Research on Propellant Performance Prediction Based on Neural Network or Algorithm Optimization

Linjing Tang, Xuying Jiao, Wei Feng, Rui Yan, Yuanbo Zhang *

Xi'an Modern Chemistry Research Institute, Wuhan, China

* Corresponding Author Email: 91717397@qq.com

Abstract. In order to analyze the four main properties of propellant, the performance prediction model based on BP neural network is established with LM algorithm and CG algorithm as the core algorithm, and the simulation calculation is carried out with the actual production process data and the performance of the model is analyzed. The results show that the mass prediction model based on BP neural network algorithm can quickly predict the properties of propellant. Compared with the prediction model based on CG algorithm, the prediction model based on LM algorithm is more suitable for propellant performance prediction and analysis.

Keywords: Neural Network, LM algorithm, CG algorithm, Matlab.

1. Introduction

The propellant production process consists of multi-process and multi-equipment, and the generated data has the characteristics of multi-source, heterogeneous, massive and multi-noise. Due to the complex chemical mechanism of its existing key processes, it is still in the "black box" state of scientific research. Therefore, it is urgent to establish a known model of the influence law between process parameters and propellant properties, so as to realize the prediction of propellant properties.

With the continuous development of artificial intelligence and big data technology, machine learning knowledge provides new ideas for propellant performance prediction [1]. Among them, as an important class of machine learning models, neural networks can establish a set of mapping relations between input and output in the absence of accurate mathematical models [2]. It is precisely because of this characteristic that neural network is very suitable for studying the nonlinear "black box" system of propellant, and establishing the mapping relationship between process parameters and final performance [3], so as to achieve the purpose of performance prediction.

At present, the application of neural network algorithm in the prediction of explosives and propellants performance has gradually become a research topic of great concern in the industry. Ma Cenrui applied neural network theory to establish a quantitative relationship model between structural state parameters and mechanical property parameters of composite solid propellants, and evaluate the aging failure of composite solid propellants [4]. Zheng Dangcheng established the BP network model of solid propellant performance parameters by using the neural network toolbox of MATLAB, and trained and tested the network model by using the data from the database [5]. Cao Xing used neural network algorithm to build a mathematical model for the quality prediction of explosive charge column, and predicted the relative density and rebound capacity of formed explosive charge column [6]. Gou Yongliang applied neural network technology to predict the concentration distribution of propellant insensitive agents, and achieved rapid and accurate prediction [7].

All the above papers are based on neural network algorithms, which predict various kinds of performance and have significant applicability. Therefore, it can be considered that using neural network algorithm to model and analyze the propellant process with relatively complex and high degree of nonlinearity and to predict the performance is a way worth considering.

2. Performance Data model establishment

2.1. Analysis of Influencing Factors and Performance Parameters

Before the establishment of the performance prediction model, it is necessary to analyze the performance influencing factors and performance parameters in the whole process of propellant.

The influencing factors of propellant performance were determined by performance attribution analysis. The final performance of propellant is mainly determined by its component uniformity, degree of plasticization and rheological properties. Among them, the component uniformity determines the mass consistency of the propellant, and the degree of plasticization and rheological properties determine the chemical properties of the propellant. Therefore, through the performance attribution analysis of the influencing factors, the main influencing factors affecting the propellant performance can be obtained, as shown in Table 1.

