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Near infrared spectroscopy octane regression fitting based on Neural Network

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Abstract: Gasoline octane is measuring gasoline antiknock ability of combustion inside the cylinder of a digital indicator, its high value shows antidetonating quality good. The near infrared spectral analysis technology is an advanced data analysis technology, its basic principle is to use the material in the C - H, N - H - H O, S, H and C = O, C = C groups of near-infrared light absorption of strong characteristics, according to near infrared spectra of the organic material information, physical and chemical characteristics of corresponding qualitative and quantitative measurement.Samples using the technology for data analysis need to be established in advance of the mathematical model between spectral data and the measured data, then put the spectrum of the sample under test data input to the data model, can get the measurement data of the sample under test.Neural network is a kind of mathematical methods simulate human neural network.Neural network can be used to establish mathematical nonlinear relationship.This article uses two types of commonly used BP and RBF neural network to establish the mathematical model between spectral values of gasoline and octane, what's more test the model,evaluation its advantages and disadvantages.
Keywords: octane;The BP neural network;RBF neural network;Regression fitting

I. INTRODUCTION

The popularity of private cars increased gasoline usage.More and more people pay attention to the quality of gasoline.The gasoline octane to a certain extent, shows the gasoline quality [1].With the expanding of gasoline using range, with a quick and convenient way to predict gasoline octane is becoming more and more important.Neural network technology matures opened up a broad road for the prediction of motor octane.

Near infrared spectroscopy is electromagnetic between visible light and infrared radiation, hydrogen containing groups of near infrared spectroscopy and organic molecules (O-H, N-H, C-H) the frequency of vibration absorption zone is consistent and all levels of frequency, by near infrared spectroscopy scanning sample, can get the characteristic information for molecular hydrogen groups in the sample, and by using near infrared spectroscopy analysis of samples with a convenient, fast and efficient, accurate and low cost, without destroying samples, no consumption of chemical reagents, no environmental pollution [2].

The neural network is used to fit the function of the neural network, and the nonlinear fitting of the unknown function is carried out. The neural network can calculate the complex relationship between the input and output results, so the fitting of the nonlinear function can be realized by the neural network [3][4].

Through the near infrared spectral analysis and prediction method of gasoline octane by using the neural network, using MATLAB software modeling, can directly forecast data and cross comparison, time and cost with fast and convenient computer saves prediction, accelerate the analysis speed and efficiency, the use of more resources to develop, at the same time the program package can provide convenience for the actual operation personnel.

2 theory introduction

2.1 BP neural network

BP (Propagation Back) neural network is a kind of multilayer feedforward neural network trained by the error back propagation algorithm, which is one of the most widely used neural network models at present [5].

Figure 2-1 shows a typical BP neural network structure, the network has a hidden layer, the input layer neurons, input layer neurons number is m, the number of hidden neurons is l, output layer neuron n (IW1,1=l*m; IW1,2=n*l; b1=l; b2=n) mining hidden layer transfer function Tansig S type (S type hyperbolic tangent transfer function), the output layer transfer function is purelin (neuron activation function).

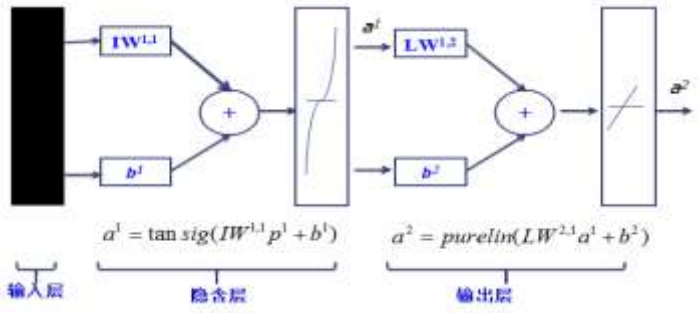

Fig. BP structure of 2-1 neural network

2.1.1 Learning algorithm of BP neural network

The error back-propagation algorithm of BP neural network learning algorithm is a typical tutor, summed up the error output and the expected output of the network weights and threshold "fault", through the back propagation error "share" to all the weight and threshold of neurons. The weights and thresholds are adjusted to the direction of the negative gradient along the direction of the error function.

