

Research on Glass Classification Based on K-means Clustering and Decision Tree

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Abstract: Ancient glass is very vulnerable to weather due to the influence of the burial environment, and its chemical composition proportion changes, which makes it impossible to correctly judge its category. In this paper, mathematical models are established based on decision tree and k-means clustering, respectively, to analyze the classification rules of high potassium glass and lead barium glass, and to find out the classification method for sub classification of the two types of glass. Finally, the mode of distinguishing the types of class cultural relics is established, which has guided significance for the identification of class cultural relics.

Keywords: Decision tree; K-means cluster analysis; A model for distinguishing the types of glass relics

1. Introduction

The appearance of ancient Chinese glass is similar to that of foreign glass products, but the chemical composition is different. Quartz sand is the main raw material of glass, and silicon dioxide (SiO₂) is the principal component of glass [1]. The stabilizer often added in ancient time was limestone, the common cosolvent was plant ash, natural soda, saltpeter and lead ore lamp, and calcium oxide (CaO) was the product of calcination of limestone. The main chemical components of glass are unique with different cosolvents added in glass production [2,3]. Due to the influence of the burial environment, ancient glass is very easy to be weathered. The classification of glass often needs to be evaluated according to its composition proportion. However, during weathering, the composition proportion of glass changes owing to a large amount of exchange between elements inside the glass and buried environmental elements, which will affect the correct judgment of glass classification.

In order to solve the above problems, this paper takes the 2022 Chinese College Students Mathematical Modeling Contest as the platform [4], based on K-means clustering and decision tree, establishes a glass cultural relic type determination model. The model has ideal stability and sensitivity, and provides guidance for the identification of chemical components of glass relics.

2. Prediction model of chemical composition content of glass relics before weathering

2.1. Relationship between surface weathering, glass type, decoration and color of glass relics

The exploration of the relationship between surface weathering, glass type, decoration and color of glass relics can be divided into correlation analysis and difference analysis. Since the four variables are categorical variables, Spearman correlation coefficient analysis and chi square test (Figure 1, 2) are adopted.

Spearman correlation coefficient [5]:

Where di represents the rank difference of each pair of observations (x,y), and n represents the number of observation pairs.

The Spearman correlation coefficient table is obtained by pairing the four variables in pairs for data analysis (Table 1):

Table 1 Spearman Correlation Coefficient

	Surface weathering	Ornamentation	Type	Colour
Surface weathering	1.000(0.000***)	0.095(0.504)	0.272(0.051*)	-0.121(0.393)
Ornamentation	0.095(0.504)	1.000(0.000***)	-0.448(0.001***)	-0.492(0.000***)
Type	0.272(0.051*)	-0.448(0.001***)	1.000(0.000***)	0.554(0.000***)
Colour	-0.121(0.393)	-0.492(0.000***)	0.554(0.000***)	1.000(0.000***)

***, **, * represent the significance level of 1%, 5% and 10% respectively

It can be seen from Table 1 that the Spearman correlation coefficient of surface weathering and type is 0.272, and the P value is 0.051 and less than 0.01, indicating that the glass type has a significant positive correlation with surface weathering. This is also the only variable that has a significant positive correlation with whether the glass surface is weathered.

Chi square statistics are defined as [6]:

χ^2 follows the chi square distribution of k-1 degrees of freedom. The greater the χ^2 value, the greater the difference between the observation frequency distribution and the expected distribution.

Color surface weathering chi square test

Set the color as variable X and the surface weathering as variable Y. The zero assumption is that there is no significant difference in color and surface weathering data. The P value of the chi square test result is $0.428 > 0.05$, so the original hypothesis is accepted, and there is no significant difference for the color and surface weathering data. Draw chi square to cross thermal diagram to show the values of crossing contingency table:

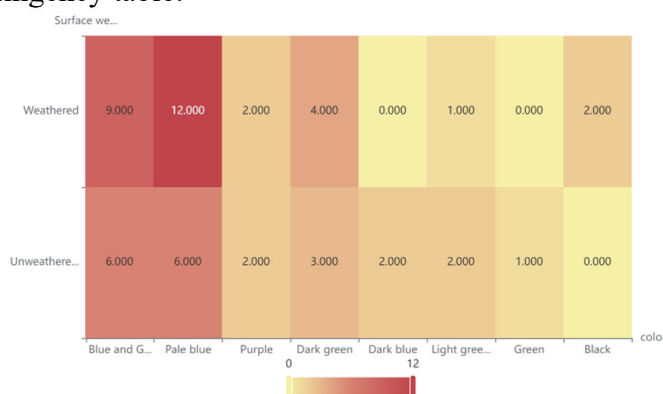


Figure 1 Color surface weathering thermal diagram

Since there is no significant difference between color and surface weathering, it does not conform to the premise of quantitative analysis of effects, so quantitative analysis of effects will not be conducted.

