Composition analysis and identification model of ancient glass products based on Spearman correlation coefficient and BP neural network

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Abstract. This paper analyzes the composition of glass products by statistical analysis of known data and then uses Spearman's correlation coefficient analysis model to analyze the composition of glass products, and uses BP neural network to build a prediction and classification model. We use BP neural network to build a prediction and classification model for the composition of glass products and classify the types. In this paper, a BP neural network classification model is constructed using C language. The number of neuron nodes in the input layer and the number of neuron nodes in the output layer are selected. The chemical composition content of the existing sample data is used as the input layer and the category is converted to the output layer after data pre-processing. Finally, a BP neural network classification model with very low classification error is obtained. The sensitivity of the classification results is obtained by sample carryover network calibration and Spearman correlation coefficient.

Keywords: Spearman correlation coefficient; BP neural net; Cluster analysis; Heat map.

1. Introduction

The earliest synthesis of real glass in China was made during the Spring and Autumn and Warring States period, when the main raw material was quartz and the flux used was a natural mineral containing lead and barium, and the glass made was called "lead-barium glass" [1], with a high content of lead oxide (PbO) and barium oxide (BaO). Potassium glass is mainly popular in Lingnan, Southeast Asia, India and other regions in China, and is made by firing with substances containing high potassium content such as grass wood ash as a flux.

At present, traditional correlation analysis methods have matured, and the more commonly used correlation analysis methods at home and abroad now include Pearson's correlation coefficient [2], Kendall's tau-b correlation coefficient [3] and Cochran's Q test [4]. However, these traditional methods generally have shortcomings such as inconsistent quantification criteria and large deviations of the estimated correlation coefficients from the overall correlation coefficients. The Spearman's correlation coefficient used in this question is closer to the estimated correlation coefficient than the Kendall 's tau-b correlation coefficient [5], and the relative error is smaller.

In this paper, we used Spearman's analysis to determine whether the significant p-value was less than 0.05 to determine the significant difference between glass type and surface weathering, but not the significant difference between ornamentation and color, and on this basis, we conducted a quantitative analysis to obtain the correlation coefficients between the relationships. Then, the statistical analysis was conducted to compare the statistical patterns of different glass types before and after weathering, firstly, the chemical content indexes before and after weathering were analyzed by descriptive statistics, and then the histograms of changes before and after weathering were drawn to observe the fluctuation of the data. At the same time, Spearman's model was used for in-depth analysis, and finally it was obtained that the main chemical components (silica, etc.) of high potassium glass showed an increasing trend after weathering, while lead-barium glass showed a decreasing trend. In addition, the surface weathering of high potassium glass is also negatively correlated with the content of potassium oxide, calcium oxide, magnesium oxide, aluminum oxide, iron oxide, lead oxide, phosphorus pentoxide and strontium oxide, and the surface weathering of lead-

barium glass is also positively correlated with the content of calcium oxide, lead oxide, phosphorus pentoxide and strontium oxide and negatively correlated with the content of sodium oxide and aluminum oxide. The BP prediction model was trained according to the existing chemical composition law, and finally predicted the chemical composition content before weathering.

2. Model assumptions and notation

2.1. Assumptions

1. It is assumed that the trends (statistical patterns) of chemical composition change before and after weathering on the surface of glass artifacts are the same, excluding environmental factors.
2. Assume that different sampling points of the same artifact need to be considered as two different samples when imported into the model.
3. assume that weathering has the same effect on the chemical composition of each unweathered surface of each glass artifact (the same degree of weathering).
4. assume that weathering has the same effect on the chemical composition of each weathered surface of each glass artifact (the same degree of weathering).
5. It is assumed that the presence or absence of weathering affects the identification of unknown classes of glass artifacts and requires separate training models.
6. It is assumed that the chemical composition of both high potassium glass and lead-barium glass is significantly different before and after weathering.

2.2. Notations

Important notations used in this paper are listed in Table 1.