Table 1. Influencing factors and performance attribution

Factors affecting	**performance attribution**	
Aluminum content	The activation energy of the reaction can be reduced by aluminum content	Uniformity of composition
Lead, nickel salt, etc	Lead and nickel salts can reduce the activation energy	
Nitrogen content of absorbent	Nitrogen content affects the explosive performance	
Absorbent nitrocotton content	Nitrocellulose affects flammability and explosive properties	
Roller spacing	The larger the material, the worse the uniformity and degree of plasticization	Degree of plasticization and rheological properties
Working roll temperature	The temperature of working shaft affects the degree of plasticization	
Empty roll temperature	Idling temperature affects the degree of plasticization	
Holding temperature	The holding temperature will affect the plasticization degree of the material	
Holding time	The holding time will affect the plasticization degree of the material	
The holding pressure	Pressure index affects the degree of material plasticization	
Dwell time	Influence pore formation	
Cylinder temperature	Affect the molding state of the material	
Stable pressure	Pressure index affects the degree of material plasticization	

Propellant performance indexes mainly include density, combustion rate, detonation heat and pressure index. Density is one of the indexes to judge the uniformity and consistency of components. As one of the production indexes of propellant, the combustion speed is also one of the influencing factors of propellant safety. Therefore, whether the combustion speed reaches the standard must be taken as the condition to judge whether the propellant is qualified. Propellant is constantly under extrusion pressure in the production process, and different pressure indexes will be produced to propellant components during propellant packaging, which affects the power of propellant, so it is necessary to analyze the pressure index of propellant. Explosive heat, also known as explosion heat, is the amount of heat given off when 1mol of explosive material explodes. Detonation heat is the root data of propellant power, so in order to make the propellant achieve a certain explosion effect, it must be guaranteed to reach the target.

2.2. Data Preprocessing

The propellant process environment is relatively complex, the data sources are relatively diverse, and the data quality needs to be improved. Therefore, it is necessary to preprocess the data firstly. The process of data preprocessing includes the processing of missing values, outliers (noise) and the reduction of data dimension. Therefore, the data preprocessing flow model is established as shown in Figure 1.

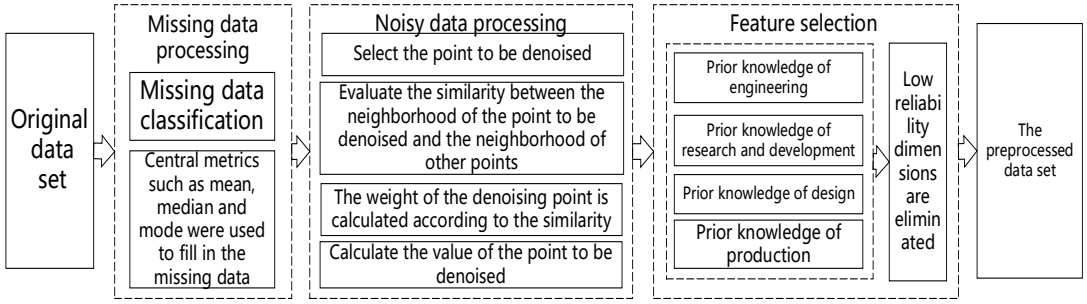


Figure 1. Pretreatment flow model

(1) Processing of missing values and outliers in multidimensional data

In the propellant production line, a lot of data are obtained through sensors, due to some objective reasons, information may be missing or phenomenon. Here, the linear interpolation method is used to fill the missing values, and the calculation formula is as follows:

$$y_a = y_s + \frac{y_E - y_s}{t_E - t_s}\left(t_a - t_s\right) \tag{1}$$

Where t_a is the moment and estimated value corresponding to the data point to be calculated; t_E and y_E is the moment and actual value corresponding to the first effective recording point after the data missing period; t_s and y_s is the moment and actual value corresponding to the most recent effective recording point before the data missing period.

For outliers, non-local mean denoising method is used to deal with the outliers, that is, the estimated value of the data points to be denoised is obtained by weighted average of the data points in the neighborhood structure similar to the data points to be denoised.

(2) Data dimension selection based on prior knowledge

In practice, not all dimensions will be beneficial for modeling. Therefore, before modeling, it is necessary to select the dimension of data according to the purpose and requirements of modeling to achieve the purpose of dimensionality reduction. This time, a priori knowledge is used to reduce the dimension by combining theory and artificial experience. The data after preprocessing are shown in Table 2.

