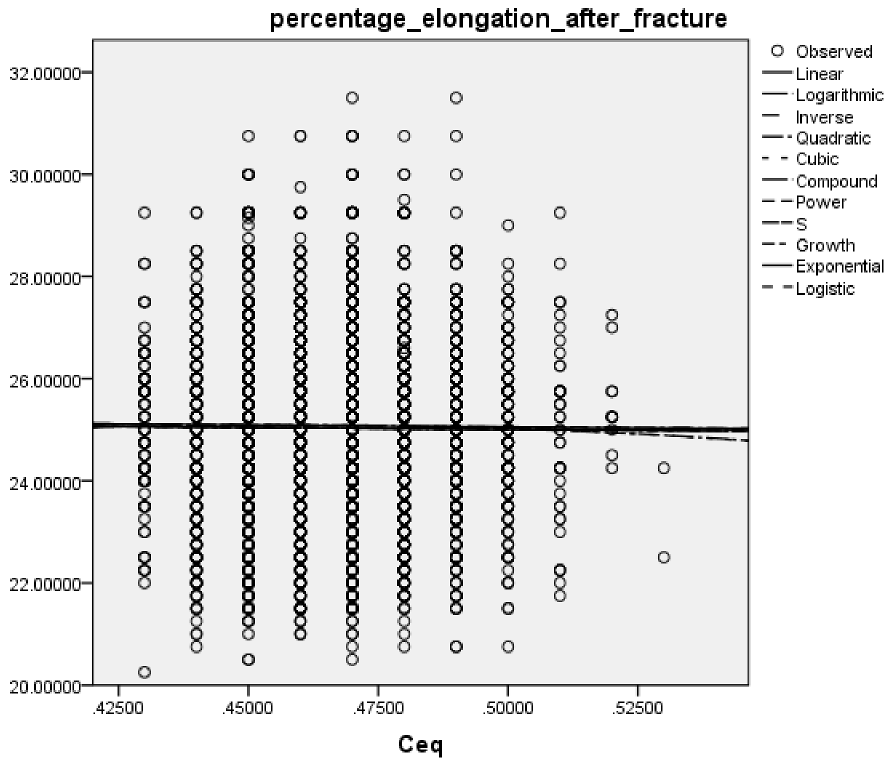

Figure 16.The scattered plot and fitted curve between element Ce_q and percentage elongation after fracture

According to the scattered plot and likely fitted curve between element $Ce_q$and percentage elongation after fracture, it is shown that the relationship is fitted by linear curve, logistic curve, compound curve and growth curve.

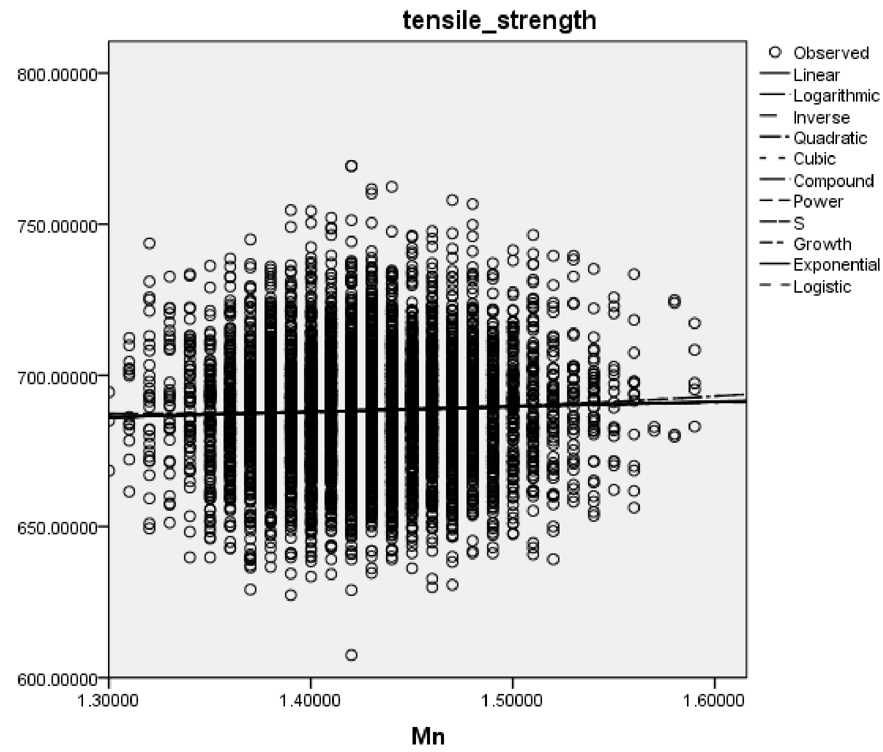

Figure 17.The scattered plot and fitted curve between element Mn and tensile strength

According to the scattered plot and fitted curve between element Mn and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

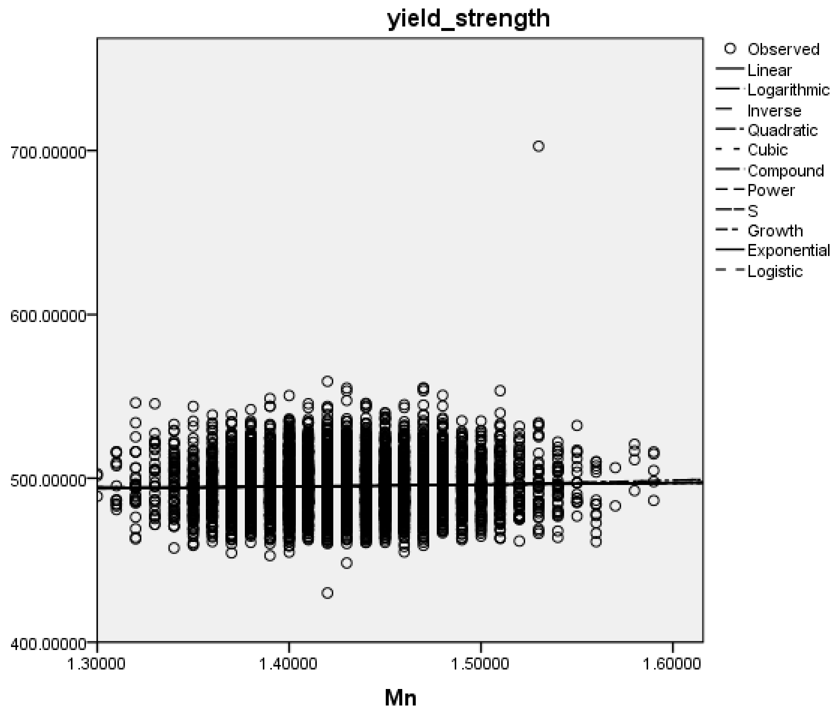

Figure 18.The scattered plot and fitted curve between element Mn and yield strength

According to the scattered plot and fitted curve between element Mn and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, compound curve and growth curve.

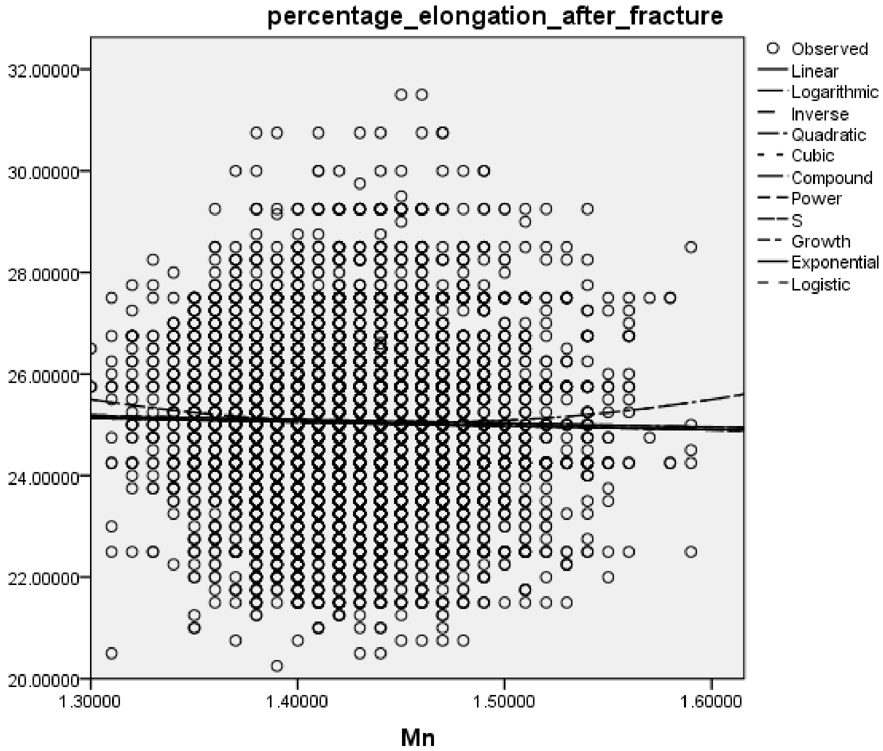

Figure 19.The scattered plot and fitted curve between element Mn and percentage elongation after fracture

According to the scattered plot and fitted curve between element Mn and percentage elongation after fracture, it is shown that the relationship is likely fitted by linear curve, logistic curve, quadratic curve and growth curve.

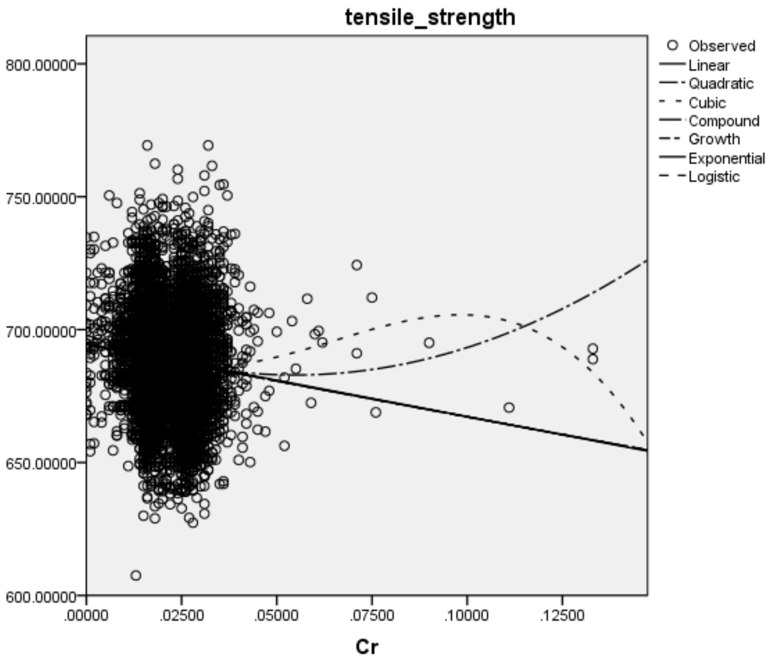

Figure 20.The scattered plot and fitted curve between element Cr and tensile strength

According to the scattered plot and fitted curve between element Cr and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve, quadratic curve and growth curve.

