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Discriminant Analysis of Soil Type by Laser Induced Breakdown Spectroscopy Combined with GA-BP Neural Network

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Abstract: Laser induced breakdown spectroscopy (LIBS) and genetic algorithm (GA) were used to optimize the neural network for classification and identification of six kinds of crop soils. Through laser-induced breakdown of soil surface to produce plasma spectrum, 100 sets of spectral data of each soil were collected by spectrometer, and the main element characteristic spectral lines were accurately calibrated with NIST atomic spectrum database as reference. In the experiment, six characteristic spectral lines are selected for analysis. After the dimension of spectral data is reduced by principal component analysis (PCA), the recognition efficiency of BP neural network is greatly improved, and the average recognition accuracy is as high as 99.5%. The study of LIBS technology and BP neural network can provide reference for finding suitable soil for crop planting.

Keywords: Spectroscopy; Laser Induced Breakdown Spectroscopy; BP Neural Network; Principal Component Analysis; Soil Identification.

1. Introduction

Trace elements such as nitrogen, phosphorus and potassium in the soil play an important role in the growth of crops. The content of trace elements in the soil required for the growth of each crop is different. Reasonable selection of the soil environment required for crop growth is of great significance to modern agricultural production. Common detection methods for measuring the content of trace elements in soil include atomic absorption spectrometry [1], inductively coupled plasma spectrometry [2], and inductively coupled plasma mass spectrometry [3]. However, the sample pretreatment process in these analytical methods is complex and cannot meet the needs of low-cost, rapid, and in-situ detection. With the further development of precision agriculture in China, there is an urgent need to develop a technology for real-time, rapid and accurate detection of soil components to meet the needs of precision planting.

Laser induced breakdown spectroscopy (LIBS) uses high-power laser to interact with the sample to generate transient plasma on the sample surface and collect the light emitted by the plasma. The wavelengths of ion spectra and atomic spectra correspond one-to-one to specific elements and have a certain quantitative relationship. From this, information such as the type and concentration of elements in the plasma can be obtained, and the element composition and its concentration can be obtained. LIBS can be used to achieve non-destructive (or minimally damaged) material, multi-element synchronization, and rapid component analysis [4-8], so it is widely used in industrial processing, biomedicine, archaeology, agriculture and other fields. Yamamoto et al. used the internal standard method to analyze Cr and Ba in soil, and the relative standard deviations were 18% and 9% respectively [9-10]. T. Edilene et al. used LIBS technology combined with the momentum-based gradient descent algorithm back propagation (Back- Propagation, BP) ANN method, detects Cu element in soil samples, uses linear regression method and encapsulation algorithm to find spectral peaks of several wavelengths in the entire spectral region as input to the neural network, some of the wavelengths found by this method are qnot Cu For characteristic spectral lines, the relative error of detection is in the range of 2.15% to 29.8% [11].

This paper uses laser induction technology combined with GA- BP neural network to discriminate and analyze different soil samples. Based on the LIBS spectral data of 6 different soils, 21 characteristic spectral lines are used as characteristic values. The GA- BP neural network is used to train the collected data. Through comparative analysis, the genetic algorithm can effectively improve the recognition accuracy of the BP network and can quickly and effectively classify the soil suitable for growing crops.

2. Experimental Materials and Methods

2.1. Sample Preparation Materials

The experimental soils were collected from various cities and counties in Gansu Province, including soil A suitable for growing tomatoes, soil B suitable for growing cucumbers, soil C suitable for growing peppers, soil D suitable for growing eggplants, soil E suitable for growing celery, and soil F suitable for growing carrots, as shown in Table 1. The samples were collected from the place of origin, naturally air-dried, ground, sieved, fully mixed, and then dried . In order to obtain a uniform laser ablation surface, the standard soil sample powder was made into round cake-shaped soil tablets using a 25 MPa desktop powder tablet press for later use. Each soil tablet has a mass of about 3g, a diameter of 25 mm, and a thickness of about 3 mm. When acquiring LIBS data, a total of 600 LIBS soil spectral data were collected in the experiment, that is, 100 for each standard soil sample.

