Study on the composition of glass artifacts based on PSO particle swarm neural network

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Abstract. The analysis of the composition of glass artifacts has always been the focus of research in related fields. By analyzing and identifying the different compositions of glass artifacts from different eras and fields can support the understanding of the history of glass artifacts, their achievements and thus their exit from human civilization. In this paper, we use multiple correlation analysis, kernel principal component analysis, BP neural network model optimized by PSO particle swarm algorithm to study the composition of ancient glass artifacts.To address the shortcomings of the conventional BP neural network model, this paper adopts the BP neural network model under the optimization of PSO particle swarm algorithm to identify and study the unknown artifact types. And different subjective assignments are made to glass artifacts with different weathering degrees to discover the level of model sensitivity.Then the S-W normal distribution test was used and it was found that most of the chemical components did not obey normal distribution. Therefore, nuclear principal component analysis was chosen to find out the correlation between different types of components. On the basis of the identified two correlation coefficients and the paired data were normally distributed, by paired sample t-test, it was found that the magnitude of the differences between the chemical components of different categories was large. This was supplemented by correlation analysis and kernel principal component analysis. Finally, the composition identification study of glass artifacts was realized, which provided a new methodological path for the composition study of glass artifacts.

Keywords: Correlation Analysis, Particle Swarm Neural Network, T-test.

1. Introduction

As one of the main categories of ancient artifacts, glass played an important role in the trade exchanges along the Silk Road and was the focus of research by scientific and technological archaeologists. The identification of the chemical composition of glass provides a sufficient scientific basis for determining its origin and classification [1].

The article uses the existing data of a batch of ancient glass relics in China, and then classifies them into two types of high potassium glass and lead-barium glass, and obtains the data of their chemical composition and weathering conditions. A BP neural network model under the optimization of PSO particle swarm algorithm is provided and combined with the type to which each cultural relic belongs, the model parameters such as the test set percentage are adjusted, and the sensitivity of the model is evaluated according to the magnitude of the effect of parameter changes on the identification results. And then evaluating the sensitivity of the classification results.

On this basis, the correlations between the chemical components of each category of glass artifact samples were analyzed by S-W normal distribution test, sample t-test, correlation analysis and kernel principal component analysis, etc. When analyzing the correlations between the chemical components of the same glass artifacts, the data should be checked for normality to select a suitable correlation analysis model. When comparing the correlations between different categories, the data should be checked for normality again to select the most suitable model for the analysis of the differences. And explore the difference of the correlation between different categories of artifacts, so as to achieve the composition of glass artifacts research identification.

2. Materials and methods

2.1. PSO particle swarm algorithm

BP neural networkBP neural network is a multilayer feedforward neural network trained according to the error backpropagation algorithm, and we selected it as the main model for classification operations because of its relatively simple structure, many adjustable parameters, richer available algorithms, and high operability [2].

However, due to the small sample size, BP neural networks also have some inherent defects: slow learning convergence, no guarantee of convergence to the global minimum, and network structure not easily determined [3]. In addition, the structure of the network, the selection of initial connection weights and thresholds have a great impact on the training of the algorithm, which requires several tests to obtain relatively optimal results and a more tedious processing [4].

Therefore, the article optimizes the BP neural network using the PSO particle swarm algorithm, a classical intelligent optimization algorithm inspired by the predatory behavior of birds, which is widely used in various optimization problems due to its simple and efficient principle [5]. By improving the weights and thresholds of the initial connections of the BP neural network, its learning convergence speed is accelerated, thus improving the accuracy of the training set under small data samples and also avoiding the processing results to fall into local extremes to some extent.

2.2. Kernel principal component analysis method

The main principle of the kernel principal component analysis method is to project the data in the original space to the high-dimensional feature space through a nonlinear mapping, which transforms the nonlinear data into linear data and performs the data processing based on principal component analysis in the high-dimensional feature space. Based on the fact that the data samples are nonlinear, we choose kernel principal component analysis [6] in order to explore the correlations between chemical components in the same class of glass artifact samples.