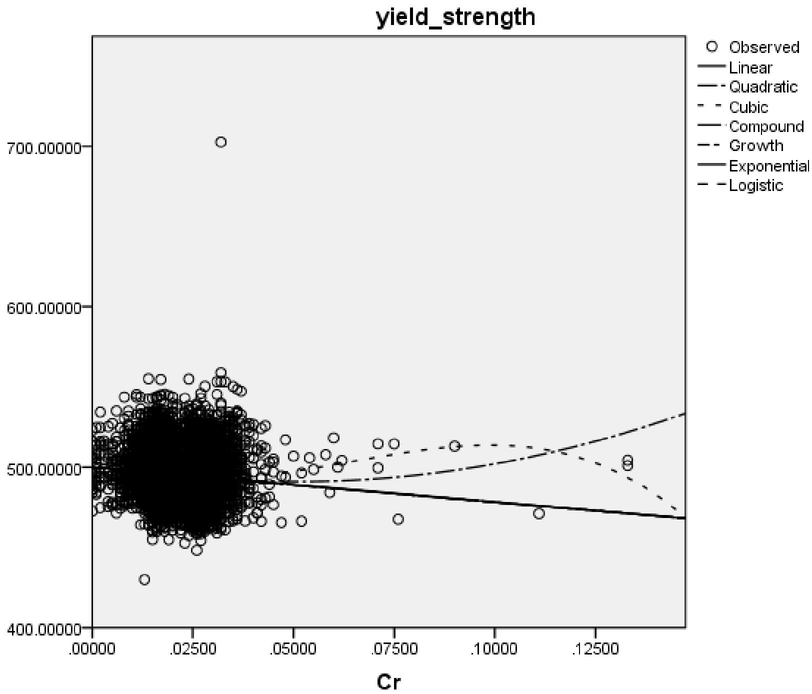

Figure 21.The scattered plot and fitted curve between element Cr and yield strength

According to the scattered plot and fitted curve between element Cr and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

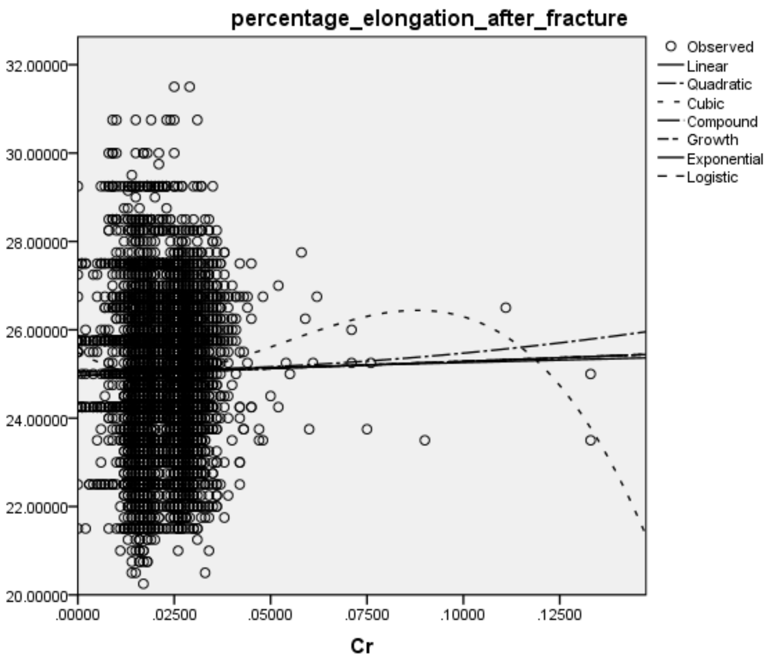

Figure 22.The scattered plot and fitted curve between element Cr and percentage elongation after fracture

According to the scattered plot and fitted curve between element Cr and percentage elongation after fracture, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

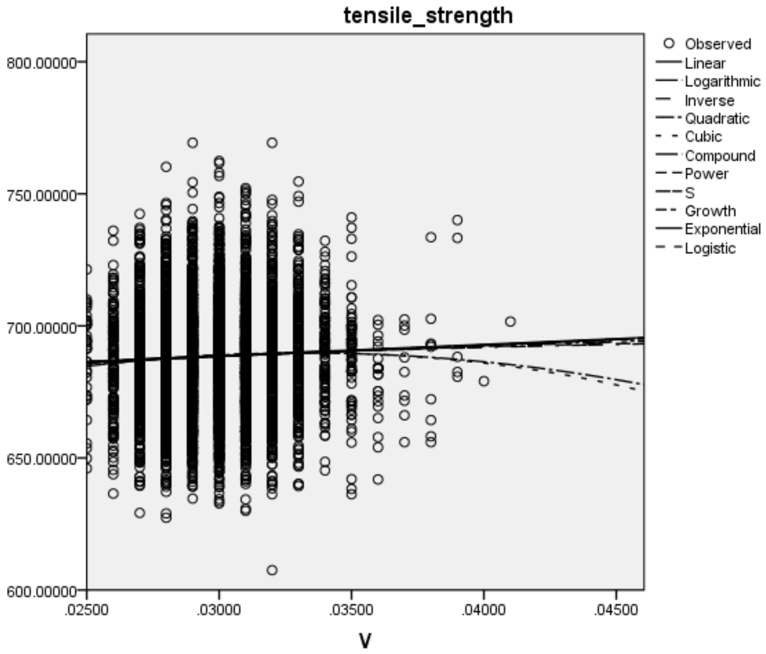

Figure 23.The scattered plot and fitted curve between element V and tensile strength

According to the scattered plot and fitted curve between element V and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

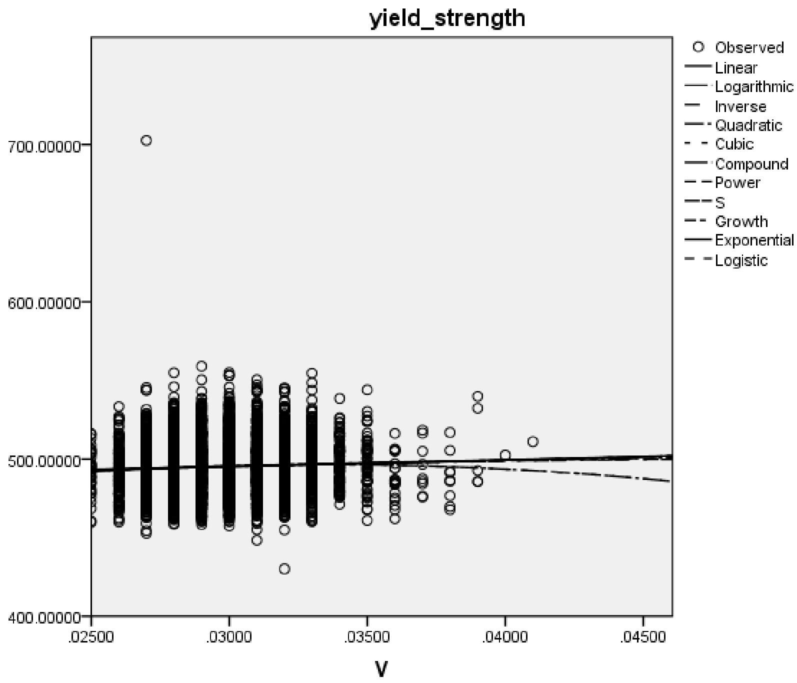

Figure 24.The scattered plot and fitted curve between element V and yield strength

According to the scattered plot and fitted curve between element V and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

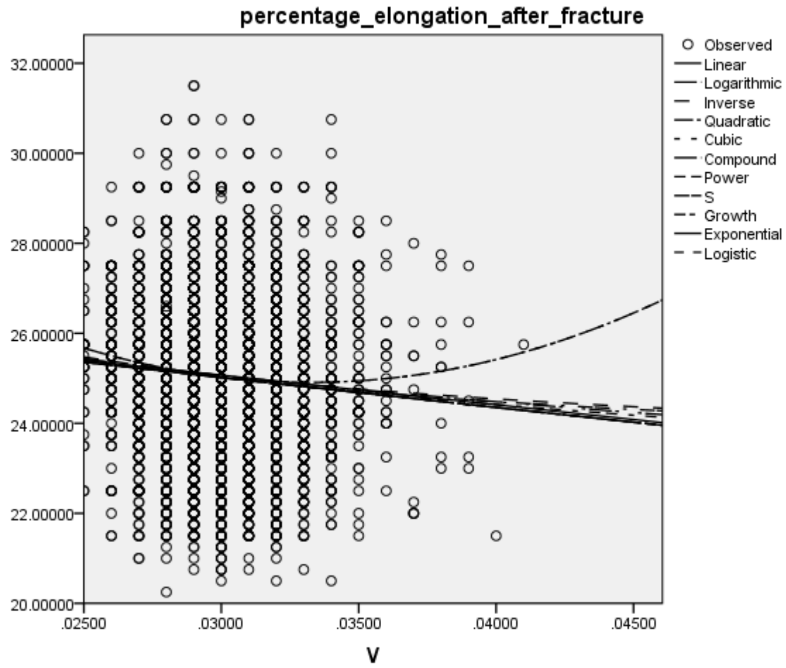

Figure 25.The scattered plot and fitted curve between element V and percentage elongation after fracture strength

According to the scattered plot and fitted curve between element V and percentage elongation after fracture strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

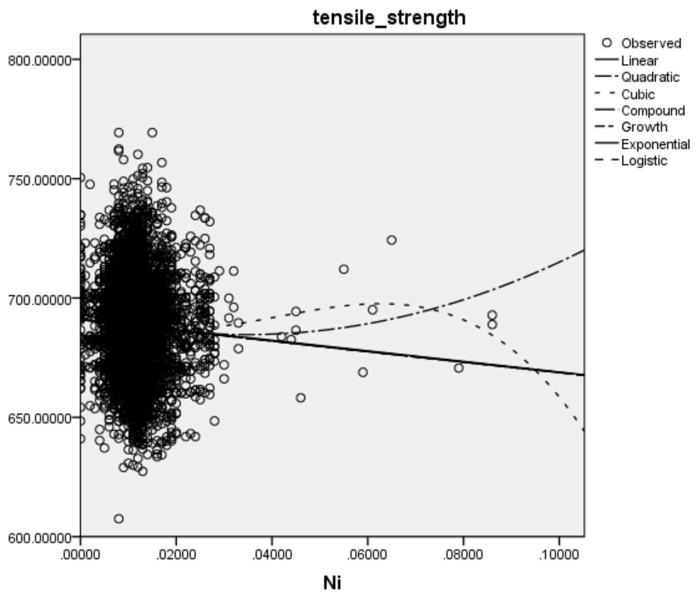

Figure 26.The scattered plot and fitted curve between element Ni and tensile strength

According to the scattered plot and fitted curve between element Ni and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