Table 1. Experimental samples

Sample ID	Sample name
Type A	Tomoto
Type B	Cucumber
Type C	Pepper
Type D	Eggplant
Type E	Celery
Type F	Carrot

2.2. Experimental setup

The LIBS test device is shown in Figure 1. It mainly includes a Dawa-100 series laser, a spectrometer (LASERTECHNK BERLIN, USA), and an enhanced charge coupled device (ICCD) detector (intensified charge coupled device, ICCD) combined with the spectrometer. Andor iStar, DH3 3 4 T), digital pulse generator (DG535, Stanford Research Systems, USA), computer, mirror, lens, optical fiber, stage, etc.

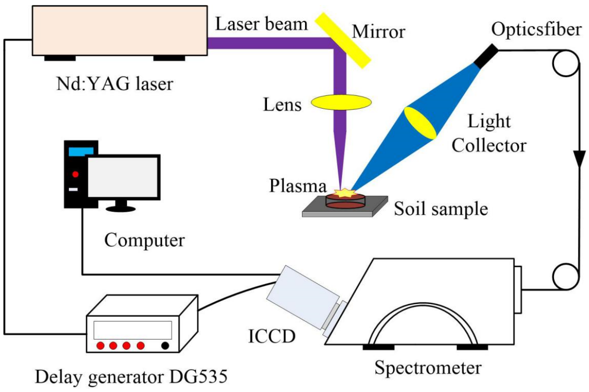


Figure 1. Schematic diagram of the spectrum collection experimental structure

This test was conducted in an air environment. A laser pulse beam is emitted by a Q -switched nanosecond-level Nd : YAG laser (excitation wavelength is 1064 nm , single pulse energy is 100 mJ, pulse width is 8 ns , frequency is 1Hz), and after reflection by the mirror, the focal length is The 50mm lens focuses on the surface of the soil sample to generate laser-induced plasma (plasma), which is collected in the optical fiber through the light collector (light collector), and at the same time transmits the optical signal to the echelle grating spectrometer (wavelength200~975 nm , resolution is about 9000), then use ICCD detector to complete photoelectric conversion, and finally transmit the electrical signal to the computer to complete later data analysis and processing. The digital pulse delay generator (Delay generator DG535) can control the delay time (delay time) of LIBS spectrum signal collection to achieve synchronization with ICCD.

During the LIBS spectrum acquisition process, the gain was set to 80, the acquisition delay time was 2 μ s, the gate width was 2 μ s, and the exposure time of the ICCD detector was 0.01 s. At the same time, in order to reduce the impact of laser pulse energy pulse fluctuations on spectral line intensity, each LIBS spectrum is the average value of 10 laser pulses accumulated at different locations in the soil sample. The soil sample is placed on the displacement platform, and the sample is kept in a "bow" shape during spectral collection to ensure that the laser pulse is evenly irradiated to different positions on the sample surface.

3. Method Theory

3.1. BP Artificial Neural Network

BP neural network plays an increasing role in data analysis due to the advantages of its feedback adjustment algorithm. It continuously adjusts the weights and thresholds of the network through backpropagation to minimize the sum of square errors of the network. A typical BP neural network structure usually consists of an input layer, a hidden layer and an output layer, as shown in Figure 2 BP neural network is trained with a certain amount of historical data to find the hidden patterns in the data, and uses this pattern to classify unknown samples. According to the theory, a typical three-layer BP neural network is used as an example to introduce the learning process of the network.

