Research on glass relics based on machine learning

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***Abstract*—The degree of weathering, chemical composition and classification of glass relics are of great significance to the research of archeologists. In this paper, the classification rules of high-potassium and lead-barium glass are constructed using the decision tree algorithm, and then the data set is determined according to the forecast demand. The problem of predicting the type of glass relics is defined as a general binary problem, which is trained by a classical neural network, multi-layer perceptron (MLP). Due to the small amount of data, the parameters were optimized by using the five-fold cross validation, and the sensitivity test was carried out. It was found that the overall robustness of the model was very strong, and the parameters had little influence on the results. After finding the optimal parameters, the prediction of MLP is highly matched with the prediction results of the decision tree, which proves that the model is reasonable.**

Keywords—Decision tree algorithm, multilayer perceptron, 5 fold cross validation

I. INTRODUCTION

Glass has good physical and chemical properties, has a wide range of uses. With the development of materials science and various analytical techniques in recent years, a comprehensive analysis of the chemical composition of glass materials can make a great contribution to the identification of glass types, regulation of the physical and chemical properties of glass and other research directions, thus making glass applicable to a wider range [1].

Based on the basic information of a batch of glass relics, in order to explore the classification rules, this paper first considers the algorithm with visualization ability and transparent decision-making process. That is, the decision tree algorithm is used as the main body for analysis and modeling, and the classification rules of high-potassium glass and lead-barium glass are obtained. In addition, in order to predict the types of unknown glass artifacts, this paper determines the data set according to the forecast requirements. The input was a 15-dimensional feature vector, including weathering markers and 14 chemical element contents; The label is the glass type mark corresponding to the data (1 for high potassium glass and 0 for lead barium glass). The prediction problem is finally transformed into a binary problem, which can be trained and learned by using traditional machine learning or neural network method, and finally output the prediction result.

II. CLASSIFICATION OF HIGH POTASSIUM AND LEAD BARIUM GLASS

In this paper, Decision Tree [2] is used to visualize the decision-making process of neural network. This method is a non-parametric supervised learning method, which can be classified by learning a series of simple strategies. The decision tree model extracts the attributes with the maximum information gain each time as the basis for division. The calculation formula of information gain is as follows:

$$Gain(D,a) = Ent(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Ent(D^v)$$

Where, D is data sample data set, Ent is information entropy function, specifically, Pk is the proportion of category label k in D, y is the total number of labels, then:

$$Ent(D) = -\sum_{k=1}^{|y|} p_k \log_2 p_k$$

After entering all training data into the decision tree for visualization, the following figure can be obtained:

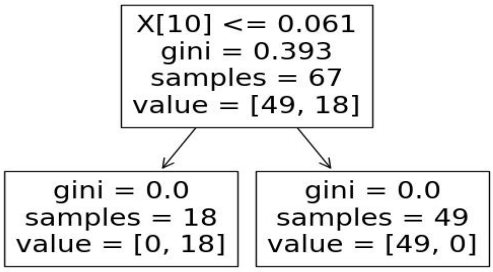

Figure 1. Classification of high potassium and lead barium glass

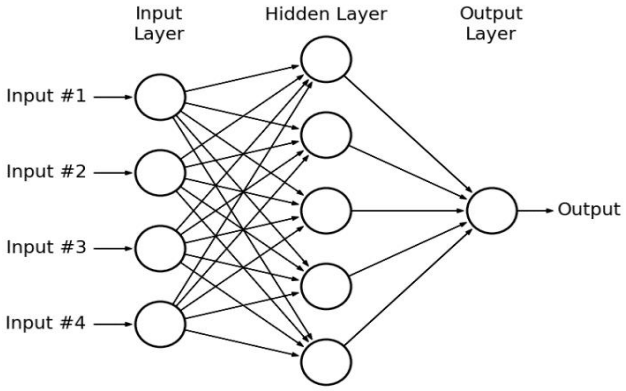

Figure 2. Schematic diagram of the multi-layer perceptron model

Where X [10] represents the tenth dimension of the input feature vector. The first dimension of the input feature is weathering marker, and the remaining 14 dimensions are chemical substances. The corresponding substance in this dimension is lead oxide (PbO). The content of this substance actually distinguishes the high-potassium glass and lead-barium glass in the data set. In the following paper, the classification rule is compared with the model results of predicting the types of cultural relics, and it is found that the results are highly consistent.