Table 1. Notations

Symbols	Meaning
X_i	Spearman's correlation coefficient independent variable
Y_i	Spearman's correlation coefficient dependent variable
$\sum d_i^2$	Sum of the variances of the equal differences between the variables and the
H_0	Assumption of correlation significance
X^2	The degree of deviation between the measured and theoretical values
ρ	Spearman's correlation coefficient
n	Sample size
N	Number of neuron nodes in the input layer
I	Number of neuron nodes in the hidden layer
J	Number of neuron nodes in the output layer
X_n	Input vector of neuron nodes in the input layer
h_i	Output vector of hidden layer neuron nodes
q_i	Total input of hidden layer neuron nodes
β_i	Bias of hidden layer neuron nodes
$\hat{Y}_i$	Output vector of output layer neuron nodes
u_j	Total input of output layer neuron nodes
λ_j	Output layer neuron node bias
w_{ni}	Connection weights between input layer and hidden layer neuron nodes
v_{ij}	Connection weights between the hidden layer and the output layer neuron
Y_j	Sample result vector

α	Momentum coefficient
k	Initial number of clusters
C_i	Initial clustering center
x	Data Objects
m	Dimension of the data object
x_j, C_{ij}	jth attribute value of x, C_i
SSE	The error sum of squares of the class cluster

3. Model construction and solving

3.1. Data pre-processing

(1) Elimination of samples with missing color data

In the solution of the relationship between color and surface weathering, this relationship cannot be determined if there is no data for color.

(2) Conversion of information to grade data

The information in the columns of "decoration", "type", "color" and "surface weathering" is sorted by intensity level Converted into numbers that the computer can calculate and process.

In order to ensure that the BP neural network prediction model has higher accuracy for prediction results, it is necessary to make the training samples infused into the network representative of the majority of ancient glass artifacts, i.e., the chemical composition data before and after weathering of the input samples conform to the statistical laws derived from the previous step.

(1) Data sample selection

According to the statistical law derived from the previous step, the chemical composition data that meet the statistical law are selected as the training samples.

(2) Sample classification

According to the question, the paired data need to be classified again, according to their different types of artifacts and whether the surface is weathered or not. and instilled into the input and output layers of two different BP neural networks, respectively.

3.2. Modeling of Spearman correlation coefficient relationship analysis

3.2.1 Introduction to Spearman's correlation coefficient

Spearman's correlation coefficient is a non-parametric measure of the correlation between two variables, which uses monotonic equations to evaluate the correlation of two statistical variables. The absolute value of Spearman's correlation coefficient is 1 when the two variables are perfectly monotonically correlated, assuming that there are no repeated values in the data.

Spearman's correlation coefficient indicates the direction of correlation between X (independent variable) and Y (dependent variable). Assuming that X increases and Y tends to increase, the Spearman correlation coefficient is positive. If X increases and Y tends to decrease, the Spearman correlation coefficient is negative. a zero Spearman correlation coefficient indicates that there is no tendency for Y to increase as X increases. As X and Y get closer to complete monotonic correlation, Spearman's correlation coefficient increases in absolute value. When X and Y are perfectly monotonically correlated, the Spearman correlation coefficient has an absolute value of 1.

Spearman's correlation coefficient is often called "non-parametric". There are two implications here. First, when the relationship between X and Y is described by any monotonic function, then they are completely Pearson correlated. Accordingly, Pearson's correlation coefficient can only give the correlation between X and Y described by the linear equation. Second, Spearman does not require a priori knowledge (i.e., knowledge of its parameters) to accurately obtain the sampling probability distributions of XandY [6].

3.2.2 Spearman correlation coefficient strength ranking principle

For the Spearman correlation coefficient calculation, $\sum d_i^2$ corresponds to the sum of the variances of the differences between the X_i and Y_i variables of the same rank. The rank, in turn, is obtained by ranking the variables by size (strength).

The original data were assigned a corresponding rank based on their average descending (or ascending) position in the overall data, corresponding to a rank difference of d_i. This is shown in Table 2 below.