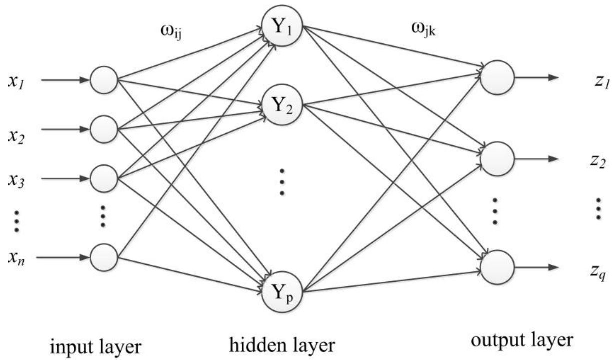


Figure 2. BP neural network structure

(1) Define variables

Taking the BP neural network topology in Figure 2 as an example, assume that the network has n input layer neurons, p hidden layer neurons, and q output layer neurons. x_i, y_j, and z_k respectively represent the input of the i -th neuron in the input layer, the output of the j -th neuron in the hidden layer, and the output of the k -th neuron in the output layer. w_{ij} and w_{jk} respectively represent the weight from the i -th neuron in the input layer to the j -th neuron in the hidden layer, and the weight from the j -th neuron in the hidden layer to the k -th neuron in the output layer. θj *and* θk respectively represent the threshold of the j -th neuron in the hidden layer and the threshold of the k -th neuron in the output layer. $f(\bullet)$ represents the activation function of the hidden layer and $g(\bullet)$ represents the activation function of the output layer.

(2) The forward propagation process of the signal

jth neuron in the hidden layer is:

$$y_j = f\left(\sum_{i=1}^{n} w_{ij}x_i + \theta_j\right) = f\left(net_j\right)$$

Among them, net_j represents the input of the jth neuron in the hidden *layer* .

kth neuron in the output layer is:

$$z_k = g\left(\sum_{j=1}^{p} w_{jk}y_j + \theta_k\right) = f\left(net_k\right)$$

Among them, net k represents the input of the kth neuron in the hidden layer.

If ok is used to represent the expected error of the k -th neuron in the output layer, then the error between the actual output of the k -th neuron and the expected output is:

$$e_k = o_k - z_k$$

The total error of the network output is:

$$E = \frac{1}{2}\sum_{k=1}^{q}(o_k - z_K)^2 = \frac{1}{2}e_K^2$$

$$d_j = \sum_{k=1}^{q} e_k \times \theta_k \times f'\left(\sum_{i=1}^{n} w_{ij}x_i + \theta_j\right)$$

If the total error E meets the termination condition of the network, the training ends; otherwise, the back propagation of the error signal will be used to repeatedly adjust the weights and thresholds of the network until E meets the termination training goal.

(3) The back propagation process of error signal

In the back propagation process of the error signal, the gradient descent method is used to adjust the weights and thresholds of neurons in each layer, making the error output by the adjusted neural network closer to the expected error. If d j is the output error of the j -th neuron in the hidden layer, its expression is:

$$d_j = \sum_{k=1}^{q} e_k \times \theta_k \times f'\left(\sum_{i=1}^{n} w_{ij}x_i + \theta_j\right)$$

The threshold of the output layer is adjusted as:

$$\theta_k(k+1) = \theta_k(k) + \eta \times e_k$$

The threshold of the hidden layer is adjusted as:

$$\theta_j(k+1) = \theta_j(k) + \eta \times d_j$$

The connection weight between the output layer and the hidden layer is adjusted as:

$$w_{jk}(k+1) = w_{jk}(k) + \eta \times e_k \times y_i$$

The connection weight between the input layer and the hidden layer is adjusted as:

$$w_{ij}(k+1) = w_{ij}(k) + \eta \times d_j \times x_i$$

Among them, is the learning rate of the neural network.

BP neural network is the most widely used neural network in the engineering field due to its excellent adaptive learning ability and nonlinear mapping ability, but it has its own limitations, such as being prone to falling into local minimum and slow convergence speed.

3.2. Genetic Algorithm Optimization of BP Neural Network

Genetic Algorithm (GA) is a computational model of biological evolution that simulates the natural selection and genetics mechanism of Darwin's theory of biological evolution. It is a method of searching for the optimal solution by simulating the natural evolution process. One of its characteristics is that since the search starts with a population of solutions, it can effectively avoid falling into the local optimum.

The solution process of genetic algorithm mainly includes: encoding, population initialization, determination of fitness function, selection, replacement, mutation, decoding and other operations.

(1) Coding

Before the genetic algorithm can start working, the problem to be solved needs to be encoded into a symbol that the genetic algorithm can recognize the operation. Putting data into a form that an algorithm can recognize is encoding.