A pair of samples (X, Y), the input layer and the hidden layer of the network between the weights of W1, hidden layer and output layer of neurons between the weights of W2. The hidden layer and the threshold of the output layer are θ^1 and θ^2.

The output of the hidden layer neuron is:

$$O_j = f\left(\sum_{i=1}^{m} \omega_{ji}^1 x_i - \theta_j^1\right) = f\left(net_j\right) \quad (1)$$

The output layer neuron output is:

$$z_k = g\left(\sum_{j=1}^{l} \omega_{kj}^2 O_j - \theta_k^2\right) = g\left(net_k\right) \quad (2)$$

The error of the network output and the expected output is:

$$E = \frac{1}{2}\sum_{k=1}^{n}\left(y_k - z_k\right)^2 = \frac{1}{2}\sum_{k=1}^{n}\left\{y_k - g\left[\sum_{j=1}^{l}\omega_{kj}^2 f\left(\sum_{l=1}^{m}\omega_{lj}^1 x_i - \theta_j^1\right) - \theta_k^2\right]\right\} \quad (3)$$

Partial derivative of the error E between the hidden layer and the output layer neurons's weight w_{kj}^2, Partial derivative of the error E between the hidden layer and the output layer neurons's weight w_{ji}^2. The adjustment formula for the weight is(η^1 and η^2 are the hidden layer and the output layer of the learning step):

$$\begin{cases} w_{ji}^1(t+1) = w_{ji}^1(t) + \Delta w_{ji}^1 = w_{ji}^1 - \eta^1 \dfrac{\partial E}{\partial w_{kj}^1} = w_{ji}^1(t) + \eta^1 \delta_j^1 x_i \\ w_{ji}^2(t+1) = w_{ji}^2(t) + \Delta w_{ji}^2 = w_{ji}^2 - \eta^2 \dfrac{\partial E}{\partial w_{kj}^1} = w_{ji}^2(t) + \eta^2 \delta_j^2 O_i \end{cases} \quad (4)$$

Error E is the partial derivative of the threshold θ_k^2 of the hidden layer neurons, and the error E is the partial derivative of the threshold θ_j^1 of the hidden layer neuron. Threshold adjustment formula for:

$$\begin{cases} \theta_j^1(t+1)=\theta_j^1(t)+\Delta\theta_j^1=\theta_j^1(t)+\eta^1\dfrac{\partial E}{\partial\theta_j^1}=\theta_j^1(t)+\eta^1\delta_j^1 \\ \theta_k^2(t+1)=\theta_k^2(t)+\Delta\theta_k^2=\theta_k^2(t)+\eta^2\dfrac{\partial E}{\partial\theta_k^2}=\theta_k^2(t)+\eta^2\delta_k^2 \end{cases} \quad (5)$$

2.2 RBF neural network

RBF neural network, which belongs to the former neural network type, it can approximate any continuous function with any precision, and is especially suitable for solving the classification problem [5].

The structure of RBF network is similar to that of multi layer forward network. It is a kind of three layer forward network. The input layer consists of signal source node; the second layer is the hidden layer, and the need to set the number of hidden units as the description of the problem, the transformation function of hidden units (RBF) is the center of radial symmetry and the attenuation of non negative nonlinear function; the third layer is the output layer, its effect on the input mode of response. The transformation from the input space to the hidden layer space is nonlinear, and the output layer space transformation from the hidden layer space is linear. The implicit layer uses the transfer function Radbas, the output layer transfer function is Purelin. The typical structure of RBF neural network as shown in the figure:

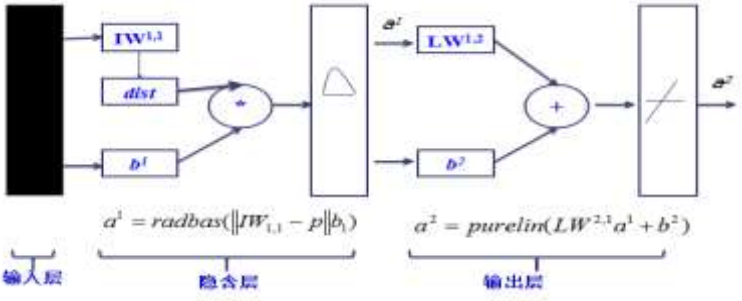

Figure 2-2RBF neural network architecture

2.2.1 Learning algorithm of RBF neural network

RBF neural network learning algorithm needs to solve the parameters have 3: the base function of the center, the variance and the hidden layer to the output layer of the weight.