Table 2. Spearman correlation coefficient intensity scale

X_i	Y_i	X_i level	Y_i level	d_i	d_i^2
3	5	2	1	1	1
8	10	5	4.5	0.5	0.25
4	8	3	3	0	0
7	10	4	4.5	-0.5	0.25
2	6	1	2	-1	1

3.2.3 P-value test for significant relationship

The significance relationship p-value is found by the chi-square test, which is the degree of deviation between the definite class variables of the statistical sample and the definite class variables. The degree of deviation between the definite class variables and the definite class variables determines the size of the chi-square value; if the chi-square value is larger, the greater the degree of deviation between the two; conversely, the smaller the deviation between the two; if the two values are exactly equal, the chi-square value is 0, indicating that the theoretical value is exactly the same. The significance p-value obtained by the chi-square test is analyzed to see if it is less than 0.05, so as to know whether there is a statistically significant relationship.

The X^2 value indicates the degree of deviation between the observed and theoretical values and is calculated as follows

$$X^2 = \sum \frac{(A-E)^2}{E} = \sum_{i=1}^{k} \frac{(A_i - E_i)^2}{E_i} = \sum_{i=1}^{k} \frac{(A_i - np_i)^2}{np_i} \qquad (i = 1, 2, 3 \ldots k) \tag{1}$$

3.2.4 Spearman correlation coefficient solution

The Spearman correlation coefficient is defined as the Pearson correlation coefficient between rank variables. The Pearson correlation coefficient between two variables is defined as the quotient of the covariance and standard deviation between the two variables, which is given by

$$\rho_{X,Y} = \frac{\operatorname{cov}(X,Y)}{\sigma_X \sigma_Y} = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X \sigma_Y} \tag{2}$$

The above equation defines the overall correlation coefficient, which is often represented by the Greek lowercase letter ρ. Estimating the covariance and standard deviation of the sample gives the Pearson correlation coefficient, commonly represented by the lowercase English letter r, which is given by

$$r = \frac{\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n} (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^{n} (Y_i - \bar{Y})^2}} \tag{3}$$

r can also be estimated from the mean of the standard scores at sample point (X_i, Y_i), yielding an expression equivalent to the above equation.

$$r = \frac{1}{n-1}\sum_{i=1}^{n}\left(\frac{X_i - \bar{X}}{\sigma_X}\right)\left(\frac{Y_i - \bar{Y}}{\sigma_Y}\right) \tag{4}$$

Since the Spearman correlation coefficient can be regarded as the Pearson correlation coefficient between rank variables, the correlation coefficient for a sample of sample size n, where n raw data are converted into rank data is calculated by the following formula.

$$\rho = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}} \tag{5}$$

3.2.5 Simplification of Spearman correlation coefficient solution

In practical applications, the link between rank variables is irrelevant and tedious to calculate, so the correlation coefficient can be calculated by using the difference between the ranks of the two variables being observed in a simple step with the formula

$$\rho = 1 - \frac{6\sum d_i^2}{n\left(n^2 - 1\right)} \tag{6}$$

3.3. Establishment of BP neural network prediction model

3.3.1 Introduction to BP Neural Networks

BP neural network, i.e., error feedback neural network algorithm, consists of three layers, including the input layer of BP neural network, the hidden layer of BP neural network and the output layer of BP neural network. Various information from the outside is transferred to the implicit layer of the BP neural network through the input layer, and the final result is obtained through the output layer. When the error between the output result of the output layer and the pre-set input value of the BP neural network is large, it enters the back propagation stage of the BP neural network and updates the network weights until the error between the output result and the desired result meets certain conditions [7].

The BP neural network has arbitrarily complex pattern classification ability and excellent multi-dimensional function mapping ability, which solves the heterogeneous or (Exclusive OR, XOR) and some other problems that cannot be solved by simple perceptrons [8].

3.3.2 BP neural network prediction model structure

Use BP neural network to build the prediction model, and the prediction model needs to be able to predict the chemical composition content before weathering based on the chemical composition data at the weathering point, so this requires our prediction model to be able to input and output all the chemical compositions through the input and output layers, so the number of nodes in the input and output layers of our prediction model needs to correspond to the number of chemical compositions. According to Annex - Form 2, there are 14 chemical components such as SiO2, Na2O, CaO, etc. Therefore, our BP neural network prediction model needs to build 14 neuron nodes in the input layer and 14 neuron nodes in the output layer. The number of neuron nodes in the hidden layer is explained later, and the BP neural network prediction model is first constructed based on the known conditions