(2) Type color surface weathering chi square test

Set the type as variable X, and color and surface weathering as variable Y. Based on the type and color. The P value is $0.001*** < 0.05$, and the null hypothesis is rejected. There is an important difference between the type and color data. Based on the type and surface weathering, the P value is $0.049** < 0.05$, and the null hypothesis is rejected. There is a noteworthy difference between the type and surface weathering data.

Display the values of cross contingency table in the form of chi square cross thermodynamic diagram (Figures 3, 4):

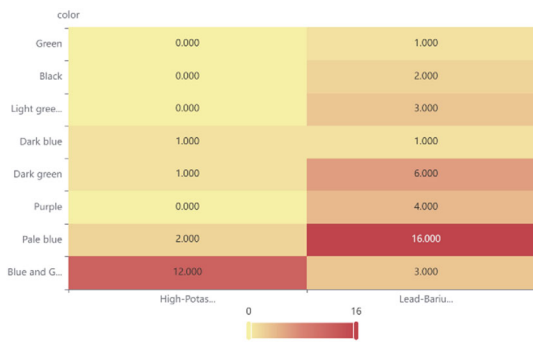


Figure 3 Type - Color Thermodynamic Diagram

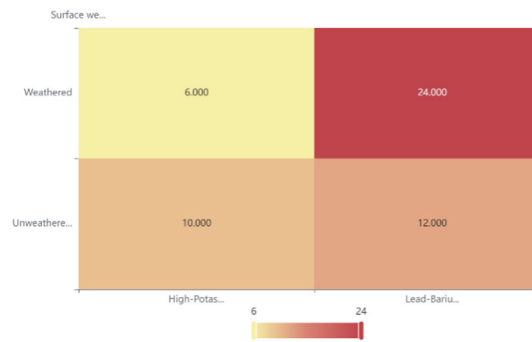


Figure 4 Type - Thermal Map of Surface Weathering

Then, quantitative analysis of effects is carried out to reflect the correlation between variables (Table 2):

Table 2 Quantitative Analysis of Type Color Surface Weathering Effect

Field name/Analysis item	Phi	Cramer's V	Contingency coefficient	Lambda
Surface weathering	0.272	0.272	0.263	0.182
color	0.707	0.707	0.577	0.294

The results of quantitative analysis of effects show that [7], the color Cramer's V value is 0.707, so the difference between color and type is strong. The surface weathering Cramer's V value is 0.272, so the difference between surface weathering and type is moderate (Table 2).

(3) Texture type color surface weathering chi square test

Set texture as variable X, surface weathering, color and type as variable Y. Based on the ornamentation and surface weathering, the P value is $0.057^* > 0.05$, so the null hypothesis is accepted, and there is no significant difference between the ornamentation and surface weathering data. Based on the patterns and colors, the P value is $0.000^{***} < 0.05$, so the original assumption is rejected, and there is a significant difference between the patterns and color data. Based on the patterns and types, significant P value is $0.000^{***} < 0.05$, so the original hypothesis is rejected, and there is a significant difference between the patterns and types.

Display the values of cross contingency table in the form of chi square cross thermodynamic diagram (Figure 5-7):