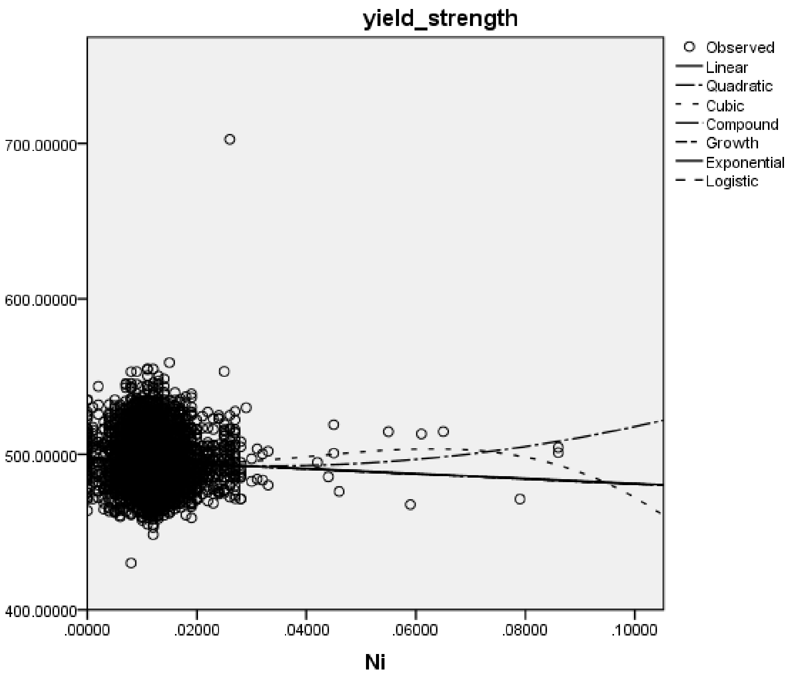

Figure 27.The scattered plot and fitted curve between element N and yield strength

According to the scattered plot and fitted curve between element Ni and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

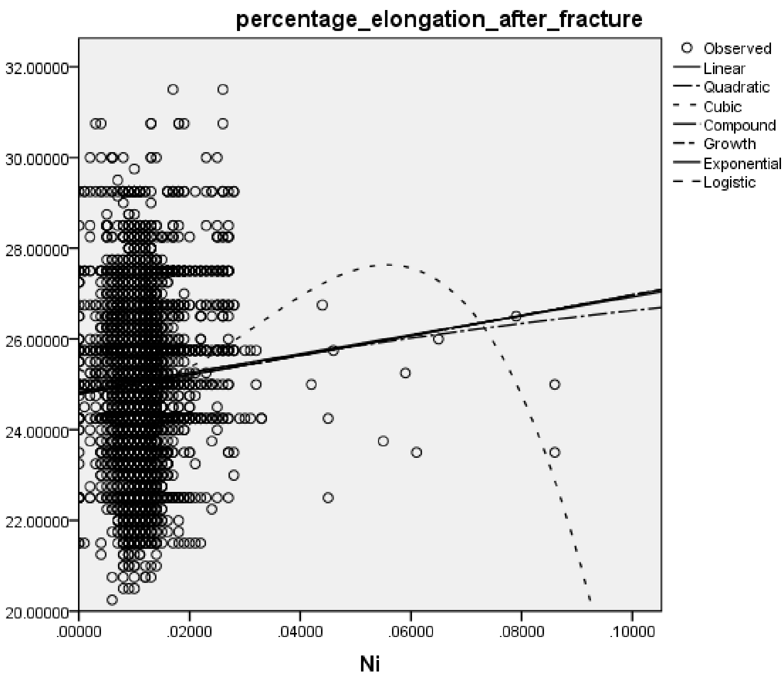

Figure 28.The scattered plot and fitted curve between element Ni and percentage elongation after fracture strength

According to the scattered plot and fitted curve between element Ni and percentage elongation after fracture strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

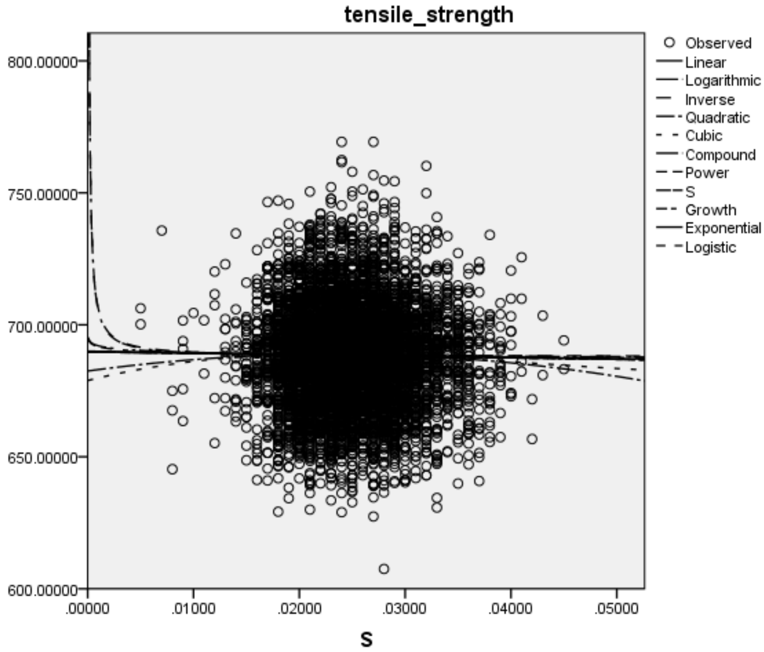

Figure 29.The scattered plot and fitted curve between element S and tensile strength

According to the scattered plot and fitted curve between element S and tensile strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

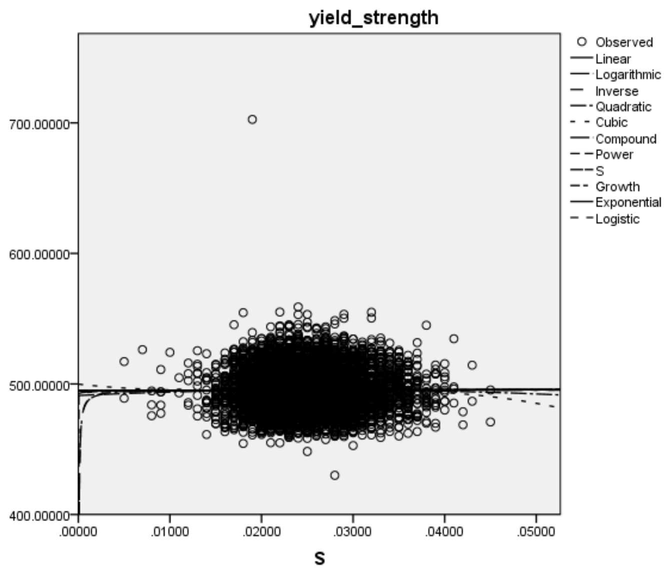

Figure 30.The scattered plot and fitted curve between element S and yield strength

According to the scattered plot and fitted curve between element S and yield strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

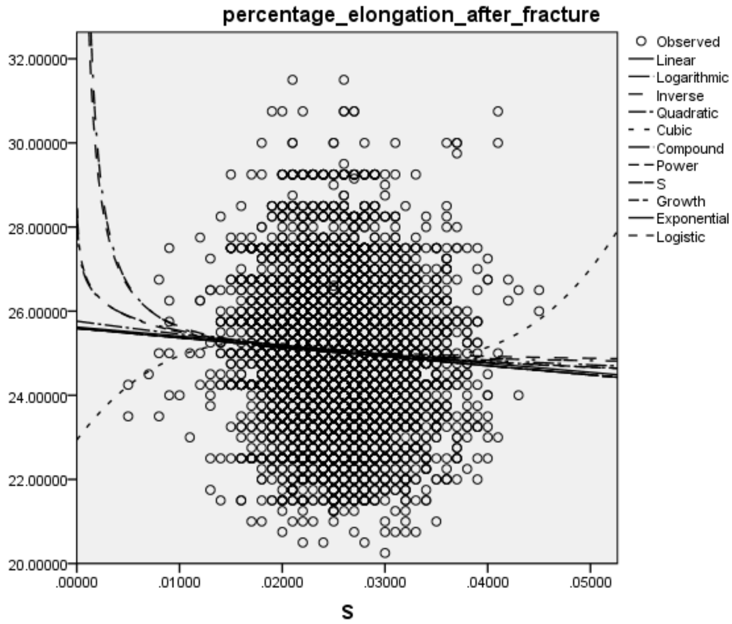

Figure 31.The scattered plot and fitted curve between element S and percentage elongation after fracture strength

According to the scattered plot and fitted curve between element S and percentage elongation after fracture strength, it is shown that the relationship is likely fitted by linear curve, logistic curve and quadratic curve.

Because the chemical compositions of No. 1 and No. 2 steel are similar, the estimated curves are approximately the same. Therefore, it is reasonable to use the approximate substitution of No. 1 steel for the estimation of chemical element and steel properties.

4.4 Establish B.P. neural network model

4.4.1 Selection of model

Regression analysis is simple and convenient when analyzing multi-factor models. However, the dependency of practical problem is often not simply a linear relationship. For example, the mapping relationship between various elements and the performance of steel bars in this problem belongs to complex multivariable coupled system, so the BP neural network method which is suitable in this situation is chosen to deal with the complicated mapping.

There are many mathematical models for predicting the relationship between the mechanical properties of steel and the alloying elements. Specifically, there are several common methods: One is simple extrapolation of trends. Alloy elements in accordance with a certain growth rate of change, which is linear growth. Although the curve of the change of alloying element content is never a linear extension, the linear model can be fitted to a small range. The second is to use common models to give predictive results. The choice of model is not in accordance with the facts that reflect the influence between chemical elements and performance of steel. The third is the average of a variety of results, which is the most common kind of error treatment: give a series of predictions, and then take the average of the forecast.

4.4.2 Artificial Neural Network

Artificial neural network(ANN) is a nonlinear system composed of a large number of computational units, which imitates the process of human brain nervous system of receiving, processing and storing to external signals, and has powerful intelligence to process information.

BP（Back Propagation）network, put forward by the research group of Rumelhart and McCelland, is a multi-layered feedforward network trained by algorithm of backward propagation of errors which is able to learn and store massive of input-output mode mapping relation and there is no need to provide it with an equation describing the mapping relation. BP neural network is a feedforward network composed by nonlinear transformation units. A multi - layer perceptron model simulating the process of brain neurons responding to external stimuli is established, which utilizes the learning mechanism of signal forward propagation and error inversion adjustment to construct an intelligent network model for non - linear information.

The picture below is a brief simulation of neural network

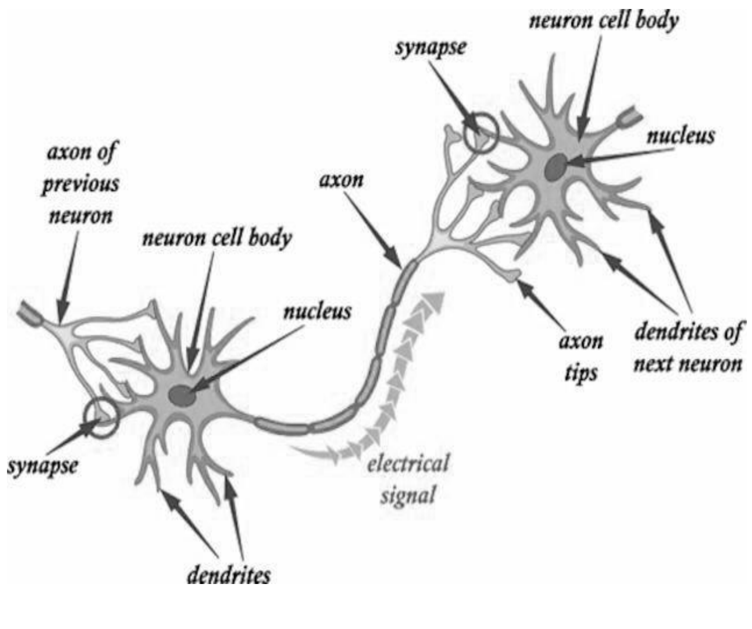

Figure 32.Neural network structure diagram

4.4.3 B.P. Neural Network Algorithm

BP neural network consists of input layer, hidden layer and output layer. The main idea is to divide the learning process into two stages: forward propagation of signal and backward propagation of error. In the forward propagation phase, the input information flows from the input layer through the hidden layer to the output layer, which produces an output signal at the output layer. The weight of the network is fixed during the forward transmission of signals, and the state of each layer affects only the state of the next neuron. If the desired output is not available at the output layer, the transition error signal propagates backwards. In the back-propagation phase, the error signal that fails to meet the accuracy requirement begins at the output end, propagates forward in a certain way, and spreads the error to all the elements of the layers,

Through the cycle of forward and backward regulation, the weights between neurons are constantly revised. When the output signal error meets the required accuracy, the learning process would stop.