3.3.3 Mathematical derivation of BP neural network prediction model

The BP neural network uses the Sigmoid function as the transformation function, and its formula is

$$f(x) = \frac{1}{1 + e^{-x}} \tag{7}$$

According to this formula, the output vector of the hidden layer neuron node, which is given by

$$h_i = f\left(q_i\right) = f\left(\sum_{n=1}^{N} X_n w_{ni} - \beta_i\right) \tag{8}$$

The output vector of neuron nodes in the output layer can then be found as

$$\hat{Y}_j = f\left(u_j\right) = f\left(\sum_{i=1}^{I} h_i v_{ij} - \lambda_j\right) \tag{9}$$

When a BP neural network is trained, an error value, which is calculated when there is a deviation (greater than the maximum allowable error for training) between the output vector of the neuron nodes in the output layer obtained after the sample has passed through the input layer, and the sample vector, is given by

$$Loss = \frac{1}{2}\sum_{j=1}^{J}(Y_j - \hat{Y}_j)^2 \tag{10}$$

After obtaining the error value, the error gradient descent method is used to calculate the weight and bias change using the bias derivative. First, the bias change of the output layer nodes is calculated , which is given by

$$\begin{aligned} \Delta\lambda_j &= -\eta\frac{\partial Loss}{\partial\lambda_j} \\ \Delta\lambda_j &= -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial\lambda_j} = -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial u_j}\frac{\partial u_j}{\partial\lambda_j} \end{aligned} \tag{11}$$

So

$$\frac{\partial Loss}{\partial\hat{Y}_j} = -\left(Y_j - \hat{Y}_j\right) \tag{12}$$

$$\frac{\partial\hat{Y}_j}{\partial u_j} = \hat{Y}_j\left(1-\hat{Y}_j\right) \tag{13}$$

$$\frac{\partial u_j}{\partial\lambda_j} = -1 \tag{14}$$

Combining equations (11) (12) (13) (14) to solve for

$$\Delta\lambda_j = -\eta\left(Y_j - \hat{Y}_j\right)\hat{Y}_j\left(1-\hat{Y}_j\right) \tag{15}$$

Then the same error gradient descent method is used to calculate the amount of connection weight change between the neuron nodes in the output layer and the neuron nodes in the hidden layer, which is calculated as

$$\Delta v_{ij} = -\eta\frac{\partial Loss}{\partial v_{ij}} = -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial u_j}\frac{\partial u_j}{\partial v_{ij}} \tag{16}$$

From equation (9), it can see that

$$\frac{\partial u_j}{\partial v_{ij}} = h_i \tag{17}$$

Solving for equations (12) (13) (16) (17) together gives

$$\Delta v_{ij} = \eta\left(Y_j - \hat{Y}_j\right)\hat{Y}_j\left(1-\hat{Y}_j\right)h_i \tag{18}$$

Continuing with the error gradient descent method to calculate the bias change of the hidden layer neuron nodes, which is calculated as

$$\Delta\beta_{ij} = -\eta\frac{\partial Loss}{\partial\beta_i} = -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial h_i}\frac{\partial h_i}{\partial\beta_i} = -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial u_j}\frac{\partial u_j}{\partial h_i}\cdot\frac{\partial h_i}{\partial q_i}\frac{\partial q_i}{\partial\beta_i} \tag{19}$$

From equation (9), it follows that

$$\frac{\partial u_j}{\partial h_i} = v_{ij} \tag{20}$$

From equation (7) (8), it is clear that

$$\frac{\partial h_i}{\partial q_i} = h_i\left(1-h_i\right) \tag{21}$$

$$\frac{\partial q_i}{\partial\beta_i} = -1 \tag{22}$$

Combining equations (12) (13) (19) (20) (21) (22) to solve for

$$\Delta\beta_{ij} = -\eta\left(Y_j-\hat{Y}_j\right)\hat{Y}_j\left(1-\hat{Y}_j\right)v_{ij}\cdot h_i\left(1-h_i\right) \tag{23}$$