(2) Generate initial population

The initial population size should be chosen appropriately. If the size of the population is too small, the genetic algorithm is prone to premature convergence, causing the global optimal solution searched by the algorithm to not represent the entire solution space. If the size of the population is too large, on the one hand, the search space will be consumed, causing the algorithm to fail to solve the problem. If the time is too long, and the population size is too large, the diversity of the population will be reduced, the distribution of feasible solutions will be sparse, and it will be difficult to search for the global optimal solution. Under normal circumstances, the initial population size is selected in the range of 20-100. After many tests, this study finally determined that when the initial population size is 50, the genetic algorithm has the best global search ability.

(3) Determination of fitness function

The fitness function is used to express the degree of adaptation of individuals in the population to the environment, and represents the ability of individuals in the population to reproduce offspring. The larger the fitness value, the stronger the adaptability of the individual in the population, and the greater the probability of inheriting offspring. After many experiments in this study, the fitness function *Fit* finally adopted is:

$$Fit = \frac{1}{SE}$$

Among them, *SE* is the sum of squared errors.

(4) Select select operation

The selection operation is to select some superior individuals from the population with a certain probability and pass them on to the next generation. Individuals with high fitness values are more likely to be passed on to the next generation, and inferior individuals are eliminated. This paper adopts the roulette strategy based on the proportion of moderate values as the selection operation of the genetic algorithm. The probability *Pi* of each individual *i is given* by the formula:

$$P_i = \frac{1/Fit_i}{\sum_{j=1}^{n}(1/Fit_i)}$$

Where$Fit_i$is the fitness value of individual i, and n is the umber of individuals.

(5) Crossover operation

Crossover operation is the core operator of genetic algorithm, which generates beneficial genes by exchanging and recombining certain genes of individuals. This article uses the real number crossover method as the crossover operation. The crossover operation on j bit between the *k* th individual ak and the lth individual al is as follows:

$$\begin{cases} a_{kj} = a_{kj}(1-b) + a_{ij}b \\ a_{ij} = a_{ij}(1-b) + a_{kj}b \end{cases}$$

Where,*b* is a random number on interval [0, 1]

(6) Mutation operation

The purpose of the mutation operation is to maintain the diversity of the population. The mutation probability is expressed as P_m. If P_m is too small, some important information may disappear prematurely. If P_m is too large, the optimization operation of the genetic algorithm will become Random search, the value of P_m in this study is 0.1.

Genetic algorithm is an optimization algorithm that has global search capabilities but does not have learning capabilities.

4. Results and Discussion

4.1. spectral Measurement

The main basis for identifying the characteristic spectral lines of elements is: 1) The element has a high probability of being excited and can be detected by the instrument in most cases, ensuring the repeatability of the results; 2) The element to be selected has a high spectral line; 3) There are no strong interfering spectral lines near the selected spectral line, which can eliminate interference caused by the spectral lines of other elements. According to this principle, the standard atomic spectrum database [11] of the National Institute of Standards and Technology (NIST) is compared one by one with the characteristic spectral lines of the main elements in the standard soil sample to obtain the content of the soil. Analyze some of the characteristic spectral line wavelengths corresponding to the elements. Different soils have different nutrient element contents, and the corresponding characteristic spectral lines have different intensities. Soils can be classified and identified through characteristic spectral lines. First, the soil spectrum is processed to extract the characteristic peaks of the six elements listed in Table 1. The six element characteristic peaks of each soil spectrum are used as a vector and correspond to its soil type label. In the experiment, 100 spectral data were collected for each soil, and a total of 600 sets of spectral data were collected for the 6 soils. Each set of spectral data has 21 characteristic attributes. Figure 3 lists the average spectral curves of 100 LIBS data measured on the six soil samples selected in the experiment.