The mathematical model of the neuron is shown in figure below.

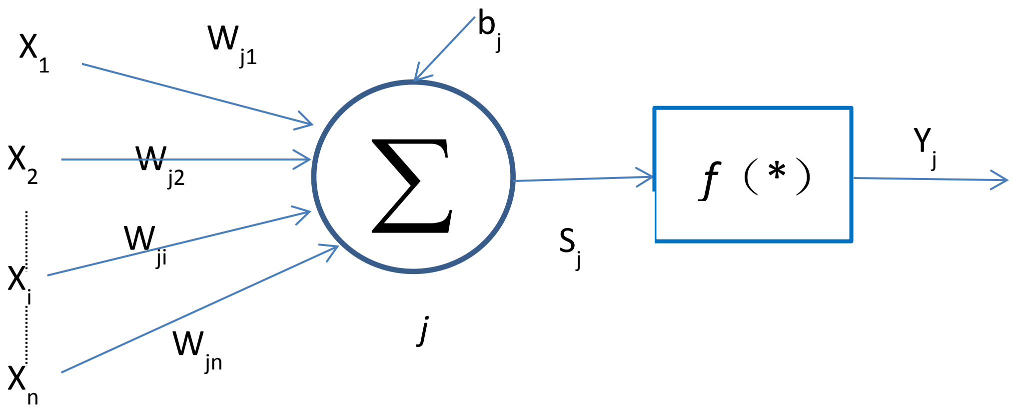

Figure 33.Mathematics model of nerve cell

In the figure, X_i refers to input; W_{ji} refers to weight; Y_j refers to output; b_j refers to threshold; f(*) refers to activation function.

Summarize the input value of the neural network:

$$S_j = \sum_{i=1}^{n} w_{ji} * x_i + b_j \tag{11}$$

Calculation of output value:

$$y_j = f(S_j) \tag{12}$$

In the transmission process, input signal passes input signal, the hidden layer nodes, and then the output node. The output of each node only affects the output of the next node, each node is a neuron structure, the unit characteristics (the transfer function) is usually s-shaped function (sigmoid) or linear function（purelin）. Sigmoid function includes log-sigmoid function and tan-sigmoid function.

The diagrams of the functions above are shown below.

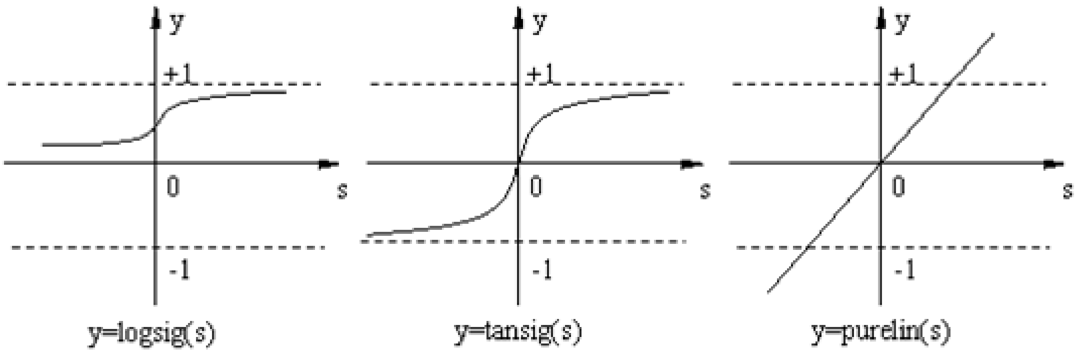

Figure 34.Diagram of Transmission functions

The input value of the Log-sigmoid function can take any value; the output value is between 0 and 1. The input value of the tan-sigmoid type transfer function tan-sig can take any value and the output value is between -1 and +1,which means it is a Monotone Differentiable Function of Continuous Value of s-shape. The input and output values of the linear transfer function (purelin) can take any value. A BP network can be seen as a highly non-linear mapping from input to output, that is, $f: R^n \to R^m, f(x) = Y$.

4.4.4 Network structure

Suppose there are n neurons in the input layer, p neurons in the hidden layer, m neurons in the output layer. The structure of the neural network is shown in figure.

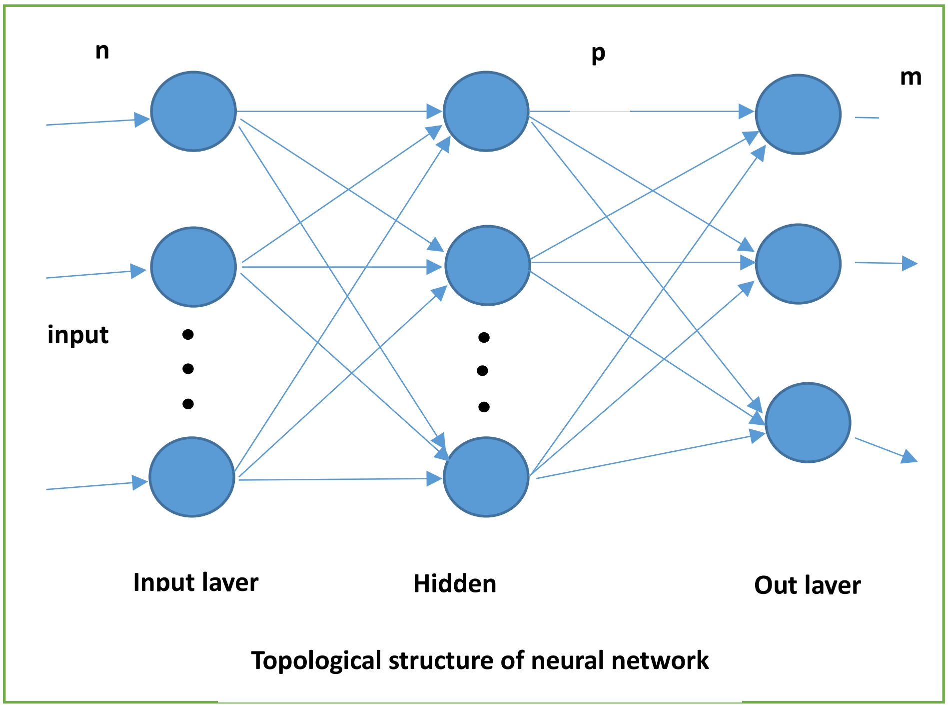

Figure 35.Topological structure of neural network

The Transfer Function Expression of BP Neural Network is shown below：

$$o = f(net) = \frac{1}{1 + e^{-net}} \tag{13}$$

4.4.5 Define Error function

The network learning error functions are divided into two categories.(t refers to expected value, y refers to output value)

Type A. The network continually learns by inputting samples one by one. This process is based on the minimum value of the single sample error (e).

$$\mathrm{E_p} = \frac{1}{2}\sum_{\mathrm{j}=1}^{m}\left(t_j^p - y_j^p\right)^2 \tag{14}$$

Type B. Batch process—Finish the grad search based on the minimum value of e after inputting all samples.

$$\mathrm{E} = \frac{1}{2}\sum_{p=1}^{p}\sum_{\mathrm{j}=1}^{m}\left(t_j^p - y_j^p\right) = \sum_{p=1}^{p} E_p \tag{15}$$

4.4.6 BP algorithm adjusts (the weight of hidden layer adjusts)

Here shows the formula of adjustment of weights of the hidden layers:

$$\Delta v_{pj} = \sum_{p=1}^{p}\sum_{j=1}^{m}\eta\left(t_j^p - y_j^p\right)f_2'\left(S_j\right)w_{jk}f_1'\left(S_k\right)x_i \tag{16}$$

Similarly, threshold adjustment of the output layer and hidden layer is the partial derivative of error function to threshold.

$$\begin{aligned}\Delta w_{jk} &= -\eta\frac{\partial E}{\partial w_{jk}} = -\eta\frac{\partial}{\partial w_{jk}}\left(\sum_{p=1}^{p}E_p\right)\\ &= \sum_{p=1}^{p}\left(-\eta\frac{\partial E}{\partial w_{jk}}\right)\end{aligned} \tag{17}$$

* η in the formula refers to the percentage of learning process.

So after the adjustment, the finally form is:

$$\Delta w_{jk} = \sum_{p=1}^{p}\sum_{j=1}^{m}\eta\left(t_j^p - y_j^p\right)f_2'\left(S_j\right)z_k \tag{18}$$

4.4.7 Steps of BP learning algorithm

Step1：Select the learning data(p=1,2,……P) , determine initial weighting matrix [W（0）]apparently.

Step2： Calculate network output with learning data

Step3： Make amendment backwards according to the formula below until all learning data had been used up.

$$\begin{gathered}w_l^{(p)}(i,j) = w_l^{(p-1)}(i,j) + \eta\delta_l^{(p)}a_{l-1}^{(p)}(j),\\ l = 1,\ldots,L,\end{gathered} \tag{19}$$

4.4.8 Hidden layer point designing

Robert Hecht-Nielsen had proved that a continuous function in any closed interval can be approximated by a hidden layer BP network. Therefore, a three-layer BP network is able to fulfill any insertion set from a dimension of m to n .

The number of hidden nodes has a certain influence on the performance of neural network. The number of nodes in the hidden layer is directly related to the number of input and output nodes. The choice of the number of hidden nodes is a very complex problem. According to experience we can refer to the following formula for design

$$l = \sqrt{n+m} + a \tag{20}$$

*L refers to number of points in hidden layer, n refers to number of points in input layer, m refers to number of points in output layer and a refers to adjustment constant varies from 1 to 10.

In order to reflect the characteristic of influence of 8 elements on tensile strength, yield strength and percentage elongation after fracture, we set up 8 input layers, including composition proportion of element C, Mn, Cr, V, Ni, S, P and Ce_q and 1 hidden layer with 10 intersection points in order to ensure accuracy and fitness. There are also three output layers- tensile strength, yield strength and percentage elongation after fracture.