III. Machine Learning

A. Model building

Based on the data of glass artifacts, the input characteristics provided are the weathering indication of the artifacts and the content of 14 chemicals, while the characteristic to be predicted is the type of glass (high potassium or lead barium). Combined with the data of glass relics, the prediction task can be transformed into a simple binary problem. Define the input feature as x and label as y.

B. Multilayer perceptron model

Perceptron is the basic model for the introduction of deep learning, which has developed from single-layer perceptron to multi-layer perceptron [3]. MLP is a feed-forward artificial neural network [4], including an input layer, a hidden layer and an output layer. Except for the input layer, all neurons adopt a nonlinear activation function. Training the model requires supervised learning using Backpropagation algorithm. Because of the abundant parameters, the multi-layer perceptron has stronger expression and learning ability than the traditional methods (such as logistic regression and support vector machine). This paper takes this model as a model with strong performance for comparative analysis.

The specific architecture of the multi-layer perceptron used in this paper is as follows:

(1) There are 15 neurons in the input layer, 32 neurons in the hidden layer, and 2 neurons in the output layer

(2) The nonlinear activation function from the input layer to the hidden layer and from the hidden layer to the output layer is ReLU (Rectified Linear Unit), which is convenient to calculate the gradient (linearity) and can accelerate the convergence of neural networks. It has a wide range of applications in neural networks. Its expression is

$$\mathrm{ReLU}(x) = max\,(0, x)$$

In this paper, the loss function is Cross Entropy Loss. The function can accurately reflect the difference between the two random variables, so as to distinguish the learning effect of the model more accurately. At the same time, the optimization of the function is convex optimization problem, which is more conducive to the learning of the model. The formula of this function is:

$$H_y(\hat{y}) = -\sum_i y_i\, log(\hat{y}_i)$$

Where y_i is the true label of the i-th category, and y_i is the predicted result.

C. Analysis of sensitivity

In order to verify the robustness of the neural network to different inputs, Cross Validation was used in this paper to evaluate the prediction effect of the model. Due to the uneven distribution of high-potassium glass and lead-barium glass in the samples, the data set was randomly rearranged during cross-validation to ensure that the two types of samples were obtained as evenly as possible. The cross-validation process is as follows:

(1) i=0 (Representative fold number)

(2) Divide the data set into five parts and rearrange the index of the data for future use.

(3) $i \leftarrow i + 1$,If i is greater than the predetermined value 5, end the cycle (turn 8).

(4) Select the first part of the data as the verification set, and connect the rest parts into a new training set.
(5) Use stochastic gradient descent to train the model on the training set.
(6) Transform the model into a prediction mode, input the data of the verification set without gradient propagation, judge the accuracy of the prediction and the prediction loss according to the label.
(7) Record the accuracy and loss of this round, go to 3.
(8) Calculate the average accuracy and loss of 5 rounds of verification, and use them as the performance effect of the model.

This paper completed two sensitivity experiments:

a. The influence of the number of iterations on the experimental results

The method of selecting the number of iterations in this paper is as follows: the number of iterations is selected every 25 from the interval [50,500], and a five-fold cross verification is automatically run to calculate the accuracy. After the experiment, it was found that the comprehensive accuracy of MLP increased with the increase of the number of iterations, and stabilized at 100% between 400 and 500 generations (the amount of experimental data was small, and it may be the case that all the verification was correct), which can be seen the model has good robustness.

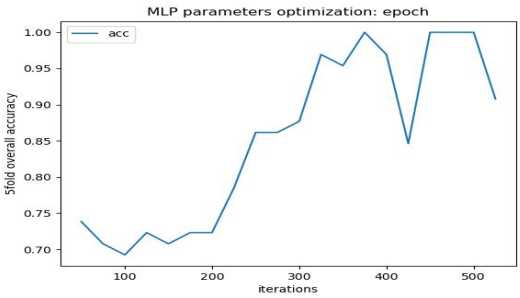

Figure 3. The influence of iteration number on validation accuracy

b. The influence of learning rate on experimental results

The learning rate selected in this paper is: [1e-4, 2e-4, 5e-4, 1e-3, 2e-3, 5e-3, 1e-2]. The number of iterations is 500.With the increase of learning rate, the validation accuracy of MLP also keeps increasing. It is stable at 100% after $1e-3$, and the verified loss is also close to 0. It can be seen that MLP has good stability under different parameters.