The error gradient descent method is then used to calculate the change in the connection weights between the neuron nodes in the hidden layer and the neuron nodes in the input layer, which is calculated as

$$\Delta w_{nij} = -\eta\frac{\partial Loss}{\partial w_{ni}} = -\eta\frac{\partial Loss}{\partial\hat{Y}_j}\frac{\partial\hat{Y}_j}{\partial u_j}\frac{\partial u_j}{\partial h_i}\cdot\frac{\partial h_i}{\partial q_i}\frac{\partial q_i}{\partial w_{ni}} \tag{24}$$

From equation (7), it follows that

$$\frac{\partial q_i}{\partial w_{ni}} = X_n \tag{25}$$

Combining equations (12) (13) (20) (21) (24) (25) to solve for

$$\Delta w_{nij} = -\eta\left(Y_j-\hat{Y}_j\right)\hat{Y}_j\left(1-\hat{Y}_j\right)v_{ij}\cdot h_i\left(1-h_i\right)X_n \tag{26}$$

Then, is summed for the number of neuron nodes in the output layer to find the final change, which is given by

$$\Delta\beta_i = \sum_{j=1}^{J}\Delta\beta_{ij} \tag{27}$$

$$\Delta w_{ni} = \sum_{j=1}^{J}\Delta w_{nij} \tag{28}$$

After the samples are input to the BP neural network, the weights w_{ni}, v_{ij} and the bias β_i、λ_j of each layer node are known (the initial assignment is a random fraction between), and the input q_i、u_j and output h_i、$\hat{Y}_j$ of each layer node can be calculated. If the error is generated, then through the above series of error gradient descent calculation, we can find the connection weights change Δw_{ni}、Δv_{ij} and change $\Delta\beta_i$、$\Delta\lambda_j$, the above changes will be applied to the BP neural network to reduce the error of the next output, so the cycle is the training process, until the error is less than required.

3.3.4 BP neural network adds momentum term

When adjusting the weights, the standard BP neural network algorithm only adjusts the gradient of the error in the descending direction at time t, but does not consider the gradient direction before the time, which often makes the training process oscillate and converge slowly. In order to improve the training speed of the network, a momentum term can be added to the weight adjustment formula. If W is used to represent the weight matrix of a layer and X represents the input vector of a layer, the expression of the weight adjustment vector with the momentum term is [9]

$$\Delta W\left(t\right)=\eta\delta X+\alpha\Delta W\left(t-1\right) \tag{29}$$

3.3.5 Number of hidden layer nodes of BP neural network

The role of the hidden nodes is to extract and store the intrinsic laws from the samples. If the number of hidden nodes is too small, the network will not be able to obtain information from the samples and will not be able to generalize and reflect the patterns of the samples in the training set; if the number of hidden nodes is too large, the network may learn to remember the non-regular content of the samples such as noise, which will lead to the so-called "overfitting" problem, but will reduce the generalization ability and increase the The training time is also increased.

At present, scholars at home and abroad have proposed a large number of methods to determine the number of nodes in the hidden layer of the BP neural network, and in this paper, we use the simplified formula of fitting by least squares method obtained by Daqi Gao [10].

$$N_{hid}=\sqrt{N_{in}\left(N_{out}+2\right)}+1 \tag{30}$$

3.4. Model solving

The information was converted according to Spearman's correlation coefficient strength rank principle, and the converted type-surface weathering, ornament-surface weathering, and color-surface weathering ranks were obtained by converting and classifying the information according to the 1-Spearman correlation coefficient rank table. After obtaining the rank correspondence table of each information, the significance p-value table of surface weathering was obtained by significance p-value calculation.

It can be concluded that: surface weathering and ornamentation, significant P-value is 0.384, accepting the original hypothesis, so there is no significant difference; surface weathering and type, significant P-value is 0.008, rejecting the original hypothesis, there is a significant difference; surface weathering and color, significant P-value is 0.421, accepting the original hypothesis, there is no significant difference.

Then the Spearman correlation coefficient between surface weathering and each factor was obtained by importing the rank correspondence table of each information into the Spearman correlation coefficient relationship analysis model.

The following correlation coefficient heat map was obtained as Figure 1.