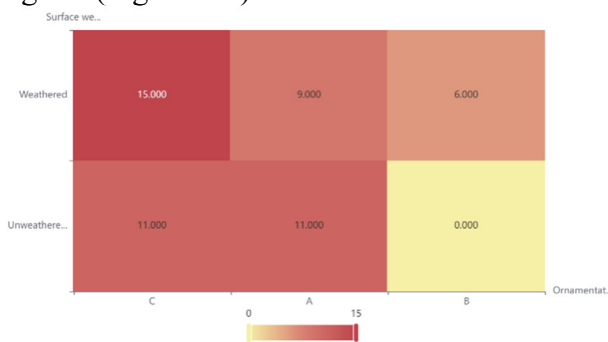


Figure 5 Texture - Thermal Diagram of Surface Weathering

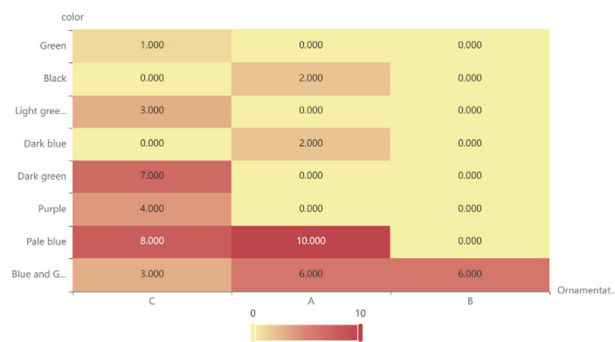


Figure 6 Pattern Color Thermodynamic Diagram

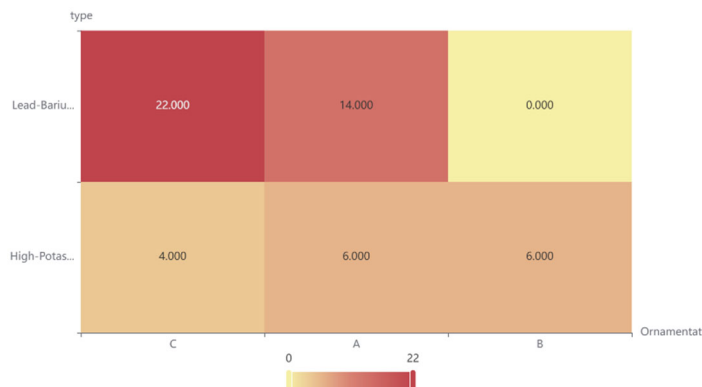


Figure 7 Pattern Type Thermodynamic Diagram

Quantitative analysis of effects on variables (Table 3):

Table 3 Quantitative Analysis of Texture Type Color Surface Weathering Effect

Field name/Analysis item	Phi	Cramer's V	Contingency coefficient	Lambda
Surface weathering	0.332	0.332	0.315	0.091
color	0.857	0.606	0.651	0.176
type	0.561	0.561	0.49	0.375

The results of quantitative analysis of effects show that the Cramer's V value of surface weathering is 0.332, so the difference between surface weathering and ornamentation is moderate. Color Cramer's V value is 0.606, so the difference between color and decoration is strong. Type Cramer's V value is 0.561, so the difference between type and decoration is strong.

2.2. Statistical law of chemical composition content of cultural relics combined with glass type

As the chemical composition of lead barium glass and high potassium glass is very different, scatter plots can be made for two different types, and their trend lines are shown in Figures 8, 9.

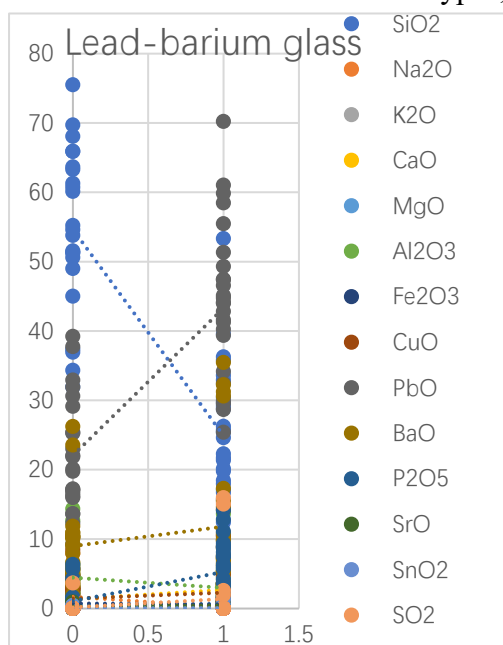


Figure 8 Fitting of weathering and chemical composition content of lead barium glass

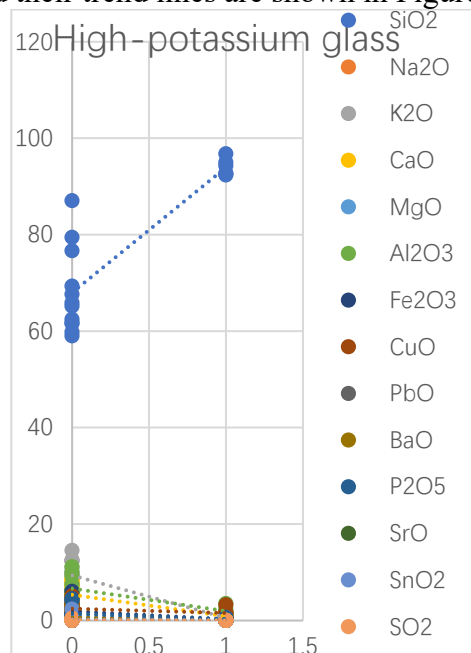


Figure 9 Fitting of weathering and chemical composition content of high potassium glass

Obviously, for lead barium glass, the content of silicon dioxide decreased significantly after weathering, and the content of lead oxide increased significantly; For high potassium glass, the content of silicon dioxide increases significantly after weathering, and the content of other components decreases (Figure 8,9).