3. Model construction and testing

3.1. PSO particle swarm algorithm model construction and testing

By dividing the pre-processed data into training and test sets, the weathered glass artifacts are assigned a value (1 for weathered and 0 for unweathered) and the class of glass artifacts is assigned a value (1 for high potassium glass and 2 for lead-barium glass). The test set was set to 20%, and the machine learning was performed using a PSO-optimized BP neural network with 30 iterations and 1000 training sessions.

Due to the small sample size of the data, we also set the cross-validation of the data for the training set with a cross-validation fold of 10, which can effectively improve the prediction performance of the model and prevent overfitting. The results of training and testing are as shown in Figure 1, Figure2, Figure3 and Figure4.

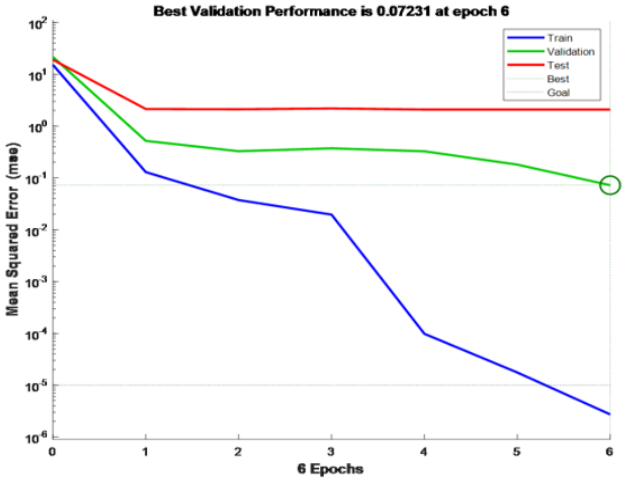

Figure 1. Model cross-validation diagram.

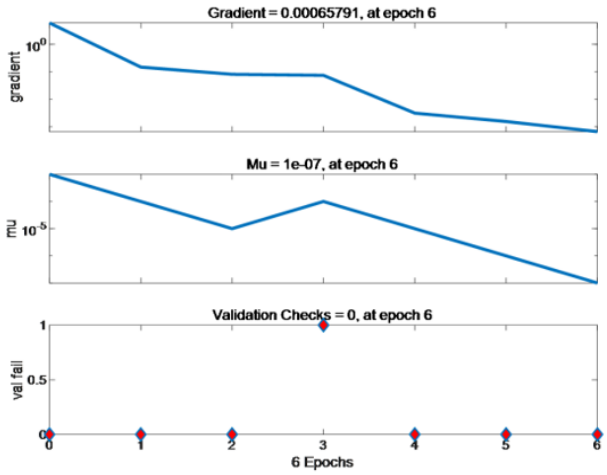

Figure 2. Model training graph.

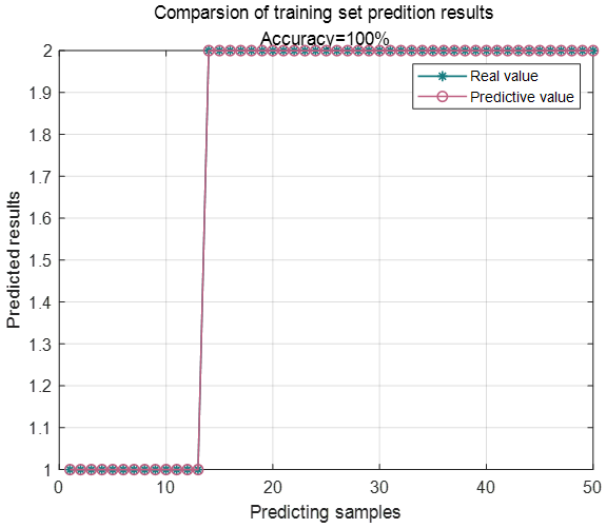

Figure 3. Comparis of results in training set.