Table 2. Cleaned data

serial number	Nitro cotton (X1)	Nitro-glycerin (X2)	...	Roller spacing (X13)	…	Cylinder temperature (X20)	Stable pressure (X21)	Density (Y1)	Combustion rate(Y2)	Pressure index (Y3)	Detonation Heat (Y4)
1	673	44.65		1.7		93	10	1.7	27.75	0.35	5050
2	675	44.6		1.7		94	10.8	1.8	28.25	0.35	5031
3	680	44.63		1.8		94	11	2	29.63	0.33	5242
…											
24	674	44.63		1.9		92	12.9	1.9	29.5	0.29	5050
25	680	44.68		1.6		95	11.5	1.8	28	0.21	5100

3. Performance prediction model construction

BP neural network is a feedforward neural network trained according to the error back propagation algorithm [8]. It uses the back propagation method to constantly adjust the weight of the network so as to minimize the sum of squared errors of the network [9]. The neuron layers of BP neural network

are connected with each other, while the neurons in the same layer are not connected [10]. The BP neural network is used to construct a prediction model with the performance influencing factors as input and the performance parameters as output to predict the propellant performance. Firstly, the main parameters of the prediction model are determined, including the training algorithm, the number of neural network layers, the number of neurons in hidden layers and the method of data set partitioning.

3.1. Selection of training algorithm

BP neural network adjusts the weight and threshold of the network through the training algorithm, so that the error between the adjusted network output and the actual value reaches the preset range. Therefore, the performance of the whole BP neural network is affected by the quality of the network training algorithm. There are many BP neural network training algorithms, the more commonly used gradient descent algorithm, Newton method, LM algorithm and CG algorithm. Among them, one of the disadvantages of the gradient descent method is that when the function gradient changes into a slender structure, the process of the gradient descent method will appear a lot of iterations. And although the direction of gradient descent is not necessarily the path of fastest convergence. Compared with gradient descent method, Newton's method has certain global prediction and better convergence property. However, the difficulty and disadvantage of Newton's method lies in the computation of Hessian matrix and its inverse matrix is very large.

However, LM algorithm and CG algorithm are between the above two algorithms, combining their advantages and optimizing their disadvantages. Therefore, LM algorithm and CG algorithm are mainly combined to establish the prediction model and analyze.

LM algorithm

LM (Levenberg-Marquardt) algorithm can provide numerical solutions for numerical nonlinear minimization (local minimization), which combines gradient descent method and Gaussian Newton method (by adjusting damping switching). The core idea is to replace the calculation of Hessian matrix with Jacobian matrix (easy to calculate), so as to improve the optimization efficiency [15-16]. When the solution BP neural network adjusts the weight and threshold of the network through the training algorithm, so that the error between the adjusted network output and the actual value reaches the preset range. Therefore, the performance of the whole BP neural network is affected by the quality of the network training algorithm. There are many BP neural network training algorithms, the more commonly used gradient descent algorithm, Newton method, LM algorithm and CG algorithm. Among them, one of the disadvantages of the gradient descent method is that when the function gradient changes into a slender structure, the process of the gradient descent method will appear a lot of iterations. And although the direction of gradient descent is not necessarily the path of fastest convergence. Compared with gradient descent method, Newton's method has certain global prediction and better convergence property. However, the difficulty and disadvantage of Newton's method lies in the computation of Hessian matrix and its inverse matrix is very large.