Because the scatter fitting trend line is only used to intuitively determine the change direction and change intensity of variables, and the independent variable has only one logical variable, which has serious collinearity, linear regression is adopted, and the glass type, texture, color and whether there is surface weathering are used as independent variables, and the chemical composition content is used as dependent variables to analyze and build a model. The author carried out linear regression analysis and ridges regression analysis respectively. Because the collinearity of independent variables is not large, and the ridge parameter k determined by the ridge trace analysis method is subjective and artificial to a certain extent, making the error larger, the linear regression analysis was selected.

It can be seen from the scatter diagram that the change trend of chemical composition content is significantly different among different glass types, and the data can be processed separately according to the class type. At this time, the independent variable texture, color and weathering are classified variables, while the linear regression can only determine the quantitative relationship of interdependence between quantitative variables, and the dummy variable transformation requires one variable as the reference term. Therefore, the independent variable is transformed into a calculable value without reference term, and the status of each value of each classified variable is equal. In this way, the status of each classification variable is equal and can be arbitrarily determined without causing change. The statistical analysis software is used to calculate the processed data, and the linear correlation analysis is performed on the content of each chemical component with the texture, color and whether there is surface weathering. The linear correlation equation is as following:

(1) Lead barium glass:

$$\text{SiO}_2: y=18.205 - 0.0A + 12.167B + 6.038C + 1.624D - 2.874E + 9.352F - 17.879G + 16.361H + 1.099J + 5.11K + 5.412L - 4.938M + 23.143N$$

$$\text{Na}_2\text{O}: y=0.499 - 0.0A + 1.089B - 0.59C + 2.07D - 1.837E - 0.158F - 2.319G + 0.602H - 0.158J + 0.217K + 2.082L - 0.232M + 0.731N$$

$$\text{K}_2\text{O}: y=0.093 - 0.0A + 0.162B - 0.069C - 0.044D - 0.227E + 0.092F + 0.43G + 0.049H - 0.07J + 0.019K - 0.156L + 0.073M + 0.02N$$

$$\text{CaO}: y=0.928 - 0.0A - 0.097B + 1.025C - 0.537D + 1.948E - 0.5F + 3.821G - 1.923H - 1.17J + 0.576K - 1.287L + 1.214M - 0.286N$$

$$\text{MgO}: y=0.255 - 0.0A + 0.271B - 0.016C - 0.262D + 0.267E + 0.317F + 0.196G - 0.234H - 0.143J + 0.374K - 0.26L + 0.232M + 0.023N$$

$$\text{Al}_2\text{O}_3: y=1.539 - 0.0A + 2.438B - 0.899C + 0.056D - 0.268E + 0.485F - 0.626G + 0.478H + 0.275J + 1.849K - 0.71L + 0.785M + 0.754N$$

$$\text{Fe}_2\text{O}_3: y=0.373 + 0.0A + 0.178B + 0.195C - 0.692D + 0.348E + 0.033F + 1.756G - 0.595H + 0.393J - 0.102K - 0.769L + 0.249M + 0.124N$$

$$\text{CuO}: y=0.837 + 0.0A + 0.42B + 0.418C - 0.458D - 0.931E - 1.559F - 1.32G - 0.579H + 5.796J + 0.035K - 0.147L + 0.775M + 0.062N$$

$$\text{PbO}: y=16.301 - 0.0A + 3.744B + 12.557C + 5.961D + 4.757E + 2.027F + 20.334G - 1.708H - 11.033J - 1.059K - 2.977L + 18.2M - 1.899N$$

$$\text{BaO}: y=5.362 + 0.0A + 3.762B + 1.601C - 0.543D - 4.128E - 2.892F - 0.334G - 1.406H + 13.638J - 3.095K + 4.122L + 3.833M + 1.53N$$

$$\text{P}_2\text{O}_5: y=1.024 - 0.0A - 0.612B + 1.635C - 1.241D + 6.102E - 0.716F + 1.361G - 3.09H - 1.051J + 1.76K - 2.101L + 2.091M - 1.067N$$

$$\text{SrO}: y=0.142 + 0.0A + 0.068B + 0.074C - 0.228D + 0.131E - 0.0F + 0.194G - 0.013H + 0.22J + 0.035K - 0.196L + 0.131M + 0.011N$$

$$\text{SnO}_2: y=0.045 - 0.0A + 0.099B - 0.054C + 0.053D - 0.166E - 0.014F + 0.321G - 0.036H - 0.014J - 0.012K - 0.087L + 0.09M - 0.045N$$

$$\text{SO}_2: y=0.101 + 0.0A + 0.043B + 0.058C - 0.221D - 0.194E - 0.209F - 0.205G + 0.404H + 0.926J - 0.2K - 0.2L + 0.039M + 0.062N$$