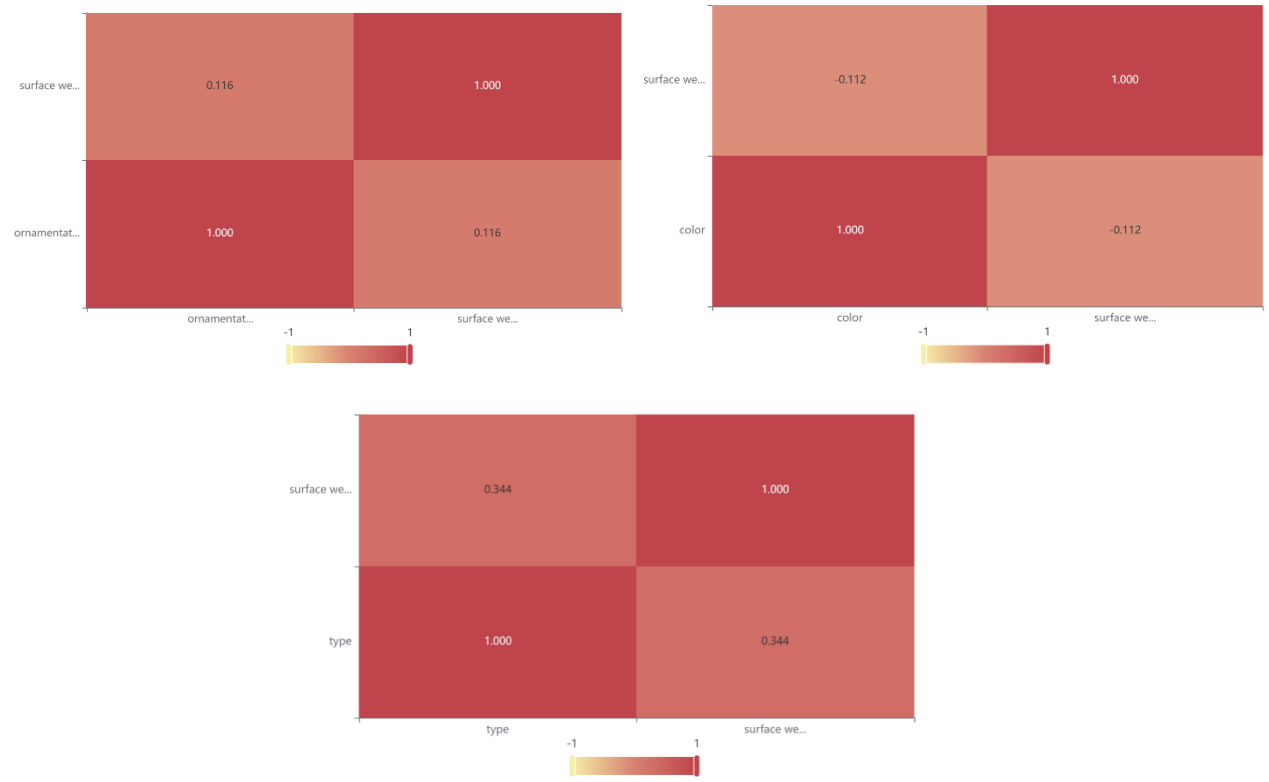

Figure 1. Surface weathering Spearman correlation coefficient thermogram (top left: ornamentation; top right: color; bottom: type)

There is a significant relationship between surface weathering and glass type (correlation exists) with a Spearman correlation coefficient of 0.344 (positive correlation). There is no significant relationship between surface weathering and glass ornamentation and color.

The Spearman correlation coefficients between surface weathering and each chemical element for each type of glass were calculated by Spearman correlation coefficients, and the corresponding coefficients were obtained to know the statistical patterns of chemical composition content before and after weathering for each type of glass. The surface weathering of high potassium glass is positively correlated with the content of silica (0.818) and the content of potassium oxide (-0.706), calcium oxide (-0.545), magnesium oxide (-0.602), aluminum oxide (-0.795), iron oxide (-0.545), lead oxide (-0.543), phosphorus pentoxide (-0.602), and strontium oxide (-0.487). negatively correlated. The surface weathering of lead-barium glass was positively correlated with the content of calcium oxide (0.445), lead oxide (0.729), phosphorus pentoxide (0.555), strontium oxide (0.312) and negatively correlated with the content of silica (-0.807), sodium oxide (-0.366), and aluminum oxide (-0.327).

