Prediction NO\textsubscript{X} Emissions for High Speed DI Diesel Engine Based on PSOBP

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**Abstract.** In this paper, BP neural network (BPNN) is studied to model and predict NO\textsubscript{X} emission of direct injection diesel engine. The model selects four parameters as input, namely rotation speed, load, exhaust temperature and fuel-air ratio. Through testing, it is concluded that the prediction performance of BPNN model will be greatly affected by the initial weight and threshold, so that the prediction accuracy of the model is not high. In order to reduce the influence of initial weight and threshold on the prediction performance of BPNN model, this paper adopts Particle Swarm Optimization (PSO) algorithm to optimize the initial weight and threshold of BPNN, and establishes the corresponding prediction model of NO\textsubscript{X} emission of diesel engine. The results show that the prediction model of BPNN optimized by PSO algorithm can effectively reduce the influence of initial weight and threshold on BPNN and make the prediction results of the model more reliable. In particular, when PSO adopts non-linear dynamic weight strategy and synchronous learning factor strategy, the prediction performance of BPNN model is more provided with reliability.

**Introduction**

Diesel engine is widely used because of its high thermal efficiency, superior dynamic performance and good economic performance [1]. However, with the aggravation of the energy crisis in recent years and the increasingly serious global environmental pollution, especially air pollution, the emission regulations of diesel engines have become increasingly stringent. For diesel engine, because of its high combustion temperature and relatively thin mixture, its NO\textsubscript{X} emissions are higher. Therefore, how to control and reduce NO\textsubscript{X} emissions is an urgent problem for diesel engine enterprises. Typically, diesel engines use selective catalytic reduction (SCR) technology to reduce NO\textsubscript{X} emissions [2]. Although SCR technology using ammonia (NH\textsubscript{3}) as reducing agent can reduce NO\textsubscript{X} emission of diesel engines efficiently, such technology may lead to NH\textsubscript{3} leakage in the working process [3], so this method needs to measure NO\textsubscript{X} emission accurately. For diesel engine enterprises, a large number of calibration tests are usually carried out to obtain NO\textsubscript{X} emission patterns under multiple working conditions. However, this process is complex, cumbersome, and costly. Therefore, in order to reduce the test cost and improve the measurement accuracy of NO\textsubscript{X}, it is a feasible and effective method to establish a prediction model based on the relationship between NO\textsubscript{X} and related operating parameters.

For this reason, many different models for predicting diesel engine NO\textsubscript{X} emissions have been put forward by scholars of various countries through a large number of studies. Jonas Asprion et al. [4] established a NO\textsubscript{X} emission model for dynamic optimization and model-based control. The structure of the model is relatively simple and the prediction results are good. Their test results showed that the relative error of NO\textsubscript{X} calculated by their model is below 10% during transient operation. C. Guardiola et al. [5] established a real-time NO\textsubscript{X} estimation model for diesel engine based on in-cylinder pressure signal and air flow. The MRE of the model is less than 10% through experiments. E. Neshat et al. [6] proposed a new multi-region model based on chemical dynamics for simulating the diesel engine closed loop. 14 reactions were used to simulate NO\textsubscript{X} formation in
their model. And their model results are in good agreement with experimental data, and the maximum error of the model for predicting NO\textsubscript{X} prediction is 12%. Stefano d’Ambrosio et al. [7] developed a fast control-oriented semi-empirical model that is capable of predicting NO\textsubscript{X} emissions in diesel engines under steady state and transient conditions. Experiments show that this method not only has low computational effort, but also can improve the predictive of capability of NO\textsubscript{X} emission. Similarly, Stelios A. Provataris et al. [8] based on Zeldovich theory, established a semi-empirical, zero-dimensional, two-zone model for predicting diesel engine NO\textsubscript{X} emissions. And the results show that the average absolute percentage errors of NO\textsubscript{X} calculated by their model for heavy and light-duty diesel engines are 18% and 20%, respectively. Roberto Finesso et al. [9, 10] proposed a control-oriented semi-empirical model and successfully applied it to light and heavy diesel engines. They found when the intake O\textsubscript{2} concentration is measured with a sufficiently level of accuracy, the variance of the NO\textsubscript{X} model could be quite good (2–8%).