Determining the radial basis function center of the hidden layer neuron,Without loss of generality, Set the training set sample input matrix P and the output matrix T respectively:

$$P=\begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1Q} \\ p_{21} & p_{22} & \cdots & p_{2Q} \\ \vdots & \vdots & & \vdots \\ p_{M1} & p_{M2} & \cdots & p_{MQ} \end{bmatrix} \quad T=\begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1Q} \\ t_{21} & t_{22} & \cdots & t_{2Q} \\ \vdots & \vdots & & \vdots \\ t_{N1} & t_{N2} & \cdots & t_{NQ} \end{bmatrix} \quad (1)$$

Among them, M is the dimension of the input variable; N is the dimension of the output variable; Q is the sample of the training set. As mentioned above, the threshold value of the hidden layer neurons in Q is: $C=P^{'}$.

To determine the hidden layer neuron threshold, for the sake of simplicity, the radial basis function center of Q hidden layer neuron is $\mathrm{b_1}=[\mathrm{b_{11}},\mathrm{b_{12}},\cdots,\mathrm{b_{1Q}}]^{'}$, among $b_{11}=b_{12}=\cdots=b_{1Q}=\dfrac{0.8326}{spread}$, spread is expansion velocity of radial basis function.

The value and threshold value of the hidden layer and the output layer are determined. When the radial basis function center and the threshold value of the hidden layer neuron are determined, the output of the hidden layer neuron can be calculated by the formula.

$$a_i = \exp\left(-\|C - p_i\|^2 b_i\right),\ i = 1,2,\cdots,Q \quad (2)$$

Among, $p_i = [p_{i1}, p_{i2}, \cdots, p_{iM}]'$ is the first i training sample vector. And marked as $A = [a_1, a_2, \cdots, a_Q]$. Suppose the connection weights between the hidden layer and the output layer W. And the threshold value of the N output layer neuron is $b_2 = [b_{21}, b_{22}, \cdots, b_{2N}]'$.

By solving the linear equations, the value W and the threshold value b_2 of the hidden layer and the output layer can be got.

$$\begin{cases} Wb = T / [A; I] \\ W = Wb(:, 1:Q) \\ b_2 = Wb(:, Q+1) \end{cases} \quad (3)$$

system program implementation

To achieve a value system by MATLAB neural network toolbox to predict gasoline octane and analysis by near infrared spectroscopy, the function provided by MATLAB neural network toolbox, can be achieved in the environment of MATLAB. Data collected by the 60 groups of gasoline samples using Fourier transform near infrared spectrometer carries on the scanning, the scanning range is 900 ~ 1700nm, the scanning interval is 2nm, the spectral curve of each sample contains 401 wavelength points. At the same time, the content of octane is determined by the traditional laboratory test method. BP neural network and RBF neural network were used to establish the mathematical model of the near infrared spectrum and the octane of gasoline samples, and to evaluate the performance of the model.

Realization of the BP neural network and RBF neural network model establishment and performance evaluation, in general can be divided into the following steps, as shown in figure 4-1.

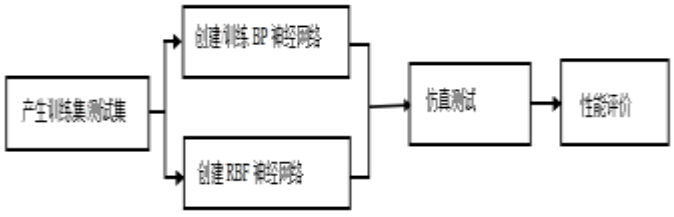

Figure 4-1 model building steps

To develop a simple and easy to understand user interface for the user to use the neural network toolbox to provide convenient call. The system generated GUI interface, as shown in figure 4-2 GUI interface.

Figure 4-2 GUI interface

After the operation can directly call the MATLAB neural network toolbox, the use of MATLAB neural network toolbox function, can be easily implemented in the MATLAB environment to achieve the forecast system.

Empty the environment variable: before the program runs, clear the variables in the work space Workspace and the commands in the Windows Command.