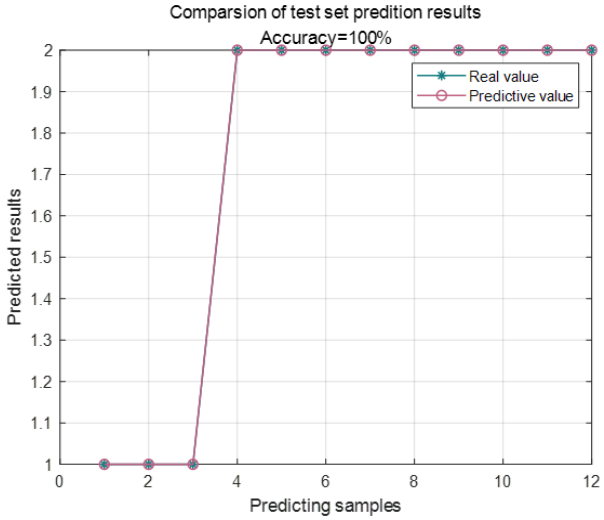

Figure 4. Comparis of results in the test set.

3.2. Kernel Principal Component Analysis Model Construction and Testing

The article adopts a nonlinear mapping function to map the set X of samples after centering in the original space to a high-dimensional space, thus realizing the mapping of linearly indivisible vectors in the original space to linearly divisible ones. It can be assumed that.

The original space is an s-dimensional space, and a higher dimensional space is constructed first, with dimension S >> s.

2. The number of samples contained in the original space is t.

The specific implementation process of the model is as follows.

The s-dimensional space is mapped to the S-dimensional space with the feature vector $\omega_i\left(i=1,\ldots,s\right)$, corresponding to the feature values $\lambda_i\left(i=1,\ldots,s\right)$. The set of samples $\Phi\left(X\right)$.

PCA in high-dimensional space Eq.

$$\Phi\left(X\right)\Phi\left(X\right)^T\omega_i=\lambda_i\omega_i\left(*\right) \tag{1}$$

Linear representation of $\omega_i\left(i=1,\ldots,s\right)$ using $\Phi\left(X\right)$.

$$\omega_i=\sum_{a=1}^{t}\alpha_i\Phi\left(X_i\right)=\Phi\left(X\right)\alpha\left(**\right) \tag{2}$$

Combining equations (*) and (**) and substituting into $\omega_i\left(i=1,\ldots,s\right)$, we get

$$\Phi(X)\Phi(X)^T \Phi(X)\alpha = \lambda_i \Phi(X)\alpha \tag{3}$$

Constant deformation.

$$\Phi(X)^T \Phi(X)\Phi(X)^T \Phi(X)\alpha = \lambda_i \Phi(X)^T \Phi(X)\alpha \tag{4}$$

The Gaussian radial basis function (RBF) kernel function is selected.

$$K(x, x_i) = e^{-\frac{\|x-x_i\|}{\sigma^2}} \tag{5}$$

The equation with and principal component analysis (KPCA) was obtained.

$$K\alpha = \lambda_i \alpha \tag{6}$$

Since K is a symmetric matrix, the resulting solution vectors are orthogonal to each other, yielding the correlation matrix as shown in Table 1.

Table 1. Kernel principal component correlation data classification association matrix.