(2) High potassium glass:

$$\text{SiO}_2: y=37.43 + 23.181A + 6.771B + 7.478C + 0.0D + 0.0E + 21.009G + 3.312H + 2.937K + 10.172L + 23.181M + 14.25N$$

$$\text{Na}_2\text{O}: y=0.695 + 0.298A + 0.199B + 0.199C - 0.0D - 0.0E - 1.291G + 2.089H + 1.189K - 1.291L + 0.298M + 0.397N$$

$$\text{K}_2\text{O}: y=3.403 - 0.9A + 0.958B + 3.344C - 0.0D - 0.0E + 0.756G + 1.23H + 2.475K - 1.06L - 0.9M + 4.303N$$

$$\text{CaO}: y=1.596 - 0.633A + 0.274B + 1.955C - 0.0D - 0.0E - 4.099G + 2.45H + 2.705K + 0.54L - 0.633M + 2.229N$$

$$\text{MgO}: y=0.265 - 0.146A + 0.44B - 0.029C + 0.0D - 0.0E + 0.415G + 0.013H - 0.387K + 0.223L - 0.146M + 0.411N$$

$$\text{Al}_2\text{O}_3: y=2.305 - 0.061A + 2.853B - 0.487C - 0.0D - 0.0E - 4.474G + 5.046H + 1.986K - 0.254L - 0.061M + 2.366N$$

$$\text{Fe}_2\text{O}_3: y=0.175 - 0.458A + 0.706B - 0.074C - 0.0D - 0.0E - 1.514G - 0.234H + 0.916K + 1.006L - 0.458M + 0.633N$$

$$\text{CuO}: y=0.371 - 0.342A - 0.201B + 0.913C + 0.0D - 0.0E - 0.882G - 1.526H + 0.904K + 1.874L - 0.342M + 0.712N$$

$$\text{PbO}: y=0.207 + 0.023A + 0.321B - 0.138C - 0.0D - 0.0E - 0.711G + 1.368H - 0.197K - 0.252L + 0.023M + 0.184N$$

$$\text{BaO}: y=0.017 - 0.139A + 0.591B - 0.435C - 0.0D - 0.0E - 0.765G + 0.261H + 0.261K + 0.261L - 0.139M + 0.156N$$

$$\text{P}_2\text{O}_5: y=0.225 - 0.253A + 0.573B - 0.095C + 0.0D - 0.0E + 0.084G - 0.448H + 0.027K + 0.562L - 0.253M + 0.478N$$

$$\text{SrO}: y=0.012 - 0.003A + 0.035B - 0.021C - 0.0D - 0.0E + 0.009G - 0.006H + 0.014K - 0.006L - 0.003M + 0.015N$$

$$\text{SnO}_2: y=0.28 + 0.12A + 0.08B + 0.08C + 0.0D - 0.0E + 1.84G - 0.52H - 0.52K - 0.52L + 0.12M + 0.16N$$

$$\text{SO}_2: y=-0.038 - 0.089A - 0.11B + 0.161C + 0.0D - 0.0E + 0.097G - 0.175H - 0.175K + 0.215L - 0.089M + 0.051N$$

Wherein, A is decoration B, B is decoration A, C is decoration C, D is color green, E is color black, F is color light green, G is color dark blue, H is color dark green, J is color purple, K is color light blue, L is color blue green, M is surface weathering point weathering, N is surface weathering point non weathering.

The above formulas can be uniformly expressed as chemical elements:

$$y=k_0+k_{AA}+k_{BB}+k_{CC}+k_{DD}+k_{EE}+k_{FF}+k_{GG}+k_{HH}+k_{JJ}+k_{KK}+k_{LL}+k_{MM}+k_{NN}$$

If the chemical composition content before (after) weathering is known (before weathering M=0, N=1; after weathering M=1, N=0), $y_{\text{after}} = y_{\text{before}} + kM - kN$ can predict the chemical composition content after (before) weathering.

The above model combines glass types to analyze the statistical laws of chemical composition content with or without weathering, which can be used to analyze and predict the chemical composition content before (after) weathering of a known place. It can also be used to roughly correct the normal chemical composition data of severe weathering points.