The following correlation coefficient heat Figure 2 was obtained.

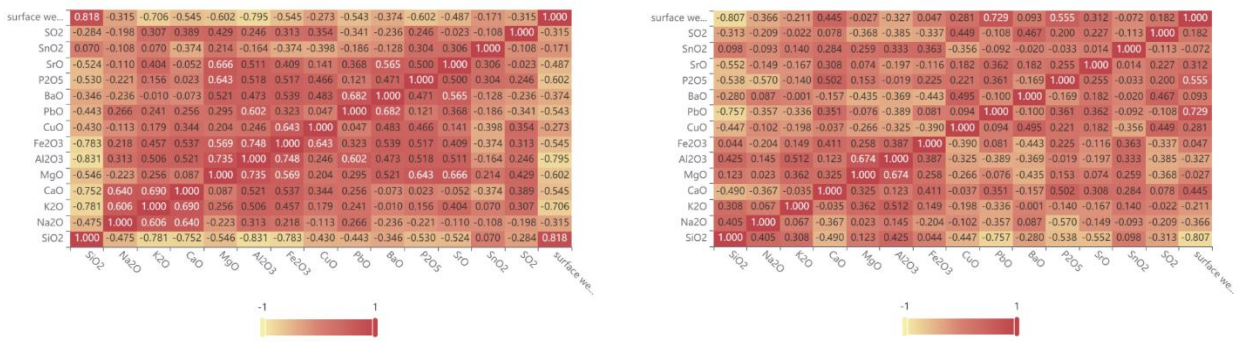

Figure 2. Spearman's correlation coefficient thermogram between surface weathering of high potassium glass and lead-barium glass and each chemical element

According to the statistical law of chemical content summarized in the previous analysis, the existing data of each type of glass were filtered and classified.

A BP neural network prediction model was constructed using Matlab, and the classified samples were injected into the BP neural network for training (post-weathering data were used as input layer samples and pre-weathering data were used as output layer samples), and a BP neural network model meeting the minimum allowable error was obtained after about 1000 cycles of training.

The trained BP neural network model was then used to predict the chemical composition content before weathering by importing the weathered chemical element content data of high potassium and lead-barium glass surfaces, respectively, and the difference between the obtained prediction results and the actual samples was calculated and solved.

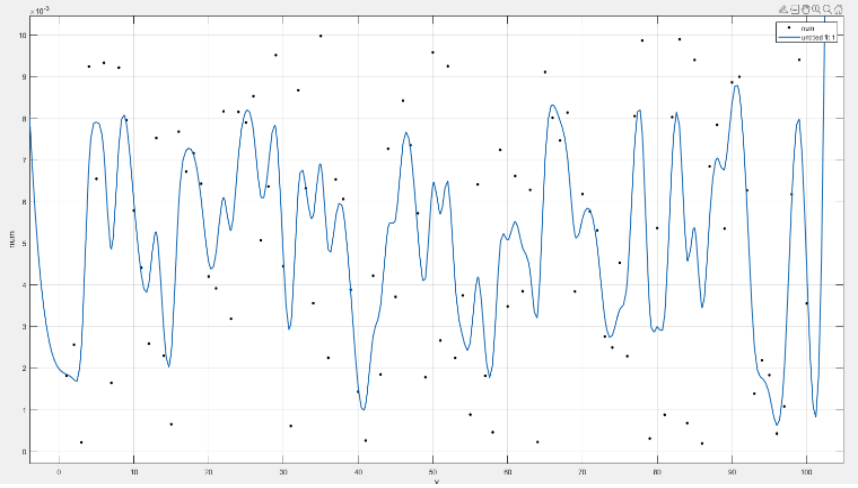

Figure 3. Prediction overall error curve of BP neural network

It can be seen that this BP neural network prediction model, in predicting more than 100 samples is, its overall error of prediction does not exceed 0.1, which meets the prediction requirements.

4. Conclusion

In summary, it is feasible to screen and classify the samples by using the statistical pattern of the chemical composition content with and without weathering on the surface of the artifact samples, and to predict the chemical composition of each type of glass before weathering using the BP neural network model.

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