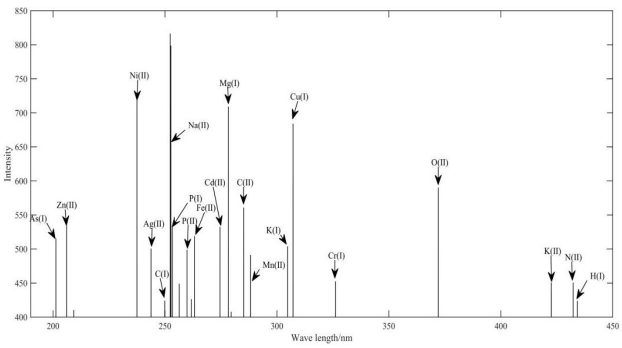


Figure 3. Plasma emission spectrum of soil sample

Table 2. Characteristic spectral lines and wavelengths

Characteristic line	Wavelength/nm	Characteristic line	Wavelength/nm
As(I)	201.3	Mg(I)	278.3
Zn(II)	206	C(II)	285.1
Ni(II)	237.5	Mn(II)	288.2
Ag(II)	243.8	K(I)	304.8
C(I)	249.9	Cu(I)	307.2
Na(II)	252.6	Cr(II)	326.1
P(I)	253.3	O(II)	372
P(II)	259.9	K(II)	422.6
Fe(II)	263.2	N(II)	432.3
Cd(II)	274.6	H(I)	434.2

4.2. Principal Component Analysis of Soil Spectrum

21 elements were selected as soil classification characteristic values. If each element is considered separately, the identification process would be cumbersome, so this paper uses the principal component analysis (PCA) method. Principal component analysis is an information compression technology that uses eigendecomposition to obtain the principal components with the largest variance to replace the original variables. It can remove the correlation between input random variables, highlight the hidden characteristics in the original data, and reduce the complexity of the data. Dimension, improve the speed and stability of modeling. In this experiment, 600 sets of characteristic spectra were obtained, and 21 characteristic spectral lines were selected for each set of spectra. Finally, a 600×21 matrix R was obtained. The resulting matrix R was subjected to PCA analysis, and the contribution rates of the first three principal components were obtained. 95.44%, 2.31%, 1.10%, the cumulative contribution rates are 95.44%, 97.75%, 98.85%. The first three principal components are enough to cover most of the information in the spectra of these six elements. The dimensionally reduced principal components PC1, PC2, and PC3 are used as input values for three-dimensional mapping. It can be seen from the figure 4 that the six soil spectra are intertwined with each other, and the discrimination is low. Effective identification cannot be achieved by directly selecting the first three principal components, so other classification algorithms need to be used to distinguish and identify them.

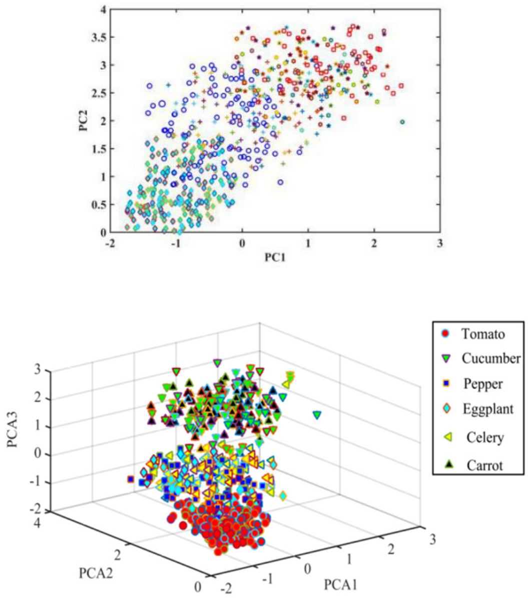


Figure 4. Scatter plot of the first three principal components of 6 soil samples

4.3. Establishment of GA-BP neural network

This article uses a genetic algorithm to optimize the BP neural network, combining the global search characteristics of the genetic algorithm with the excellent learning ability and nonlinear mapping ability of the BP neural network to achieve the purpose of improving the network output accuracy. The optimization process of GA-BP neural network mainly includes two processes: first, the genetic algorithm global search obtains the global optimal value of the BP neural network weights and thresholds; second, the BP neural network uses the global optimal value searched by the genetic algorithm for network training, the nonlinear relationship between input data and output data is obtained. The specific process is shown in Figure 5.