3. Classification model of glass chemical composition

3.1. Analysis of classification rules of high potassium glass and lead barium glass based on decision tree model [8,9]

Set all chemical compositions and weathering conditions as variable X and glass type as variable Y, as shown in Table 4:

Table 4 Glass Decision Tree

X	SiO ₂	Na ₂ O	K ₂ O	CaO	MgO	Al ₂ O ₃	Fe ₂ O ₃	CuO	PbO	BaO	P ₂ O ₅	SrO	SnO ₂	SO ₂	Weather or not
Y	Type														

Because there are both continuous variables (content data of each element) and discrete variables (whether or not) in X variables, the algorithm is classified according to the type of variables, and c4.5 algorithm is used to build the decision tree. For discrete data, it is seen as the expansion of ID3, the

information gain rate of the calculator. For continuous variables, the data are processed in discrete form. Take the adjacent average of n data to obtain n-1 partition points. Then calculate the information gain rate of these n points, select the maximum information gain rate point as the division point, and use this point as the benchmark to discretize the continuous data. Finally, set the data [4] into the model and run the Python program. It was found that only lead oxide (PbO) played a crucial role in the decision tree classification. Lead oxide (PbO) is the root node of the decision tree. The decision tree structure is shown in Figure 10:

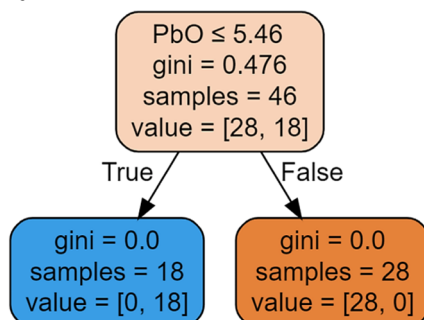


Figure 10 Decision tree structure

When the lead oxide (PbO) content of the glass is less than or equal to 5.46, the glass is judged as high potassium glass; When the lead oxide (PbO) content of the glass is greater than 5.46, the glass is judged as lead barium glass.

3.2. Subclass division method based on K-means clustering algorithm [10]

Using Python and statistical analysis software, K-means cluster analysis is used to iterate the samples for high potassium glass, which requires a total of three iterations. The final results are shown below. The final clustering results in two types of cluster_1 and cluster_2, accounting for 44.44% and 55.56% respectively. As a whole, the distribution of the two groups is relatively uniform, indicating that the clustering effect is good (Table 5).

Table 5 Summary of Cluster Categories of High Potassium Glass

Clustering category	frequency	%
cluster_1	8	44.44%
cluster_2	10	55.56%
Total	18	100%

In order to explore the specific characteristics of each category, each iteration will use ANOVA to study the differences of each category group. In each iteration, chemical components with P value greater than 0.05 in variance analysis will be eliminated, because P value greater than 0.05 indicates that the chemical components do not show significant, and such substances do not play a role in cluster analysis. Table 6 shows the comparison results of cluster category variance difference in the final iteration. Clustering category population shows significance for all studies, indicating that its characteristics in research items have noticeable differences (Figures 11,12).

Table 6 Comparison Results of Variance Analysis of Cluster Categories of High Potassium Glass

	Cluster Category ANOVA Difference Comparison Results (Mean ± SD)		F	p
	cluster 1(n=8)	cluster 2(n=10)		
SiO2	91.29±5.55	64.93±5.32	104.984	0.000
K2O	2.23±3.35	9.74±4.09	17.495	0.001
CaO	0.90±0.68	6.20±2.54	32.426	0.000
MgO	0.34±0.55	1.14±0.63	7.985	0.012
Al2O3	2.34±1.14	7.23±2.24	31.373	0.000
Fe2O3	0.20±0.14	2.32±1.55	14.697	0.001

p<0.05 p<0.01

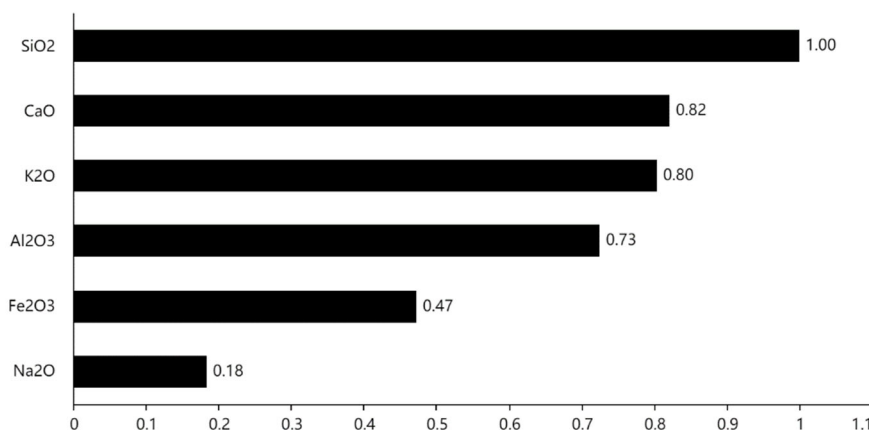


Figure 11 Importance comparison of cluster items of high potassium glass

K-means clustering is used to analyze the lead barium glass samples, and two iterations are made, and two groups of clusters are finally divided_3 and cluster_4. The specific results are as follows (Table 7, 8; Figure 13, 14):