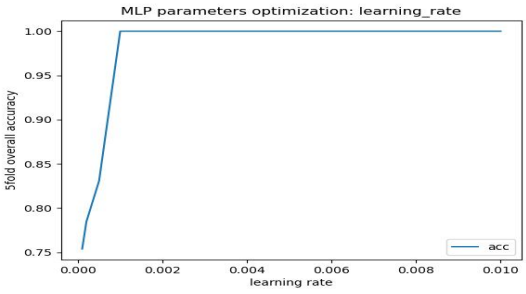

Figure 4. The influence of learning rate on validation accuracy

For comparison, this paper selects a neural network with only one fully connected layer (equivalent to a linear model) for comparison, and carries out parameter tests in the same learning rate interval, as shown in the following figure:

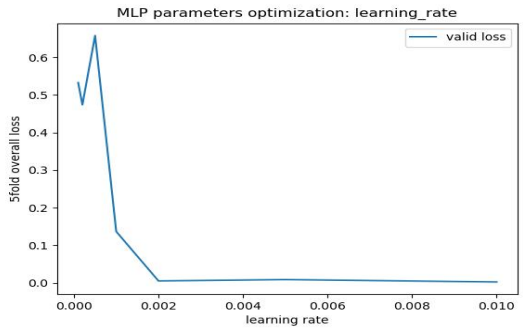

Figure 5. The effect of learning rate on validation loss of MLP

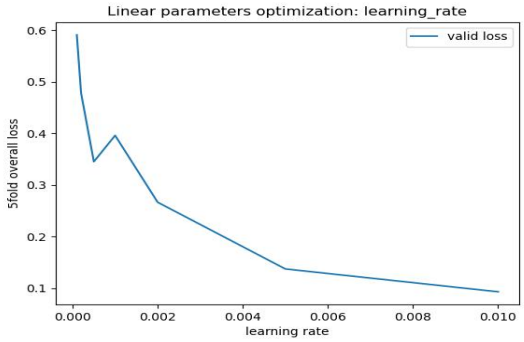

Figure 6. Effect of learning rate on validation loss of linear models

It can be observed that the validation loss decreases much faster in the MLP model than in the linear model, and good validation results can be obtained with very small learning steps.

D. Predict the outcome

The final training of the neural network adopts the Stochastic Gradient Descent (SGD), where the stochastic step length (learning rate) of each descent is $1e-3$ and the number of iterations is 500. Training is performed on all training data. The final output prediction results are shown in the following table:

TABLE I. PREDICTION RESULTS OF MULTI-LAYER PERCEPTRON MLP

Types of cultural relics	Type
A1	High in potassium
A2	Lead barium

A3	Lead barium
A4	Lead barium
A5	Lead barium
A6	High in potassium
A7	High in potassium
A8	Lead barium

E. Compare with Decision tree model

In order to test the rationality of MLP classification, this paper also loaded the test data into the decision tree model for prediction, and found that the prediction results were consistent with MLP. By matching the content of lead oxide in cultural relics in the test set, it can be found that the level of this component content is directly related to the judgment of the type (high lead oxide belongs to lead-barium glass, and vice versa belongs to high-potassium glass), which explains the rationality of the results.

TABLE II. COMPARATIVE ANALYSIS OF DECISION TREE PREDICTION RESULTS AND LEAD OXIDE CONTENT

Types of cultural relics	Type	Lead oxide content ratio (%)
A1	High in potassium	0.00
A2	Lead barium	34.30
A3	Lead barium	39.58
A4	Lead barium	24.28
A5	Lead barium	12.23
A6	High in potassium	0.00
A7	High in potassium	0.00
A8	Lead barium	21.24

IV. CONCLUSIONS

In this paper, the decision tree algorithm is used to construct the classification rules of high-potassium and lead-barium glass, and it is found that the content of lead oxide (PbO) is the characteristic material to distinguish high-potassium glass and lead-barium glass in the data set. Aiming at the unknown category of glass relics, this paper establishes a multilayer perceptron model to predict the type of glass relics. Specifically, the cross entropy loss function is used to accurately reflect the difference between the two random variables, so as to distinguish the learning effect of the model more accurately.

Due to the small amount of data, the parameters were optimized by using the five-fold cross validation, and the sensitivity test was carried out. It was found that the overall robustness of the model was very strong, and the parameters had little influence on the results. The final training of the neural network adopts stochastic gradient descent, and the predicted result is that A1, A6, A7 and A8 are high-potassium glass, and the remaining unknown glass types are lead-barium glass. Finally, the prediction results of the multi-layer perceptron are substituted into the decision tree model for prediction, and the results are consistent. It is found again that the type of glass relics is related to the content of lead oxide. If the lead oxide is high, it belongs to lead barium glass, and if the lead oxide is high, it belongs to high potassium glass.

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