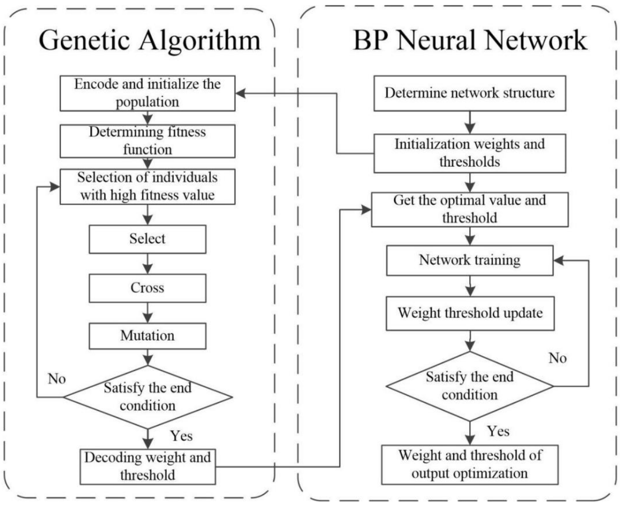


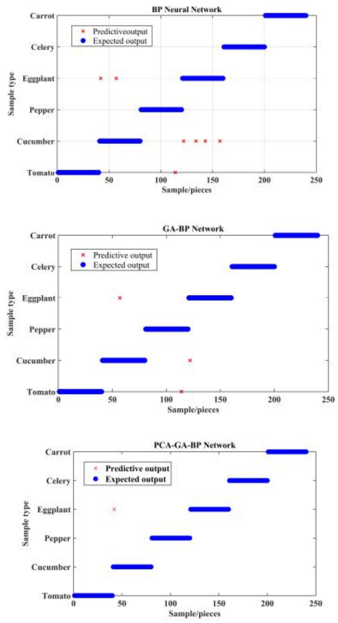
Figure 5. GA-BP neural network

The evaluation of GA-BP network is mainly divided into determining the structure of BP neural network, determining GA optimization parameters, finding the optimal target, calculating errors, and obtaining prediction results. Determine the BP neural network structure according to the number of input and output data, and determine the length of the genetic algorithm individual. Genetic algorithm is used to optimize the weights and thresholds of BP neural network. Use the fitness function to calculate the fitness value of an individual, and find the individual corresponding to the optimal fitness value through operations such as selection, intersection, and mutation.

This paper uses GA- BP neural network to classify and identify the collected LIBS spectra of six types of soil. In the experiment, 100 sets of LIBS spectral data were collected for each soil, with a total of 600 sets of LIBS data. Each set of LIBS spectral data extracted 21 Characteristic element spectral lines form a 600×21-dimensional data matrix. PCA is used for dimensionality reduction. The contribution rate of the first three principal component components is 98.85% , which contains most of the information of the original data. Therefore, the first three principal components are used As the input vector of the BP neural network, a 900×3-dimensional data matrix is formed. After multiple training selections on the GA-BP neural network, the tansig function was finally selected as the excitation function of the hidden layer neurons, and the purelin function was used as the excitation function of the output layer neurons. The maximum training value of the network was 2000, and the target error was set to 0.01. The number of iterations in the genetic algorithm is 40, the population size is 50, the crossover probability P_c is 0.1, and the mutation probability P_m is 0.2.

This paper randomly selected 360 spectra from 600 soil spectra to train the established BP neural network, and used the remaining 240 spectra as the prediction set. The prediction results are shown in Figure 6."O " in the figure represents the expected output of each set of spectral data, and "X " represents the predicted output of each spectral data. When "O " coincides with "X ", it means the prediction result is correct. The experimental results using the BP neural network algorithm are shown in Figure 6(a). The results show that the test set is more likely to be misjudged, and the recognition accuracy is 97.08 %. Figure 6(b) The experimental results using the GA-BP neural network algorithm show that there are 2 Cucumber recognition errors in the test set, 1 Pepper spectrum is recognized incorrectly, and the other spectra are correctly recognized. Therefore, its recognition accuracy is 98.75 %. Figure 6(c) shows the result when the three principal components after PCA dimensionality reduction are used as the input of the BP neural network. It can be seen that only one Cucumber element is identified as Eggplant at this time, and other spectra can be correctly identified. At this time the recognition accuracy is 99.58%.

The soil classification prediction ability of GA-BP neural network based on principal component analysis has been greatly improved.