From the training set / test set: 60 samples of the spectra and the octane of data stored in the spectra_data.mat file, the file contains two variables: matrix NIR as sample spectral data of 60 rows and 401 columns, octane 60 rows of 1 octanes. The required spectral data and octane of the system is part of the data of the NIR data set and octane data set. Without loss of generality, random method is used to generate training set and test set, that is, 50 samples are randomly generated as training set, and the remaining 10 samples are used as test set. Because of the randomness of the training set and the test set, the results are different at each time. N (n) is used to generate a random sequence of positive integers with a length of randperm.

Create / training BP neural network, RBF neural network and simulation test: the use of MATLAB neural network toolbox function, MATLAB neural network toolbox interface as shown in figure 4-3. It can facilitate the BP neural network and RBF neural network creation, training and simulation test. Before the training, it can set the known training parameters,it can also take the default settings.

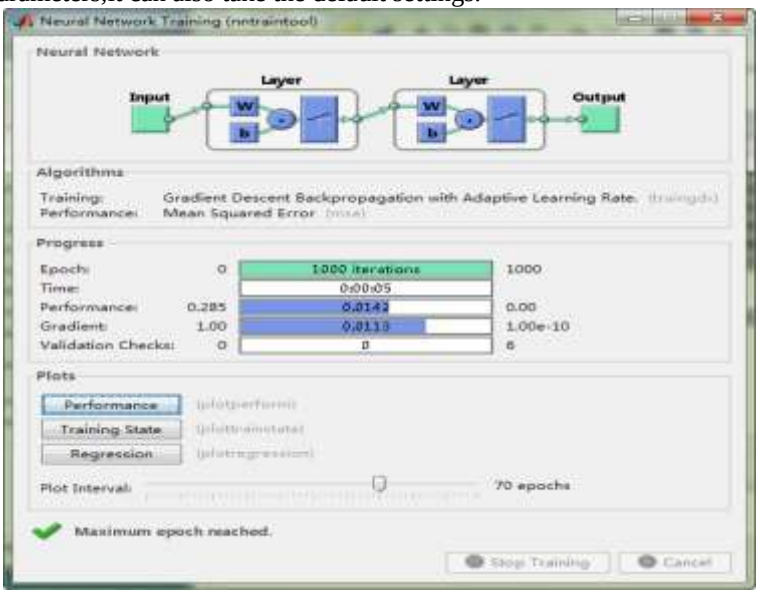

Figure 4-3 neural network toolbox

Performance evaluation: BP neural network and RBF neural network simulation test is finished, the deviation of the value and the true value can be evaluated by the computer, and the generalization ability of the network can be evaluated.

The smaller the relative error, the better the performance of the model. The coefficient of determination in the range [0,1], the more close to 1, showed that the model performance is better; and the more close to 0, indicating that the model's performance is worse.

Two evaluation indexes are selected as the relative error and the coefficient of determination:

$$E_i = \frac{|\hat{y}_i - y_i|}{y_i}, \; i = 1,2,\cdots,n \tag{1}$$

$$R^2 = \frac{\left(l\sum_{i=1}^{l} \hat{y}_i y_i - \sum_{i=1}^{l} \hat{y}_i \sum_{i=1}^{l} y_i \right)^2}{\left(l\sum_{i=1}^{l} \hat{y}_i^2 - \left(\sum_{i=1}^{l} \hat{y}_i \right)^2 \right)\left(l\sum_{i=1}^{l} \hat{y}_i^2 - \left(\sum_{i=1}^{l} y_i \right)^2 \right)} \tag{2}$$

Among, $\hat{y}_i (i = 1, 2, \cdots, n)$ is the predictive value of i sample; $y_i (i = 1, 2, \cdots, n)$ is the real value of i sample; n is sample number.

Figure 4-4 shows the performance, the vertical axis represents the numerical variance, the abscissa represents 4 time points, the blue line is the training data, the red curve is a direct test of the data, after training the blue curve fall that the relative error is more and more small, the red curve in (0, 1) within the scope of more and more close to 1, indicating that the model performance is better, this time through a randomly generated training and test sets at variance is 0.14894 cut in the time point of three has the best performance.