Table 7 Summary of Basic Information of Clustering Categories of Lead Barium Glass

Clustering category	Frequency	%
cluster_3	5	10.20%
cluster_4	44	89.80%
Total	49	100%

Table 8 Comparison Results of Variance Analysis of Clustering Categories of Lead Barium Glass

	Cluster Category ANOVA Difference Comparison Results (Mean ± SD)		F	p
	cluster_3(n=5)	cluster_4(n=44)		
Q2- SiO ₂	16.04±11.90	41.47±17.53	9.899	0.003
Q6- MgO	0.00±0.00	0.72±0.62	6.517	0.014
Q9- CuO	7.24±3.63	1.27±1.37	56.376	0.000
Q11- BaO	31.16±3.32	8.14±4.60	117.183	0.000
Q15- SO ₂	7.10±7.72	0.08±0.55	41.349	0.000

$p < 0.05$ $p < 0.01$

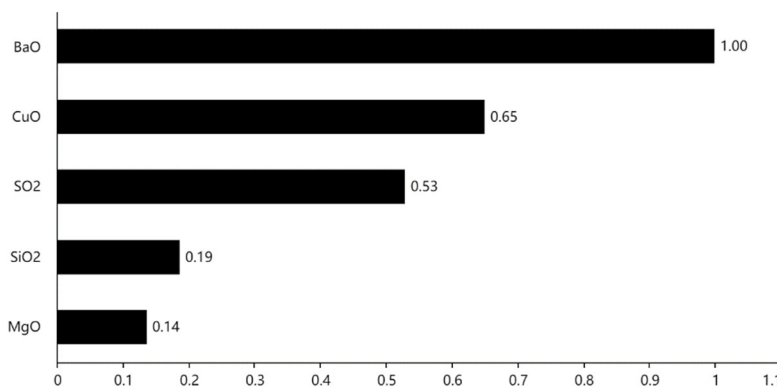


Figure 13 Importance comparison of cluster items of lead barium glass

3.3. Rationality analysis and sensitivity analysis

In this study, the internal evaluation index group internal error square (SSE) is selected for model rationality analysis, which is also called "elbow method". SSE represents the average distance of point pairs in the cluster, which can reflect the cohesion of the cluster. The formula is:

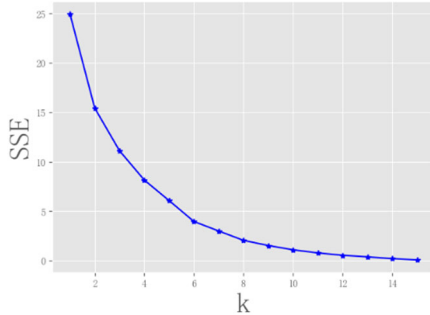


Figure 15 "Elbow Diagram" of High Potassium Glass

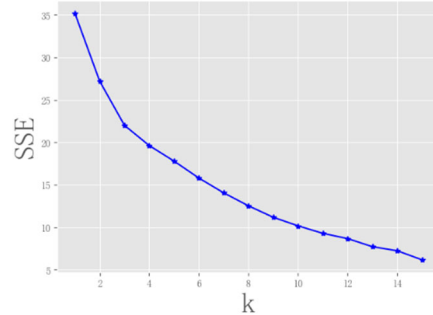


Figure 16 "elbow diagram" of lead barium glass

As the number of clusters k increases, the degree of aggregation of each cluster increases, and then the sum of squares of errors SSE decreases. When k is less than the optimal number of clusters, because the increase in k will greatly improve the degree of aggregation of each cluster, the decrease of SSE will be large. When k reaches the optimal number of clusters, the increase in k will not greatly improve the aggregation of each cluster, so the decrease of SSE will be greatly reduced, and then the curve tends to be flat with the increase of k value. The relationship curve between SSE and k looks like an elbow, and the corresponding k value of the elbow is the optimal cluster number. The "elbow diagram" of elevated potassium glass and lead barium glass was made with python. The k value was two, which was consistent with the cluster analysis results. Therefore, the model was reasonable (Figures 15,16).