Data 1	Data 2	Data 3	Data 4	Data 5	Data 6	Data 7	Data 8	Data 9	Data 10	Data 11	Data 12	Data 13	Data 14
1	-0.4637	-0.5496	-0.6968	-0.1874	-0.6717	-0.6371	-0.4906	-0.2148	-0.2256	-0.2257	-0.1633	0.4948	-0.1173
0.0243	1	0.6973	0.5896	-0.5772	0.1435	-0.2105	-0.0104	0.5810	-0.3136	-0.4326	-0.4230	-0.2130	-0.4144
0.1677	-0.0994	1	0.7261	-0.2232	-0.0372	-0.1524	0.1169	0.1187	-0.4687	-0.5379	-0.2953	-0.0592	0.1070
-0.1970	-0.2448	0.4190	1	-0.2937	0.1161	0.1961	0.3708	0.1922	-0.4717	-0.4574	-0.4854	-0.5469	0.3387
0.1178	0.0238	0.2323	0.5300	1	0.4859	0.4094	-0.0648	-0.1668	0.5253	0.5541	0.6909	0.2140	0.3306
0.2873	-0.0322	0.2073	0.3363	0.4494	1	0.5573	0.0880	0.4073	0.7132	0.5759	0.5162	-0.4659	-0.1526
-0.0190	-0.3246	0.2081	0.4977	0.3020	0.2275	1	0.4945	-0.1590	0.5667	0.7278	0.5181	-0.3594	0.1273
-0.3829	0.0153	0.0187	-0.1976	-0.2714	-0.2084	-0.2059	1	-0.3969	0.0740	0.2203	-0.0951	-0.4358	0.4279
-0.5870	-0.0643	-0.3098	0.0686	-0.1549	-0.4501	-0.0401	-0.3116	1	0.0098	-0.1410	-0.1553	-0.1789	-0.3480
-0.4652	0.0398	-0.1862	-0.4281	-0.4105	-0.2990	-0.2825	0.7751	-0.1992	1	0.9246	0.7959	-0.1636	-0.3183
-0.1235	-0.2436	-0.0047	0.5029	0.2719	0.1236	0.3362	-0.0230	-0.1308	-0.1434	1	0.8105	-0.0289	-0.2280
-0.5391	0.0605	-0.1656	0.1114	0.0655	-0.1340	-0.0501	0.1631	0.3786	0.1856	-0.0707	1	0.2261	-0.2357
0.1125	-0.1069	0.1711	0.2449	0.2302	0.4507	0.2370	-0.1624	-0.1976	-0.1076	-0.0693	-0.0565	1	-0.2162
-0.0645	-0.1349	-0.0214	-0.1733	-0.2639	-0.1721	-0.1837	0.5264	-0.2622	0.4295	-0.1107	0.0306	-0.0761	1

The article takes the automatically generated correlation matrix of high potassium glass compounds as an example. A positive correlation indicates that the two compounds are positively correlated and vice versa; the larger the absolute value, the stronger the correlation.

4. Results and Analysis

4.1. PSO particle swarm algorithm model results analysis

The prediction results of the training and test sets before optimization are compared with those after optimization, and the results show that the BP neural network model with PSO optimization has a significant advantage in prediction accuracy compared with the neural network model without optimization; the convergence speed of machine learning is also improved.

To accommodate the type of input values to the algorithm, we assigned subjective values to certain variables, weathered glass artifacts (1 for weathered and 0 for unweathered), and categories of glass artifacts (1 for high potassium glass and 2 for lead-barium glass). Considering that the manual subjective assignment may affect the classification of unknown categories of glass artifacts in the previous analysis, we re-assigned values to the above variables and repeated the experiment to conduct sensitivity analysis of the table2.

Table 2. Experimental table of sensitivity of assignment of glass differentiation categories.

	Experiment 1	Experiment 2	Experiment 3	Experiment 4	Experiment 5	Experiment 6
Weathering Assignment	1, 0	1, 0	2, 1	2, 1	0, 1	0, 1
Category assignment	2, 1	1, 2	2, 1	1, 2	2, 1	1, 2
Classification 1	2	1	2	1	2	1
Classification 2	1	2	1	2	1	2
Classification 3	1	2	1	2	1	2
Category 4	1	2	1	2	1	2
Category 5	1	2	1	2	1	2
Classification 6	2	1	2	1	2	1
Classification 7	2	1	2	1	2	1
Category 8	1	2	1	2	1	2

From the above table, it can be concluded that the sensitivity of the model and the results of the classification is low, i.e., the model has a strong stability.

We also changed the number of populations in the PSO particle swarm optimization algorithm several times in the range of [21, 30], and the final classification results were exactly the same 10 times.