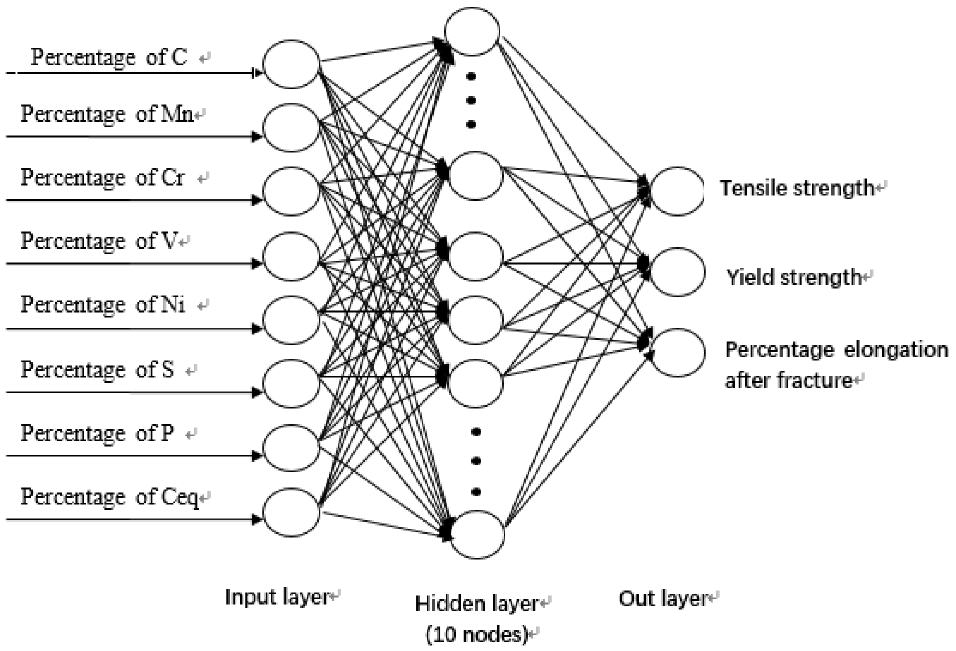

Figure 36.Neural network of relationship between chemical elements and properties of deformed steel bar

4.5 Modification of B.P. Neural Network Model

The method of heuristic improvement is to improve the parameters of BP neural network on the basis of gradient descent method, so as to overcome the shortcoming of network in learning process. The core idea of this method is to make the adjustment of weights to the maximum adaptation to error reduction requirements. In this paper, the additional momentum method is used to modify the BP neural network.

The additional momentum method is making a superposition of theoretical weight adjustment amount in this study and a portion of the last weight adjustment in the backpropagation stage and turning the value into the actual amount of weight adjustment in this study. The essence of this algorithm is to transfer the impact of weight changing through the momentum factor m_c into this adjustment. When the value of m_c is zero, the weights are adjusted according to the gradient descent method. When the value of m_c is L, the new weight adjustment is equal to the change of the previous weight, and the adjustment generated by the gradient descent method is ignored directly. Therefore, when the momentum term is added, $\nabla f(w(n))$ will become small when the network weight approaches the flat area at the bottom of the error surface, then in order to prevent w(n+1)=0 from appearing, w(n+1)≈w(n), which helps the network to jump out of the local minimum.

Weight adjustment formula is:

$$\Delta w(n+1) = m_c[w(n) - w(n-1) - (1 - m_c)\eta\nabla f(m(n))] \qquad (21)$$

*n refers to training times, m_c refers to momentum factor, η refers to the percentage of learning process.

The BP neural network model is modified with the additional momentum method to fit the nonlinear function at the preset error of 0.000001.

4.6 Model Solution

4.6.1 group 1

As for product 1, single-layer BP network has strong nonlinear mapping ability, so we choose single-layer neural network model, containing 10 hidden neurons and 3 output neurons.

We apply systematic sampling method to extract 8 initial values of elements for there are 8 input neurons in the system.

The initial values are：

[0.22; 1.43; 0.022; 0.03; 0.012; 0.024; 0.027; 0.47]

In order to improve the accuracy of the neural network, the number of iterations is 50000, and the training result is displayed every 2000 step length. In the network, the momentum factor is 0.7, the minimum error of the training target is 0.0000001, and the learning rate is 0.015. The above data is used to check the neural network performance. Use MATLAB program to work out the results.

The results are shown in figure below.

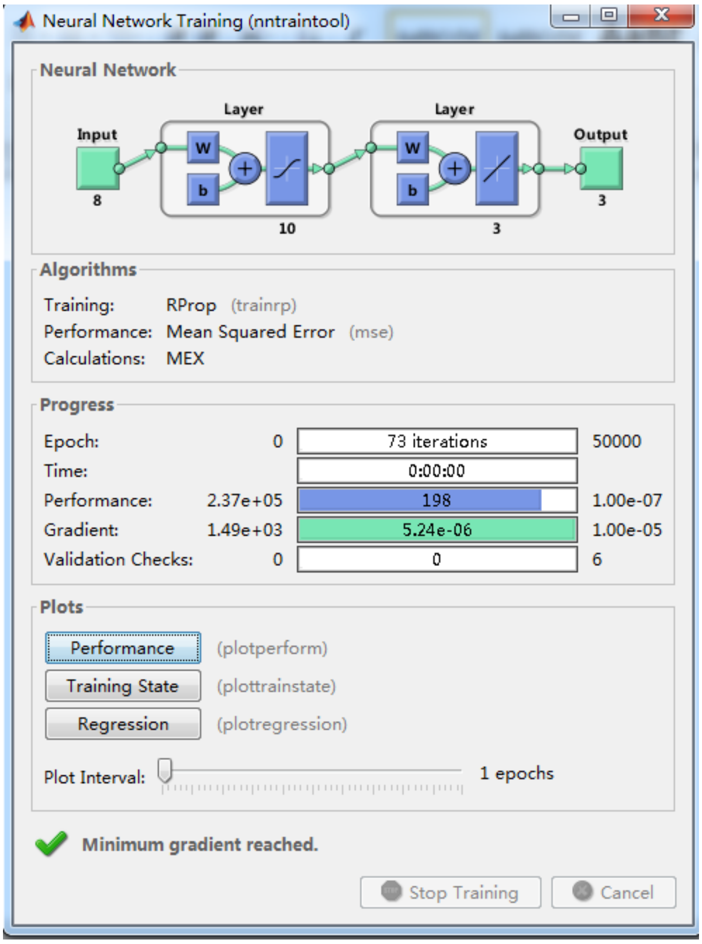

Figure 37.Training of product 1

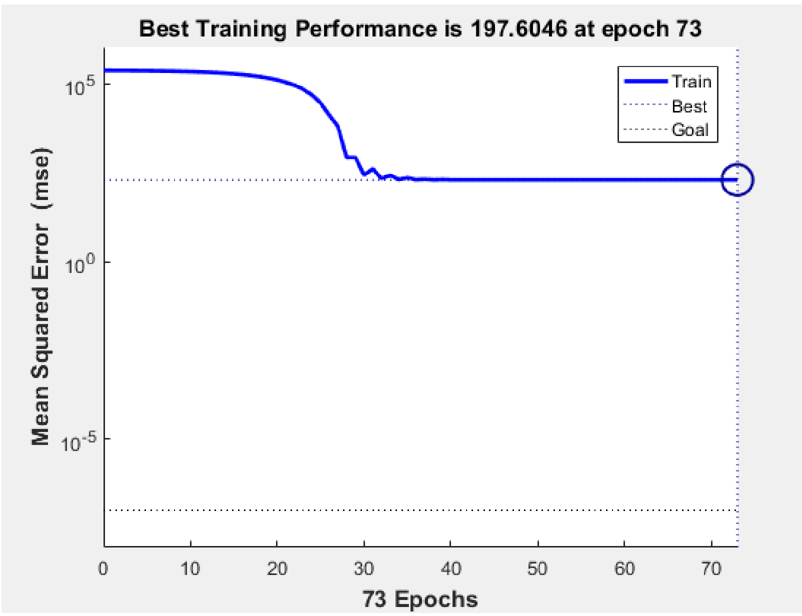

Figure 38.Performance of product 1

In the toolbox, data are divided automatically into three sets: training set, validation set and test set. There aren't any overlaps between these data sets. After training, the system will enter the data in the validation set and output a deviation. According to the number of steps the validation set, such as 50000echo, the system will determine whether the error in the 50000 consecutive test declines, if not decreased or even increased, indicating training set training error has no longer reduced. Then the training stops in order to prevent over learning.

From the figure38, it is apparent that the system gets best training performance when the epoch reach 66 iterations, whose value is 200.8237, and gradient reaches initial 1.74e +03. When the error value dropped to the default value 1e-05, stop training and after multiple iterations reaches 6.95e-06 which fulfills the demand. In the training, the weight vector solution is not unique, each step of the weight correction will make the error decreases, intuitionistic view is that the weight vector components along the gradient decreases in the direction of advance, the gradient limit is the requirement of iterative termination. Through the curve can be seen, with the training process, the curve gradually gets close to the best curve.

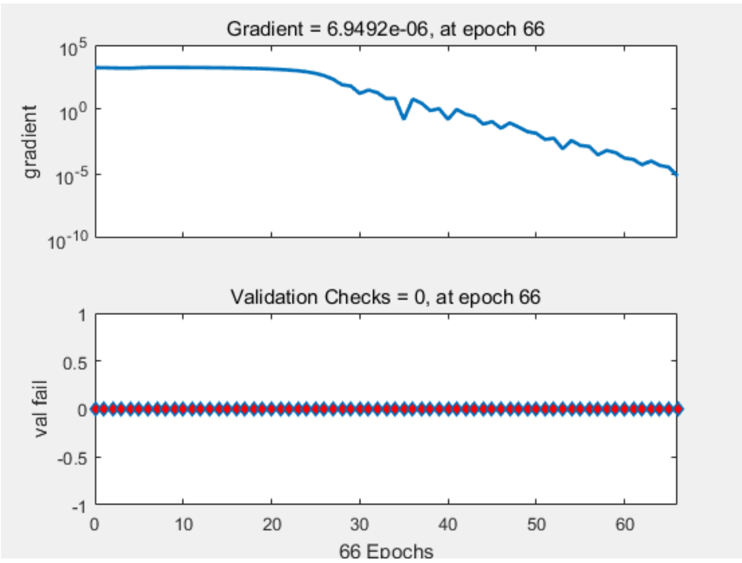

Figure 39.Gradient and val fail of product 1

From the figure39, it can be concluded that the original grad value is larger, and gradually decreases in the training process, so that the error is gradually reduced, so as to ensure the accuracy of the model.