Xavier Tauzia et al. [11, 12] proposed a 0D semi-physical model too. To saving calculation time, their model does not evaluate emissions on a crank-angle base but only at the exhaust valve opening (EVO). NO\textsubscript{X} predictions of their model are within ±20% of measured values for 95% of the tested operating points. C. Quleire et al. [13] proposed a semi-physical model for predicting NO\textsubscript{X} emissions from diesel engines. This model is based on the simplification of zero-dimensional thermodynamic model of only considering main phenomena taking part in NO\textsubscript{X} formation. In this model, the maximum burned gas temperature sub-model is coupled to an averaged NO\textsubscript{X} formation kinetic model (based on the Zeldovich mechanism) to form a mean-value model for NO\textsubscript{X} computation. Rok Viha et al. [14] established a control-oriented thermodynamic model capable of predicting NO\textsubscript{X} emissions in diesel engines, their model is derived from zero-dimensional combustion model using in-cylinder pressure as the input. Emre Ozgui et al. [15] developed a fast NO\textsubscript{X} emission prediction methodology by utilizing one-dimensional models generated in GT-Suite software.

The numerical model is another method for NO\textsubscript{X} emission prediction. Unlike the above models, the data model does not need to understand the generation mechanism of NO\textsubscript{X}, it has a relatively simple structure, good fitting performance and low labor consumption. Jiaxin Ma et al. [16] established a linear and nonlinear auto-regressive model with exogenous inputs (GNARX) for NO\textsubscript{X} prediction. Gokhan Alcan et al. [17] proposed a nonlinear model for a heavy-duty diesel engine NO\textsubscript{X} emission formation. Sigmoid based nonlinear autoregressive with exogenous input (NARX) model is employed to predict NO\textsubscript{X} emissions with given input set under both steady-state and transient cycles. Experimental results show that the steady-state and the transient validation accuracies for the majority of the obtained models are higher than 80% and 70%, respectively.

Artificial Neural Network (ANN) is a bionic model that simulates the neural structure and behavior of the human brain. ANN model is also often used to predict the emission of NO\textsubscript{X} from diesel engines. By establishing the relationship between input and output basic data, ANN model can predict the combination of input data which has never been seen before [18]. Moreover, when there are many input parameters, it is difficult to establish the relationship between input and output variables. At this time, the ANN model is also an appropriate choice [19]. Obodeh O [20] evaluated the capabilities of ANN as a predictive tool for multi-cylinder diesel engine NO\textsubscript{X} emissions. They found the Levenberg-Marquardt (LM) algorithm with 11 neurons produced the best results. Hamid Taghavifar et al. [21] established an ANN model with two hidden layers. Combining with different training functions, NO\textsubscript{X} emission was predicted at engine speed of 2000 rpm, 3000rpm and 4000rpm. By combining ANN with ant colony optimization (ACO) algorithm, J. Mohammadhassani et al. [22] established a prediction model for NO\textsubscript{X} and soot. And their model could model the exhaust NO\textsubscript{X} emissions with the correlation factors of 0.98. R. Rahimi Molkdaragh et al. [23] used wavelet neural network (WNN) and stochastic gradient algorithm (SGA) to predict diesel engine performance and emissions.

BP Neural Network (BPNN) [24], as one of the most mature neural network algorithms, is widely used in various research fields because of its good self-learning, self-adaptation, robustness
and generalization ability [25]. In BPNN, the prediction results can be more accurate by re-calculating the connection weights and thresholds of neurons in the hidden layer by propagating the errors back to the hidden layer in the output layer. However, the initial weights and thresholds of traditional BPNN are randomly generated, and its performance depends on the selection of initial weights and thresholds [26]. In document [26], Niu Xiaoxiao et al. obtained the neural network prediction model with the best prediction performance by using Genetic Algorithm (GA) to optimize the initial weights and thresholds of BPNN. Although this method can stabilize the performance of BPNN to a certain extent, the training time of BP neural network is greatly increased due to the complex operations such as GA mutation and hybridization, and the convergence speed is slowed down when approaching the optimal solution, even the phenomenon of early convergence occurs. N.S. Rosli et al. [27] pointed out through tests that the precision of BPNN optimized by particle swarm optimization (PSO) is higher than that optimized by GA. Although PSO is an excellent global optimization algorithm, there are premature convergence and local optimum problems in traditional PSO when solving complex problems [28].