4.2. Analysis of nuclear principal component analysis model results

The correlation patterns of six compounds, magnesium oxide, aluminum oxide, iron oxide, barium oxide, phosphorus pentoxide and strontium oxide, in the high potassium and lead-barium samples were analyzed by the kernel principal component analysis model as follows.

In the high potassium samples, all six compounds showed positive correlations with each other, with strong positive correlations among barium oxide, phosphorus pentoxide, and strontium oxide; in addition, three compounds, sodium oxide, potassium oxide, and calcium oxide, also showed significant positive correlations with each other. Silicon dioxide showed negative correlations with all compounds except for some positive correlations with tin oxide, and significant negative correlations with potassium oxide, calcium oxide, aluminum oxide, and iron oxide

In the lead and barium samples, all five compounds, potassium oxide, calcium oxide, magnesium oxide, aluminum oxide and iron oxide, showed positive correlation with each other. Copper oxide showed a significant positive correlation with barium oxide and sulfur dioxide. Silicon dioxide showed a significant negative correlation with lead oxide and strontium oxide

We analyzed the variability of the principal components of the chemical composition association between the two glass types using kernel principal component analysis, and found that the difference in contribution between the principal components and non-principal components was larger for high potassium glass and relatively small for lead-barium glass as shown in Figure5 and Figure6.

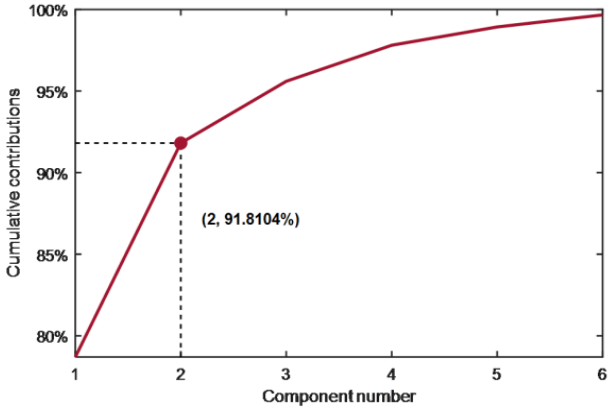

Figure 5. Contribute graph high potassium glass.

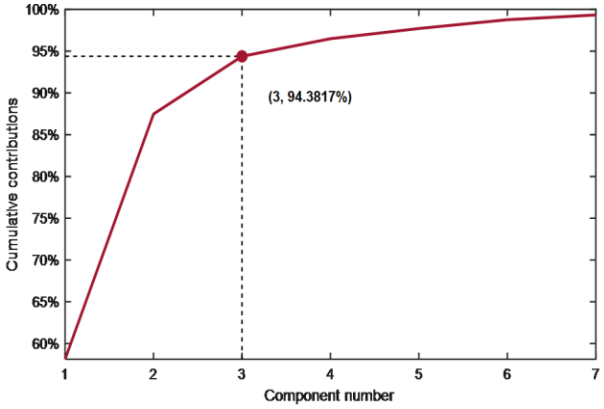

Figure 6. Contribute graph lead-barium glass.

From the images, it can be concluded that the cumulative principal component contribution of high potassium glass reaches more than 90% in the second principal component, while lead-barium glass reaches more than 90% in the third principal component. Compared with the high potassium glass, the contribution of each component of lead-barium glass is more average.

5. Conclusion and Discussion

5.1. Model Advantages

The cross-validated PSO-optimized PB neural network classification model with completely independent training and testing sets is used to build a more reasonable model on the one hand, and to improve the convergence speed and accuracy of classification for small sample data on the other hand.

Kernel principal component analysis was used to screen the variables for nonlinearity and the construction of the correlation matrix with good robustness to non-normally distributed data in the topic.

5.2. Deficiencies of the model and improvements

Since the particle swarm optimization neural network algorithm needs to use cross-checking to improve the convergence speed when dealing with small sample data, and the excessive cross-checking folds and number of iterations will cause it to run very slowly and the efficiency is not outstanding. Therefore, the model accuracy can be improved by increasing the number of training samples and the number of iterations.

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