4.6.2 Group 2

As for No.2 steel, the initial values are：

[0.22; 1.43; 0.022; 0.03; 0.012; 0.024; 0.027; 0.47]

While other parameters are the same as those in No.1

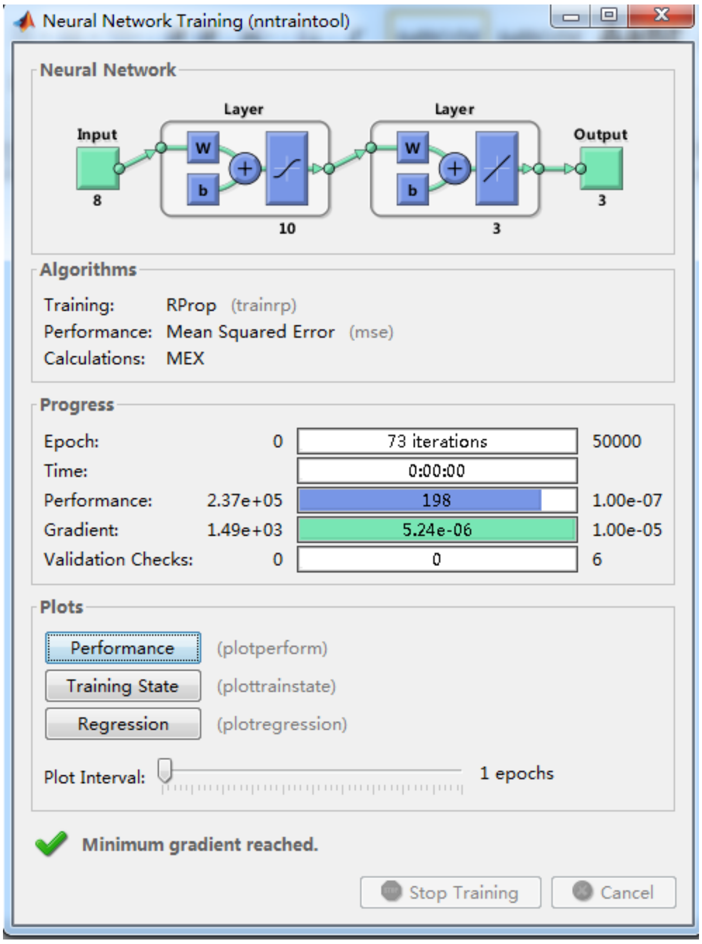

Figure 40.Training of product 2

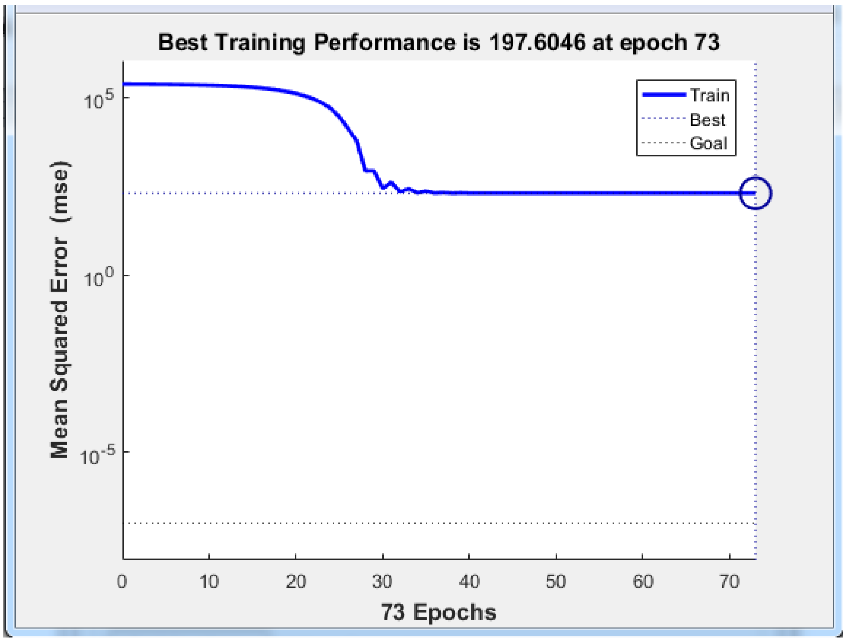

Figure 41.Performance of product 2

From the figure, it is apparent that the system gets best training performance when the epoch reach 73 iterations, whose value is 197.6046, and gradient reaches initial 5.24e-06. When the error value dropped to the default value 1e-05, stop training and after multiple iterations reaches 6.95e-06 which fulfills the demand. In the training, the weight vector solution is not unique, each step of the weight correction will make the error decreases, intuitionistic view is that the weight vector components along the gradient decreases in the direction of advance, the gradient limit is the requirement of iterative termination. Through the curve can be seen, with the training process, the curve gradually gets close to the best curve.

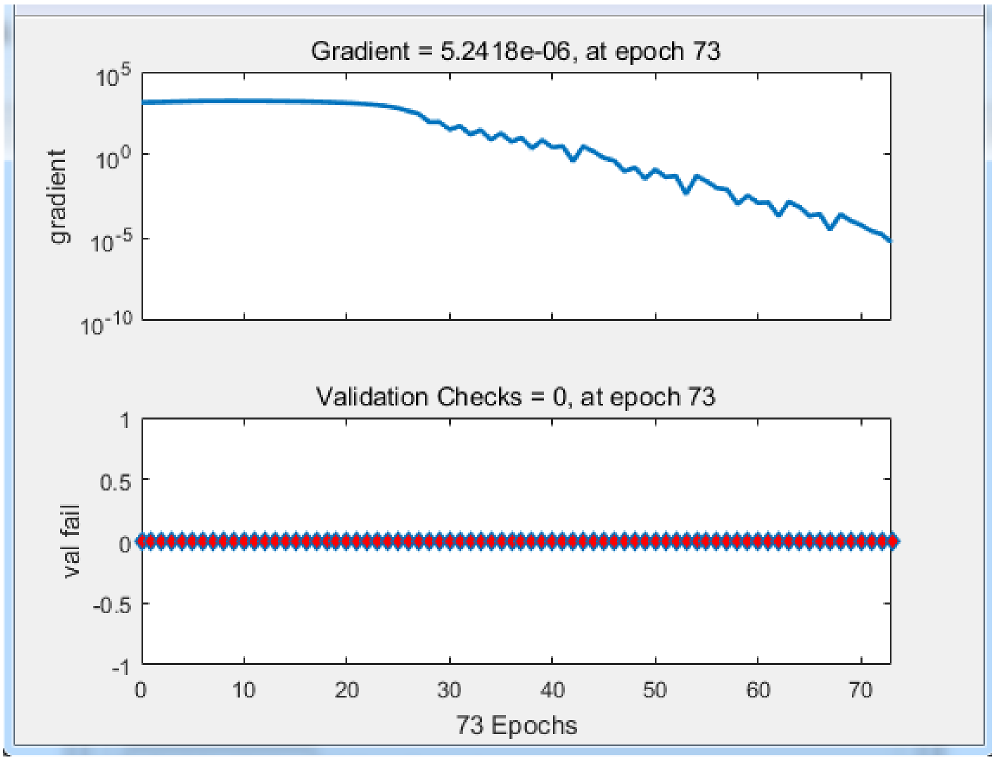

Figure 42.Gradient and val fail of product 2

The training level of the No.2 steel is similar with No. 1, so the modified BP neural network model given by this paper can be used by both No. 1 and No. 2.

4.7 Analysis of problem 3

The modified BP neural network model is obtained from Problem 2. On the basis of this ,loop statements are increased（shown in appendix）in order to realize that with the increase of the content of Cr, the content of Mn and V can be reduced by taking the appropriate step length under the premise that the performance of the deformed bar is little changed.

From the data in Attachment 1, the Cr content ranges from 0 to 0.133%, the Mn content ranges from 1.3 to 1.59% and the V content ranges from 0.025 to 0.041%.

These three elements are evenly take 30 values from the chart into the calculation.

4.7.1 Influence on chemical properties of Mn and Cr elements

As for steel No.1, the three-dimensional scatter grams of influence of Mn and Cr elements on tensile strength, yield strength and percentage elongation after fracture are displayed as follows

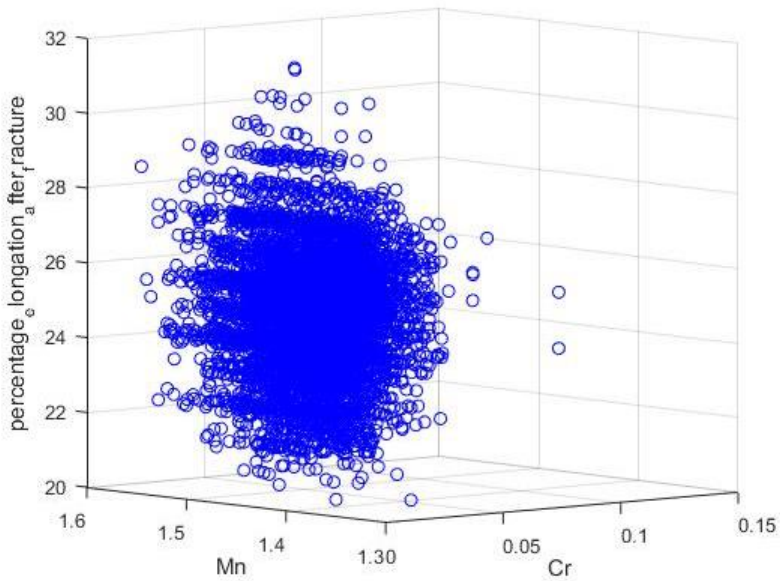

Figure 43. Influence on percentage elongation after fracture of Mn and Cr in 1

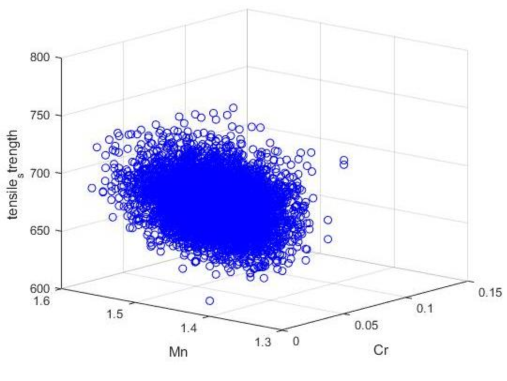

Figure 44. Influence on tensile strength of Mn and Cr in 1

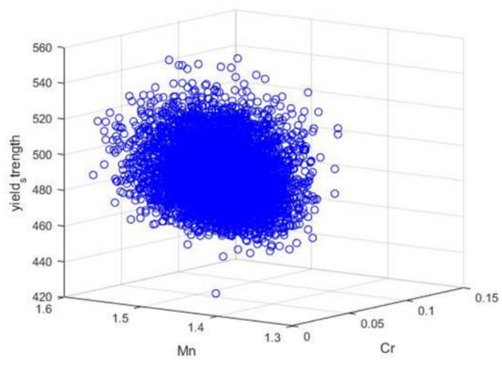

Figure 45. Influence yield strength on of Mn and Cr in 1

The three-dimensional scatter grams of influence of Mn and Cr elements on tensile strength, yield strength and percentage elongation after fracture are displayed as follows