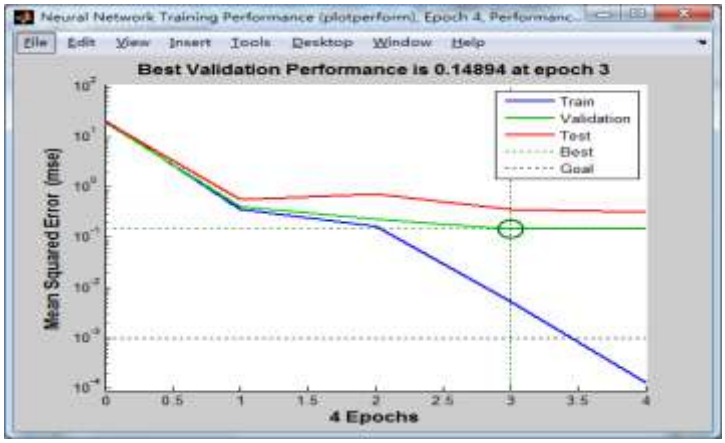

Figure 4-4 performance

Figure 4-5regression shows ,Each distribution is close to 1, so the decision coefficient R2, close to 1, determine the coefficient in the range [0,1], the more close to 1, showed that the model performance is better.

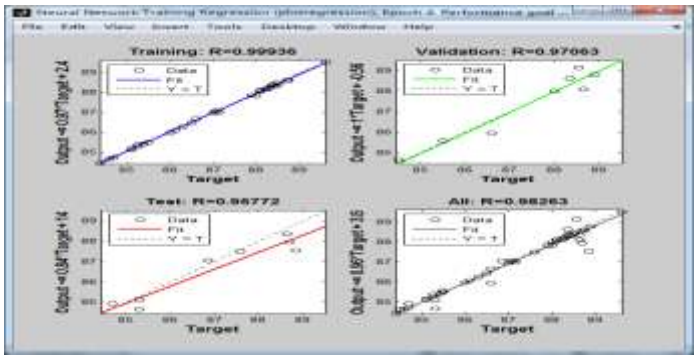

Figure 4-5 regression

In order to observe and analyze the results more directly, the results will be presented in the picture. Since the training set and the test set are randomly generated, the results of each operation will be different. After the

image formation, we can clearly see the situation of BP neural network and RBF neural network to realize the prediction of octane.

Figure 4-6 prediction sample comparison shows, forecast value and real value through the traditional laboratory tests no fundamental difference sample 1,5,8 BP/RBF neural network; prediction value with a very small error by traditional laboratory test the true value of sample 6,7,9,10 BP/RBF neural network; prediction and sample 2,4 although the forecast value and the real value gap with other prediction the sample is large compared to the BP/RBF neural network, but accounted for a relatively small sample and within the allowable error.

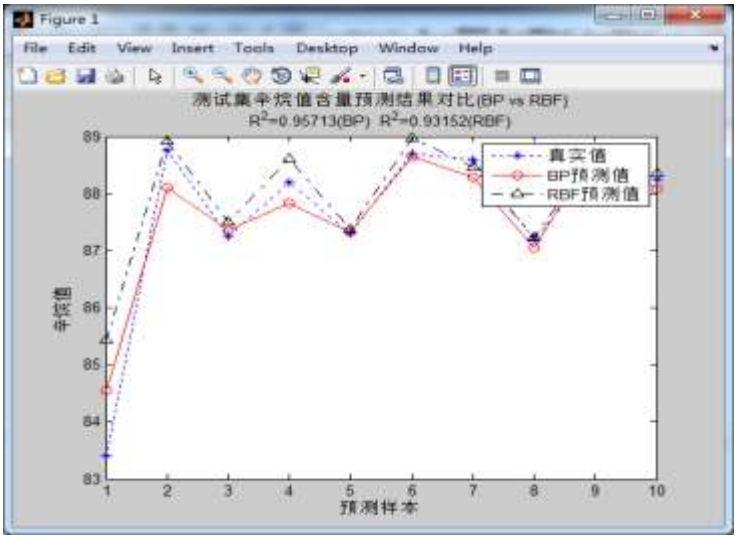

Figure 4-6 prediction sample comparison

After the operation, after the discovery, although the training set and test set randomly generated, and each time the results are different, but the value is very close to the true value, the prediction of BP neural network and RBF neural network can better realize the content of gasoline octane.

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