begin
$k := 0;\ \upsilon := 2;\ \mathrm{x} := \mathrm{x}_0$
$\mathbf{A} := \mathrm{J}(\mathrm{x})^{\mathrm{T}}\mathrm{J}(\mathrm{x});\quad \mathrm{g} := \mathrm{J}(\mathrm{x})^{\mathrm{T}}\mathrm{f}(\mathrm{x})$
$found := (\|\mathrm{g}\|_{\infty} \le \varepsilon_1);\quad \mu := \tau * \max\{a_{ii}\}$
while (**not** *found*)**and**$(k < k_{\max})$
$k := k + 1;\quad Solve(\mathbf{A} + \mu\mathbf{I})\mathrm{h}_{lm} = -\mathrm{g}$
if $\|\mathrm{h}_{lm}\| \le \varepsilon_2(\|\mathrm{x}\| + \varepsilon_2)$
$found := \mathbf{true}$
else
$\mathrm{x}_{new} := \mathrm{x} + \mathrm{h}_{lm}$
$\rho := (F(\mathrm{x}) - F(\mathrm{x}_{new}))/(L(0) - L(\mathrm{h}_{lm}))$
if $\rho > 0$
$\mathrm{x} := \mathrm{x}_{new}$
$\mathbf{A} := \mathrm{J}(\mathrm{x})^{\mathrm{T}}\mathrm{J}(\mathrm{x});\quad \mathrm{g} := \mathrm{J}(\mathrm{x})^{\mathrm{T}}\mathrm{f}(\mathrm{x})$
$found := (\|\mathrm{g}\|_{\infty} \le \varepsilon_1)$
$\mu := \mu * \max\left\{\frac{1}{3}, 1 - (2\rho - 1)^3\right\};\ \upsilon := 2$
else
$\mu := \mu * \upsilon;\ \upsilon := 2 * \upsilon$
end

CG algorithm

The Conjugate Gradient method was originally proposed by computational mathematician Hestenes and geometrician Stiefel [17], which is a method between the steepest descent method and Newton's method. Only through the information of the first derivative, it not only improves the slow convergence of the steepest descent method, but also avoids the super-large computation requirement of Newton's method for Hesse matrix [18]. It will decompose the objective function in different directions and then obtain the extreme values and then set them. If it is a quadratic optimization problem, the conjugate gradient method can theoretically guarantee that the optimal solution will be found in at most n steps. The pseudo-code of CG algorithm is as follows:

$r_0 \triangleq b - Ax_0;\ p_0 = r_0;$
repeat
for $k = 0,1...$ **do**
if $p_k = 0$ **then**
return x_0
end
else
$a_k = \frac{r_k^T r_k}{P_k^T A P_k};\ x_{k+1} = x_k + a_k p_k;$
$r_{k+1} = r_k - a_k A p_k;\ b_k = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k};$
$p_{k+1} = r_{k+1} + b_k p_k;$
end
end
until *convergence*;

3.2. The number of neural network layers is determined

The universal approximation theorem shows that a feedforward network with a linear output layer and at least one hidden layer with any "compressed" activation function can approximate any Borel measurable function from one finite dimensional space to another with any nonzero error as long as there are enough hidden layer neuron nodes [11]. Comprehensive analysis shows that the BP neural network with three layers has a faster operation speed and better effect. Therefore, in this paper, the neural network with one hidden layer is adopted, that is, it only contains the input layer, the hidden layer of one layer and the output layer.

3.3. Number of neurons in hidden layer

There is still a lack of certain scientific theories on the selection of the number of hidden layer neurons. At present, most of them determine the general range according to the empirical formula and determine the most suitable number of hidden layer neurons for application scenarios through a certain number of tests. In this paper, combined with Nielsen's node number estimation formula [12] :

$$h = \sqrt{p+q} + a \tag{2}$$

And the estimation formula of the number of high starting nodes [13]:

$$h = \sqrt{0.43pq + 0.12q^2 + 2.54p + 0.77q + 0.35} + 0.51 \tag{3}$$

It is determined that the number of neurons in the input layer and output layer of this prediction model is 21 and 4, then the number of neurons in the hidden layer is set as 12 according to the above equation (where p and q are the number of neurons in the input and output layers respectively).

3.4. Partitioning the data set

The set aside method was used to divide the sample data set, and 70% of them were randomly selected as the training set, while the validation set and test set accounted for 15% of the remaining data respectively.