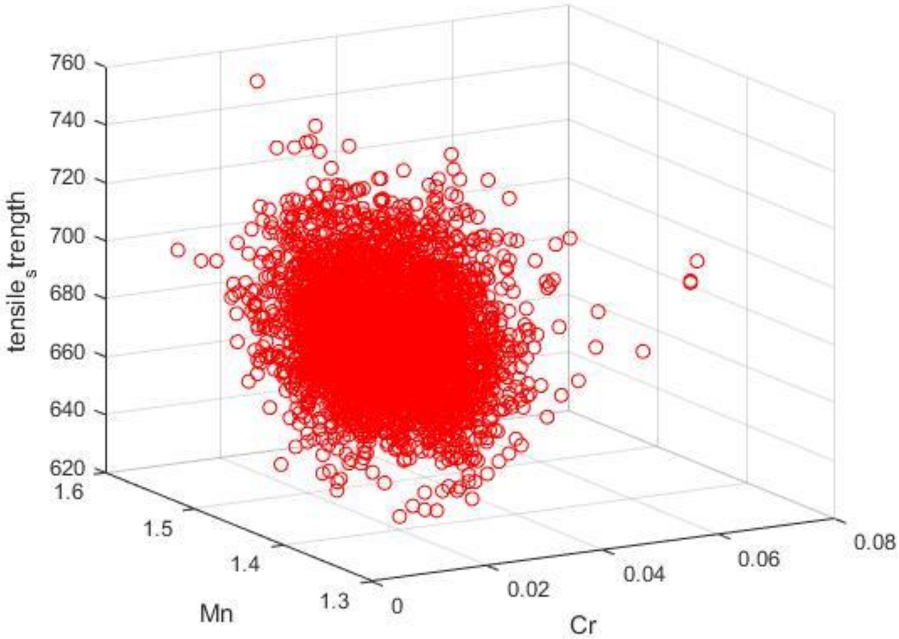

Figure 46. Influence on tensile strength of Mn and Cr in 2

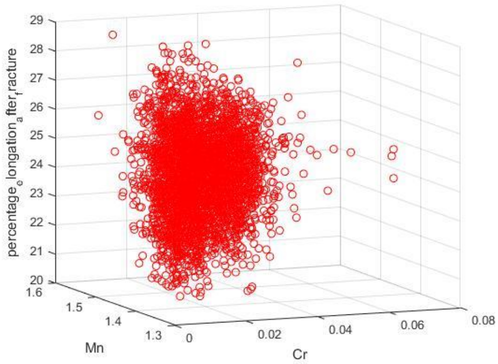

Figure 47. Influence on percentage elongation after fracture of Mn and Cr in 2

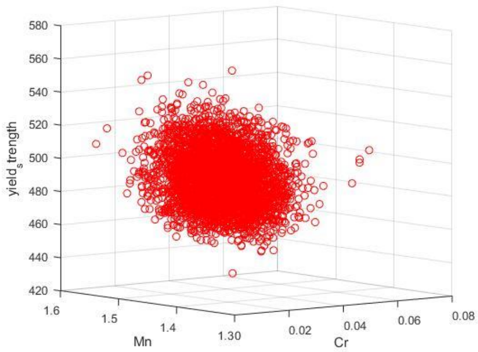

Figure 48. Influence yield strength on of Mn and Cr in 2

4.7.2 Influence on chemical properties of V and Cr elements

Evidence shows that cutting down contents of Mn while increasing the content of Cr, tensile strength, yield strength and percentage elongation after fracture will decrease slowly but not rapidly. The properties of the material decreases rapidly when the contents of Mn decreases by 8.24%.

The three-dimensional scatter grams of influence of V and Cr elements on tensile strength, tensile strength, yield strength and percentage elongation after fracture are showed as follows

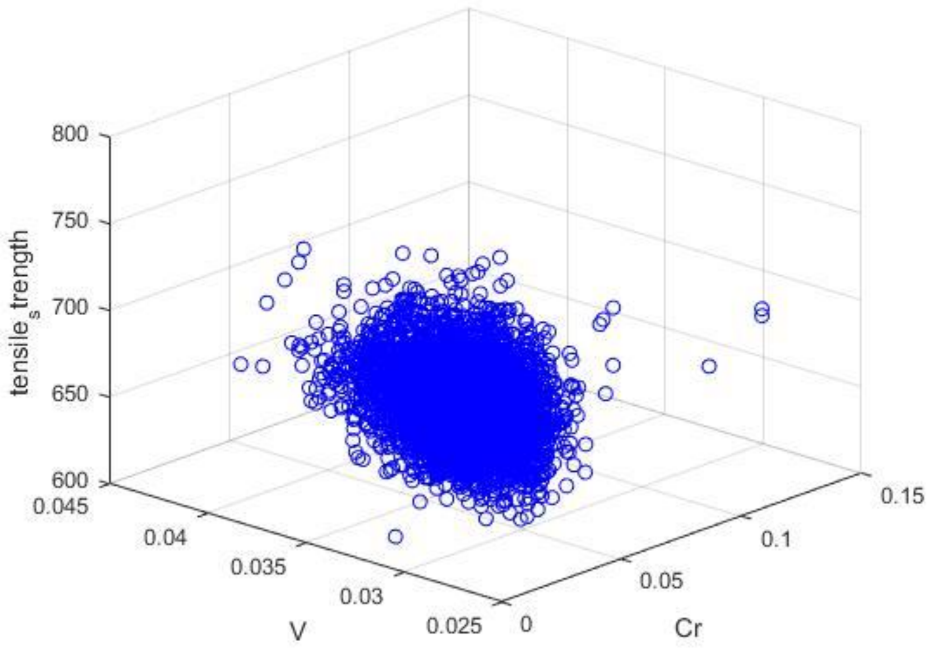

Figure 49. Influence on tensile strength of V and Cr in 1

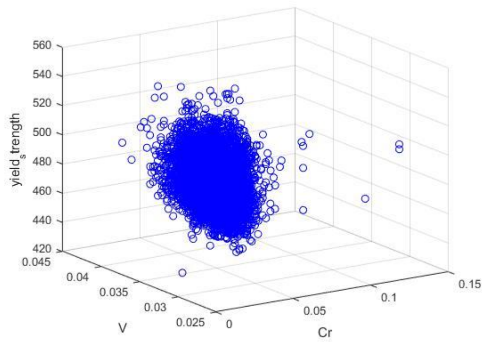

Figure 50. Influence on yield strength of V and Cr in 1

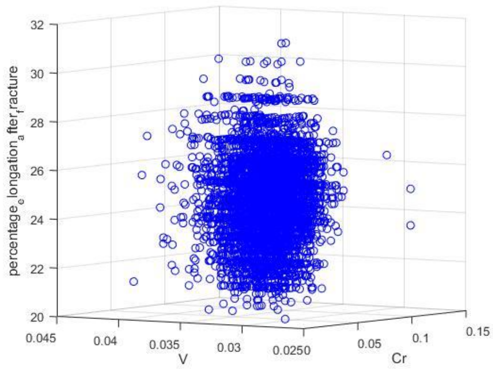

Figure 51. Influence on percentage elongation after fracture of V and Cr in 1

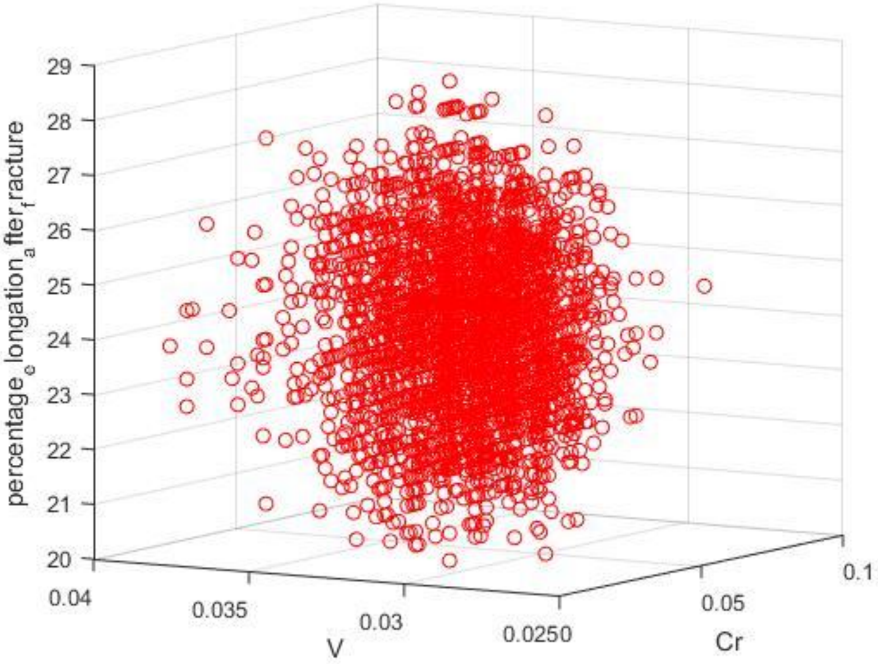

Figure 52. Influence on percentage elongation after fracture of V and Cr in 2

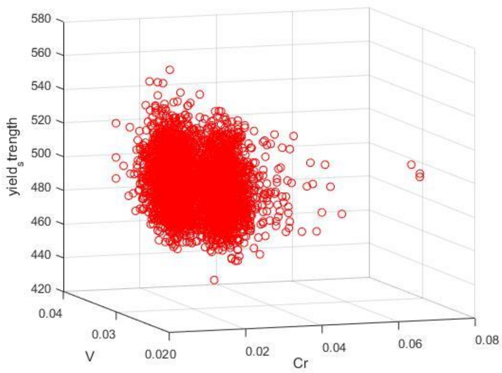

Figure 53. Influence on yield strength of V and Cr in 2

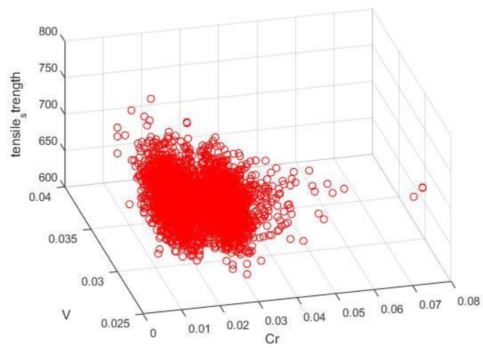

Figure 54. Influence on tensile strength of V and Cr in 2

Experiment shows that cutting down contents of V while increasing the content of Cr, tensile strength, yield strength and percentage elongation after fracture will decrease slowly but there are not big influences on steel bar’s performance. The properties of the material decreases rapidly when the contents of V decreases by 5.97%.

The allowable reductions of Mn and V with the increasing of Cr content can be calculated using the MATLAB program, and the results are shown in the appendix.

4.8 Conclusion

When the Cr, Mn and V values are determined, the yield strength of the corresponding reinforcement can be predicted. With this yield strength as a reference, a 10% downside is allowed for the performance reduction range. Control the Cr, Mn content of the same, reducing the V content until the yield strength exceeds the allowable range, obtained V content of the allowable reduction. Similarly, the allowable reduction of Mn is obtained.

5.Model evaluations

5.1 Advantages

1. The data are analyzed and filtered to remove the invalid data, which improves the accuracy of the model

2. Mathematics model of problem 1 uses multiple regression analysis method to find out principal chemical elements and sub factor. Only consider the influence of the main elements on the performance of the steel bar in the following analysis makes contribution to simplification of the model.

3. Mathematics model of problem 2 uses BP neural network, which is highly credible. Meanwhile it is able to predict three main performance indexes with only a slight modification on input layer value.

4. Mathematics models are described with graphs and data, which make the model more clear and intuitive.

5. Use control variates method to establish models of factors that influence properties of deformed steel bar

6. Use MATLAB to calculate the program to find the optimal composition of steel contents

5.2 Improvements needed

Due to the limitation of computer speed, the model only considers the main elements, but the other elements have some influence on the performance of deformed steel bar. If the conditions permit, more elements can be considered and optimized on the basis of the original model and program.

6. Promotion and application of the model

The model can effectively and quickly analyze the composition optimization scheme which satisfies the performance requirements of steel bars, and provides theoretical support for the production of the steel plant. It plays a positive role in reducing the cost, improving the efficiency and saving energy.

It can also be used to predict the development trend of these systems, which can be used to analyze and analyze the relationship between the components and the overall performance and quality.

7. Conclusion

The arrival of the big data era makes the adjustment and optimization of practical problems become feasible and necessary. However, many traditional methods are based on rich experience, and there is no reliable theoretical basis.

Through the research of this paper, the following conclusions are drawn:

(1) The correlation of chemical elements to the properties of deformed steel bars is analyzed with the data from actual production. The results shows that C, Mn, Cr, V, Ni, S, P and Ce_q are the principal factors Influence factors, while other elements have less influence.