In general, the performance of machine learning models has a strong relationship with the size of prediction modeling data sets, and the increase of training data sets can often lead to performance improvement. Therefore, it is theoretically feasible to achieve model sensitivity test by evaluating the performance of prediction problem models with data set size.

In order to realize the sensitivity analysis of k -means clustering algorithm used in the division of two glass subcategories, it is used as a prediction model. At the same time, in order to evaluate the model on the dataset, the function based on the best practice of repeated hierarchical k -fold cross validation is selected for evaluation.

The K -fold cross method is used for verification. The data set is divided into k copies. The k copies of data are divided into 1 test set and $k-1$ training set. The mean square error MSE_i of the model on each test set is calculated. Finally, the cross validation parameter $CV(k)$ is obtained:

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^k MSE_i \quad (1)$$

In order to fully show the sensitivity of data set size and model performance evaluation, data visualization is adopted, and the change trend of the two is shown in Figure 17 below.

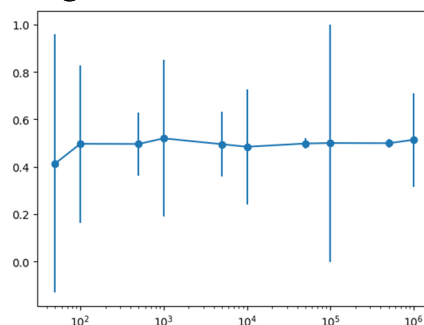


Figure 17 Sensitivity Analysis Chart

The abscissa represents the order of magnitude of the model, and the ordinate represents the performance parameters of the model. As showed in Figure 17, the k-means clustering algorithm used for glass subcategory classification is relatively stable, and the classification performance of the algorithm will not vary greatly due to different dataset sizes. Even if the data set is low, better classification results can be obtained.

4. Classification judgment model of glass relics

4.1. Model identification of unknown glass types based on K-means clustering

To identify the category of unknown glass cultural relics, just put the data [4] into the cluster analysis model calculated in Section 3.

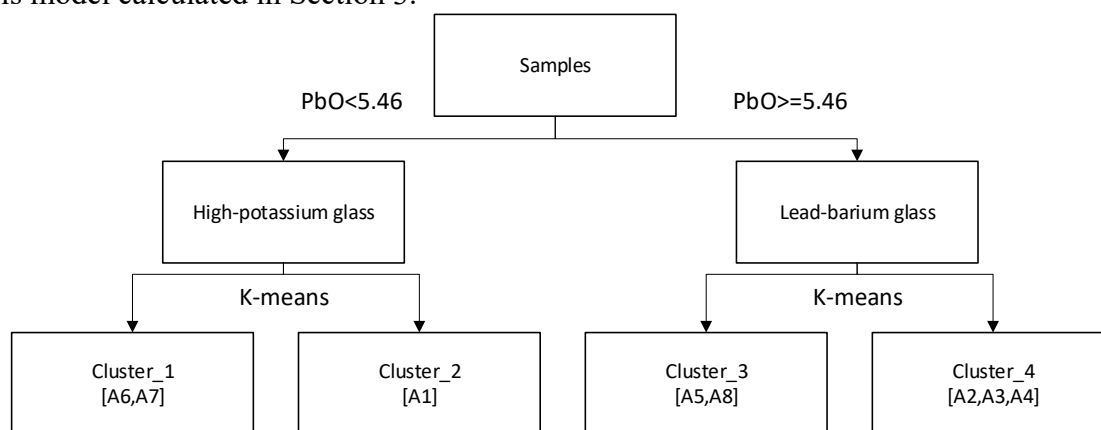


Figure 18 Identification Results of Unknown Glass Cultural Relics

It can be seen from Figure 18 that among the unknown types of glass relics in the given data [4]. There are two subclasses of high potassium glass and two subclasses of lead barium glass. Belongs to high potassium glass cluster_ The cultural relics of Class 1 glass relics are numbered A6 and A7, belonging to the high potassium glass cluster_ The cultural relic number of Class 2 glass relics is A1; It belongs to lead barium glass cluster_ The cultural relics of Class 3 glass relics are numbered A5 and A8, belonging to the lead barium glass cluster_ The cultural relics of Class 4 glass relics are numbered A2, A3 and A4.

4.2. Sensitivity analysis of classification results

The sensitivity of the analysis classification results is the sensitivity of the analysis model. In Section 4, the sample data [4] is put into the K-means clustering based model in section 3 to get the classification results. The sensitivity test of the model has been submitted in Section 3.3, so this question will not be repeated.

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