(a) BP neural network (b) GA-BP neural network (c) PCA-GA-BP neural network

Figure 6. BP neural network prediction results

Due to the randomness of the genetic algorithm, a random training result in the experiment is selected for analysis (Figure 6).

It can be seen that the optimal fitness curve value of the genetic algorithm gradually decreases, gradually becomes stable around 12 generations, and the convergence speed is fast; Figure c: GA-BP neural network training performance curve, the error accuracy trend after 90 steps of network training It is stable, the training results are very close to the accuracy set by the network, and the global search ability is strong. It can avoid the neural network from falling into local minima to a large extent, and effectively improve the recognition accuracy of the network.

In this experiment, BP neural network, GA-BP neural network and PCA-GA-BP neural network were used to conduct 50 repeatability recognition tests on 360 sets of spectral data in the test set. Record the number of errors each time identified. As shown in Figure 8, the recognition accuracy of PCA-GA-BP neural network is basically more than 99.8%. At the same time, the waveform stability is strong, the network convergence performance is good, and the number of errors is stable, which can better Used in classification and identification of soil samples. The statistical results in Table 3 show that the recognition accuracy of soil samples has been greatly improved, but the classification and recognition time is long. Through dimensionality reduction, the network training time can be reduced, and the recognition accuracy is also improved.

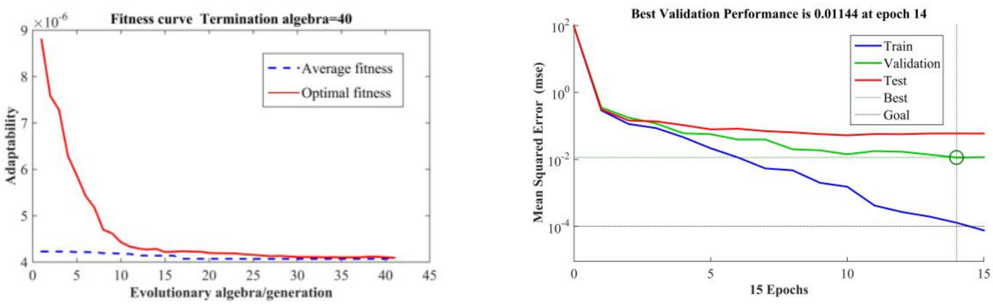


Figure 7. A random training result

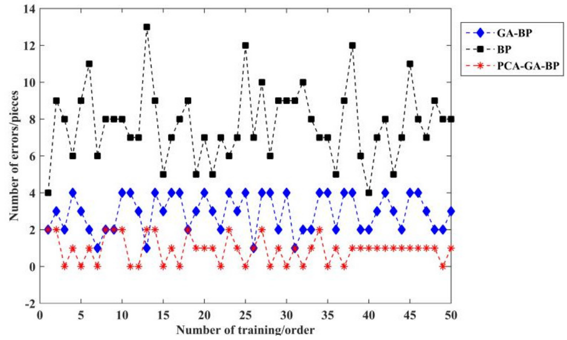


Figure 8. Number of errors identified by three types of neural networks

Table 3. Training results of three types of neural networks

Neural networks	Total-error/pieces	Mean-error/pieces	Total training-time/s	Average-time/s	Average recognition-accuracy
BP	387	7.74	38.46	0.77	97.85%
GA-BP	145	2.9	104.13	2.09	99.19%
PCA-GA-BP	46	0.92	73.53	1.47	99.74%

5. Conclusion

Using laser-induced breakdown spectroscopy technology combined with GA-BP neural network, in the air environment, using the defocus distance.

The spectral data of 6 soil samples were collected for 1.5mm, and 21 characteristic spectral lines were selected as characteristic analysis spectral lines. PCA dimensionality reduction processing was performed on the data, and GA-BP neural network was used to identify and analyze the 360 sets of tested data. The average recognition accuracy was 99.82%, and the time for network modeling was also reduced. When directly using BP neural network for identification analysis, the average accuracy is 98.31%. Therefore, using GA to optimize the BP neural network can overcome the premature convergence of the BP neural network, prevent the network from entering a local minimum, and make the training classification performance more stable. Therefore, the combination of LIBS technology and GA-BP neural network provides a theoretical basis for soil classification identification and rational utilization of farmland.

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