.

(2) A linear model between steel properties and chemical composition is established by multiple linear regression method, however, after analysis, there is a complex coupling between the two nonlinear relationships. Therefore, a modified BP neural network algorithm is used to establish the mapping relationship between steel properties and chemical elements, and a model of analysis and optimization problems is given, which makes the algorithm more accurate.

(3) According to the BP neural network model, it can be concluded that by increasing Cr content and cutting down Mn and V contents appropriately, the material properties can be kept within the permissible range and has little effect on its practical application, which could help steel plants to save costs of production.

The BP neural network model provides an effective reference for customization and mass production of the factory, which has typical practical significance. In addition, BP neural network model also played a positive role in new product composition control and performance prediction,

8.Reference Documentation

[1] WANG MJ,LIU XB,LI ZM. Study on Mechanical Properties and Components of 20MnSi Steel. 2000,1-2.

[2] Yuan ZX,Yu ZS,Li SQ,Li DX,Wu J. Study on the Relationship between Chemical Compositions and Mechanical Properties of Steels Made by Wuhan Iron and Steel Corporation. Journal of Wuhan Yejin University of Science and Technology. [TF701.3]. 1998. 406-410.

[3] Long YY. Fast prediction of cast iron property base on BP neutral network. 2012,32-51.

[4] Paulito P.Palme,Yaiehi Hayasaka,Shiro Usui. Mutation-Based Genetic Neural Network [J].IEEE Transactions on Neural Networks,2005,16(3).

[5] SU LY,DENG Y,RAN XZ. Statistical Modeling and Analysis of High_strength Low_alloy Steel between Mechanical Properties and Chemical Composition. [O211.4]. 2008,37-40.

[5] LIU TS. The Research and Application on BP Neural Network Improvement.2011,9-21.

[6] Ashok Kumar Goel,Suresh C． Saxenax,Surekha Bhanot．． A fast learning algorithm for training feedforward neural networks[J]． International Journal of Systems Science． 2006,37(10):70-722.

[7] J. Kennedy, R. Eberhart. Particle Swarm Optimization. Proceedings of IEEE International Conference on Neural Networks, 1995,4:1942-1948

Appendix (program of MATLAB)

BP Neural network model of steel 1

```
clear;
load bpnerve1.mat;
Input_layer=Input_layer';
Output_layer=Output_layer';
net=newff(minmax(Input_layer),[10,3],{'tansig','purelin'},'trainrp');
net.trainParam.epochs=50000;
net.trainParam.show=2000;
net.trainParam.lr=0.15;
net.trainParam.mc=0.7;
net.trainParam.goal=0.0000001;
net=train(net,Input_layer,Output_layer);
Y=sim(net,Input_layer);
x=[0.22;1.43;0.022;0.03;0.012;0.024;0.027;0.47];
y=sim(net,x)
```

BP Neural network model of steel 2

```
clear;
load bpnerve2.mat;
Input_layer2=Input_layer2';
Output_layer2=Output_layer2';
net=newff(minmax(Input_layer2),[10,3],{'tansig','purelin'},'trainrp');
net.trainParam.epochs=50000;
net.trainParam.show=2000;
net.trainParam.lr=0.15;
net.trainParam.mc=0.7;
net.trainParam.goal=0.0000001;
net=train(net,Input_layer2,Output_layer2);
Y=sim(net,Input_layer2);
x=[0.21;1.35;0.02;0.033;0.5;0.46;0.03;0.035];
y=sim(net,x)
```

Optimization algorithm among Cr,Mn and V of steel 1

```
clear;
load bpnerve1.mat;
Input_layer=Input_layer';
Output_layer=Output_layer';
net=newff(minmax(Input_layer),[10,3],{'tansig','purelin'},'trainrp');
net.trainParam.epochs=50000;   % 50000 epochs
net.trainParam.show=2000;
```

```
    net.trainParam.lr=0.15;
    net.trainParam.mc=0.7;
    net.trainParam.goal=0.0000001; % the min error is 
0.0000001
    net=train(net,Input_layer,Output_layer);
    Y=[769.31322;558.99737;31.5];
    i=0;a=[];
    for Cr=0:0.05:0.133
        for Mn=1.59:-0.05:1.30
            for V=0.041:-0.005:0.025
                   x=[Cr;Mn;V];
                   y=sim(net,x);
                   diff=(y-Y)./Y;
                   diff=abs(diff);
             if diff(1)<=0.1&&diff(2)<=0.1&&diff(3)<=0.1
                  i=i+1;
                  a(i,:)=x';
                   end
               end
           end
       end
```

Optimization algorithm among Cr,Mn and V of steel 2

```
    clear;
    load bpnerve2.mat;
    Input_layer=Input_layer';
    Output_layer=Output_layer';
    net=newff(minmax(Input_layer),[10,3],{'tansig','pureli
n'},'trainrp');
    net.trainParam.epochs=50000;   % 50000 epochs
    net.trainParam.show=2000;
    net.trainParam.lr=0.15;
    net.trainParam.mc=0.7;
    net.trainParam.goal=0.0000001; % the min error is 
0.0000001
    net=train(net,Input_layer,Output_layer);
    Y=[769.31322;558.99737;31.5];
    i=0;a=[];
    for Cr=0:0.05:0.133
        for Mn=1.59:-0.05:1.30
            for V=0.041:-0.005:0.025
                   x=[Cr;Mn;V];
                   y=sim(net,x);
                   diff=(y-Y)./Y;
```

```
                diff=abs(diff);
            if diff(1)<=0.1&&diff(2)<=0.1&&diff(3)<=0.1
                i=i+1;
                a(i,:)=x';
                end
            end
        end
    end
a
```

Relationship of Cr and Mn on tensile strength of steel 1

```
clear
load question_steel1.mat
plot3(Cr,Mn,tensile_strength,'bo')
grid on;
xlabel('Cr');   % the x label is Cr
ylabel('Mn');   % the y label is Mn
zlabel('tensile_strength');  % the z label is
tensile_strength
```

Relationship of Cr and Mn on tensile strength of steel 2

```
clear
load question_steel2.mat
plot3(Cr,Mn,tensile_strength,'ro')
grid on;
xlabel('Cr');   % the x label is Cr
ylabel('Mn');   % the y label is Mn
zlabel('tensile_strength');  % the z label is
tensile_strength
```

Relationship of Cr and Mn on yield strength of steel 1

```
clear
load question_steel1.mat
plot3(Cr,Mn,yield_strength,'bo')
grid on;
xlabel('Cr');   % the x label is Cr
ylabel('Mn');   % the y label is Mn
zlabel('yield_strength');  % the z label is
yield_strength
```

Relationship of Cr and Mn on yield strength of steel 2

```
clear
load question_steel2.mat
plot3(Cr,Mn,yield_strength,'ro')
```

```
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('Mn');   % the y label is Mn
    zlabel('yield_strength'); % the z label is
yield_strength
```

Relationship of Cr and Mn on percentage elongation after fracture of steel 1

```
    clear
    load question_steel1.mat
    plot3(Cr,Mn,percentage_elongation_after_fracture,'bo')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('Mn');   % the y label is Mn
    zlabel('percentage_elongation_after_fracture');  % the
z label is percentage_elongation_after_fracture
```

Relationship of Cr and Mn on percentage elongation after fracture of steel 2

```
    clear
    load question_steel2.mat
    plot3(Cr,Mn,percentage_elongation_after_fracture,'ro')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('Mn');   % the y label is Mn
    zlabel('percentage_elongation_after_fracture');  % the
z label is percentage_elongation_after_fracture
```

Relationship of Cr and V on tensile strength of steel 1

```
    clear
    load question_steel1.mat
    plot3(Cr,V,tensile_strength,'bo')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
    zlabel('tensile_strength');  % the z label is
tensile_strength
```

Relationship of Cr and V on tensile strength of steel 2

```
    clear
    load question_steel2.mat
    plot3(Cr,V,tensile_strength,'ro')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
```

```
    zlabel('tensile_strength');  % the z label is
tensile_strength
```

Relationship of Cr and V on yield strength of steel 1

```
    clear
    load question_steel1.mat
    plot3(Cr,V,yield_strength,'bo')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
    zlabel('yield_strength');  % the z label is
yield_strength
```

Relationship of Cr and V on yield strength of steel 2

```
    clear
    load question_steel2.mat
    plot3(Cr,V,yield_strength,'ro')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
    zlabel('yield_strength');  % the z label is
yield_strength
```

Relationship of Cr and V on percentage elongation after fracture of steel 1

```
    clear
    load question_steel1.mat
    plot3(Cr,V,percentage_elongation_after_fracture,'bo')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
    zlabel('percentage_elongation_after_fracture');  % the
z label is percentage_elongation_after_fracture
```

Relationship of Cr and V on percentage elongation after fracture of steel 2

```
    clear
    load question_steel2.mat
    plot3(Cr,V,percentage_elongation_after_fracture,'ro')
    grid on;
    xlabel('Cr');   % the x label is Cr
    ylabel('V');   % the y label is Mn
    zlabel('percentage_elongation_after_fracture');  % the
z label is percentage_elongation_after_fracture
```

Optimal algorithm among Cr， Mn and V of steel 1

steel 1	chemical composition	
Cr	Reduction of Mn（%）	Reduction of V（%）
0	2.89	3.21
0.0046	3.13	3.69
0.0092	3.37	4.13
0.0138	3.66	4.55
0.0184	3.91	5.05
0.023	4.12	5.51
0.0276	4.41	5.98
0.0322	4.66	6.43
0.0368	4.92	6.89
0.0414	5.12	7.35
0.046	5.39	7.86
0.0506	5.66	8.27
0.0552	5.89	8.73
0.0598	6.12	9.19
0.0644	6.39	9.65
0.069	6.64	10.12
0.0736	6.88	10.57
0.0782	7.12	11.03
0.0828	7.39	11.51
0.0874	7.64	11.95
0.092	7.89	12.39
0.0966	8.14	12.87
0.1012	8.41	13.33
0.1058	8.64	13.77
0.1104	8.89	14.25
0.115	9.15	14.71
0.1196	9.39	15.06
0.1242	9.63	15.63
0.1288	9.89	16.08
0.1334	10.14	16.55

Optimal algorithm among Cr， Mn and V of steel 2

steel 2	chemical composition	
Cr	Reduction of Mn （%）	Reduction of V （%）
0	2.86	3.17
0.0046	3.12	3.65
0.0092	3.34	4.08
0.0138	3.63	4.51
0.0184	3.88	5.01
0.023	4.08	5.47
0.0276	4.38	5.95
0.0322	4.63	6.39
0.0368	4.89	6.85
0.0414	5.09	7.31
0.046	5.36	7.81
0.0506	5.63	8.23
0.0552	5.86	8.69
0.0598	6.09	9.15
0.0644	6.36	9.61
0.069	6.61	10.08
0.0736	6.85	10.53
0.0782	7.03	10.99
0.0828	7.36	11.47
0.0874	7.61	11.91
0.092	7.86	12.35
0.0966	8.11	12.86
0.1012	8.38	13.29
0.1058	8.61	13.72
0.1104	8.86	14.21
0.115	9.12	14.67
0.1196	9.36	15.02
0.1242	9.6	15.61
0.1288	9.86	16.04
0.1334	10.11	16.51