4. Simulation an analysis

The neural network toolbox included in MATLAB software is based on the basic artificial neural network, which has good function optimization effect and easy operation for nonlinear data. As long as according to their own needs, call the relevant function, you can complete the prediction model network design and training. Therefore, MATLAB is used to conduct simulation analysis on the established prediction model [14]. The neural network model is shown in Figure 2.

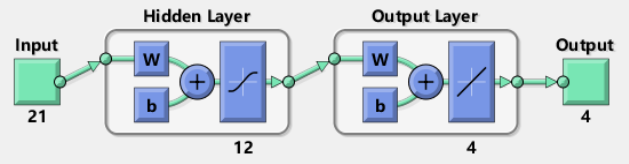
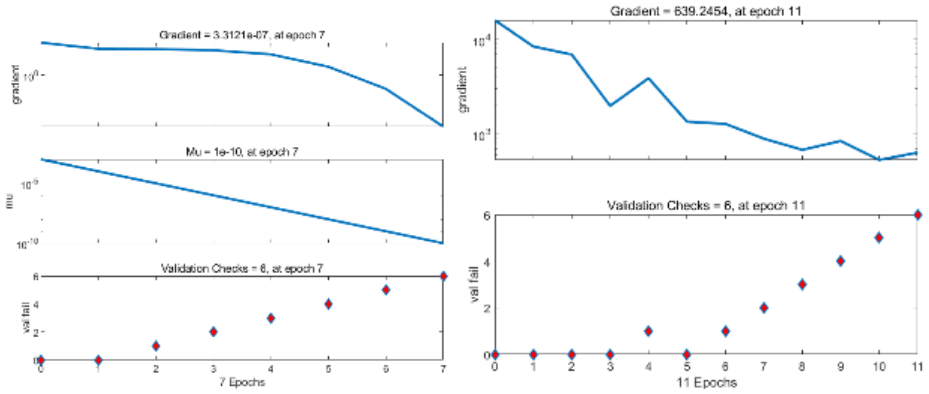


Figure 2. Structure diagram of artificial neural network model

Firstly, the changes of three important model parameters in the training process of the two algorithms are compared and analyzed. Validation Checks to verify generalization ability. Mu is only reflected in the LM algorithm, indicating whether the algorithm currently chooses the approach gradient descent method or Newton's method. It can be seen from fig. 3 that the gradient of the LM algorithm prediction model starts to decrease rapidly in the fourth round of training, and the gradient decreases to the minimum after 7 rounds of training. Starting from the fifth round, the validation set error showed an upward trend for three consecutive rounds, so the training was judged to be over. Although the gradient of CG algorithm prediction model has been declining, the gradient has been stable since the 10th round, and the stable value is about 250. However, from the sixth round, the validation set error showed an upward trend for five consecutive rounds, so it was judged that the training was stopped after 11 rounds of training.



(a) LM algorithm (b) CG algorithm

Figure 3. State diagram of parameters change during model training

Next, the prediction error ratio of each sample under the two algorithms is analyzed. The larger the value, the larger the prediction error. Here, the prediction error ratio is expressed as:

$$\eta(M,N)=\left|\frac{M_i-N_i}{N_i}\right|\times 100\% \tag{4}$$

Where, M is predicted data and N is actual data. i means the ith sample.

As can be seen from Figure 4, the error ratio of the prediction model of LM algorithm is relatively small on the whole. Among them, the error ratio of burning rate and explosion heat is basically kept within 5%. Seventy-five percent of the burning rate samples had an error ratio of less than 10 percent. The error ratio of the charge density is slightly larger than that of the other performance indicators, with only about 75% of the samples predicting an error ratio less than 15%. But the maximum error was only 25 percent. The error ratio of CG algorithm prediction model is generally large. Among the four performance indicators, only the explosive heat error ratio has always remained within 10%. The error ratio of the burning rate varies from 3% to 25%. The error ratio of charge density and pressure index is very large, most of them exceed 20%, and some of them even exceed 60%.

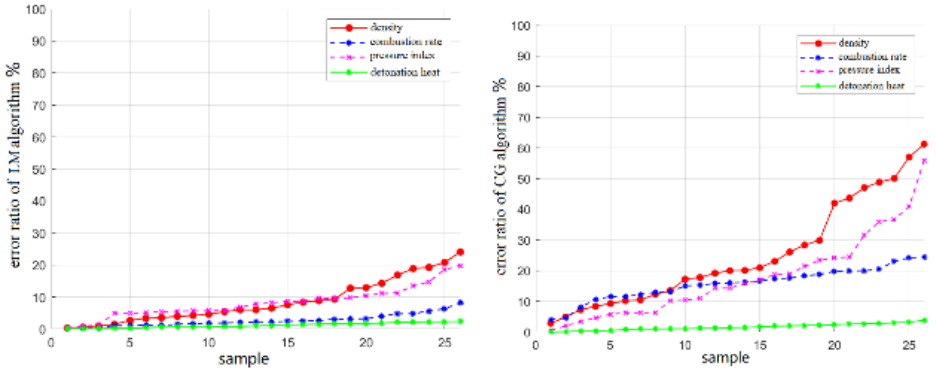


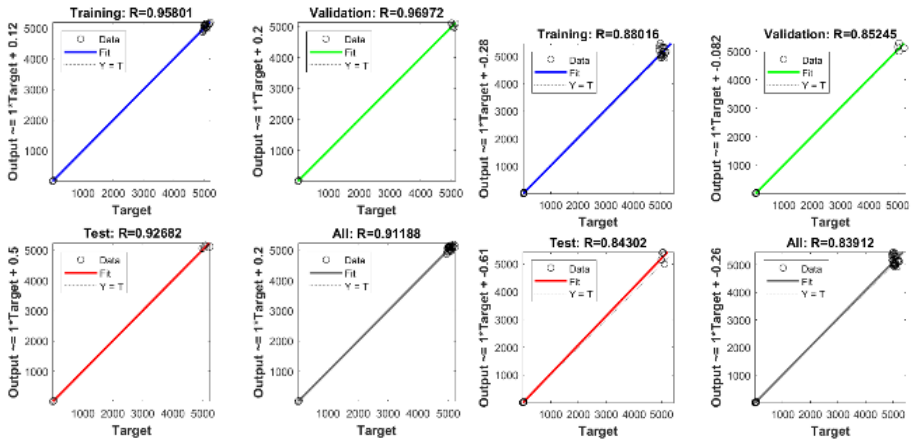
Figure 4. Comparison of prediction error ratio

MATLAB uses the R value to judge the correlation. R value is the complex correlation coefficient, which ranges from 0 to 1. The larger the value, the better the prediction effect. Its prediction expression is:

$$R(M,N)=\frac{Cov(M,N)}{Var[M]Var[N]} \tag{5}$$

Where, Cov denotes covariance, Var denotes variance.

As can be seen from fig.5, the results of R values of the predicted and experimental values of the LM algorithm prediction model on the training and validation sets are relatively good, both above 90%. However, the prediction result of CG algorithm prediction model is relatively poor, which is less than 90%.



(a) LM algorithm (b) CG algorithm

Figure 5. The results diagram of artificial neural network model

5. Conclusion

(1) The neural network performance prediction model constructed based on BP neural network algorithm can be preliminarily used to quickly predict the density, combustion rate, detonation heat and pressure index.

(2) Compared with the neural network with CG algorithm as the training algorithm, the BP neural network model with LM algorithm as the training algorithm is more suitable for the performance prediction analysis of propellant. But the BP neural network model with LM algorithm as the training algorithm needs to be further optimized on the current basis to obtain higher prediction accuracy.

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