Based on this, a model for predicting NOX emission of diesel engine is established by using PSO algorithm to optimize the initial weight and threshold of BPNN. In this model, PSO algorithm optimization adopts non-linear dynamic weight strategy and synchronous learning factor strategy, namely PSOBP model.

**Experimental Setup and Data Collection**

In this study, experiments were performed on a 7L supercharged, electronically controlled, high-pressure common rail diesel engine. The main specifications of the experimental engine are presented in Tables 1.

| Form                                  | Six Cylinders, Four Strokes, Water Cooling Four Valves |
|---------------------------------------|-------------------------------------------------------|
| Displacement (L)                      | 7.14                                                  |
| Cylinder Diameter×Stroke (mm×mm)      | 108×130                                                |
| Connecting Rod Length (mm)            | 210                                                   |
| Compression Ratio                     | 18:1                                                  |
| Rated Power (kW@rpm)                  | 199@2300                                               |
| Maximum Torque (N.m@rpm)              | 1080@1300~1600                                        |
| Idle Speed (rpm)                      | 600±50                                                 |
| Explosive Pressure Limit (MPa)        | 16.5                                                   |
| Fire Order                            | 1-5-3-6-2-4                                           |
| Emission Limitation Phase             | Standard VI after SCR matching                        |

In order to get enough training and test data, more than 30 hours were spent on the test-bed. In the test-bed test results, 120 operating points are selected. In addition, 85 of the 120 selected operating points are selected as training data of the model, and 35 operating points are selected as test data of the model. Some of the test data are shown in Table 2 below.

**BPNN Prediction Model Optimization Method**

When PSO algorithm is adopted to optimize the initial weights and thresholds of BPNN network, the initial weights and thresholds of BPNN model are taken as optimization objectives. For ease of understanding, the particles that need to be optimized can be regarded as a chromosome, while the weights or thresholds that need to be optimized can be regarded as genes on the chromosome, and their length is the number of optimized values, as shown in Figure 1.
Table 2. Data of some test sample points.

| Serial Number | Speed (rpm) | Load (%) | Fuel-Air ratio (-) | Exhaust Temperature (°C) | NOX (ppm) |
|---------------|-------------|----------|--------------------|--------------------------|-----------|
| 1             | 700         | 10.      | 0.14               | 164                      | 378.69    |
| 2             | 800         | 40       | 0.37               | 287                      | 1104.68   |
| 3             | 900         | 50       | 0.49               | 357                      | 1532.39   |
| 4             | 1100        | 90       | 0.83               | 514                      | 1292.54   |
| 5             | 1200        | 10       | 0.19               | 239                      | 388.30    |
| 6             | 1300        | 75       | 0.73               | 498                      | 2152.75   |
| 7             | 1400        | 60       | 0.62               | 454                      | 2004.89   |
| 8             | 1500        | 60       | 0.61               | 436                      | 2376.00   |
| 9             | 1700        | 10       | 0.23               | 252                      | 527.39    |
| 10            | 1800        | 60       | 0.57               | 416                      | 2198.93   |
| 11            | 2100        | 92       | 0.52               | 403                      | 1784.14   |
| 12            | 2300        | 90       | 0.56               | 457                      | 1771.54   |

Among them, $W_1$ is the number of weights between input neurons and hidden layer neurons, $T_1$ is the threshold number of neurons in the hidden layer, $W_2$ is the number of weights between the neurons in the hidden layer and those in the output layer, $T_2$ is the threshold number of neurons in the output layer, $D$ is the dimension of particles.

In addition, before optimization, particle swarm optimization algorithm needs to initialize all individual particles, each particle contains a set of initial weights and thresholds. In the process of optimization, Root Mean Square Error (RMSE) is used as the fitness function of a single particle in particle swarm optimization. The ultimate goal of optimization is to find the initial weight and threshold value when the root mean square error is minimum. When the number of iterations reaches the maximum, the optimal initial weights and thresholds are assigned to BPNN and trained. When the training time reaches the maximum or the preset error, the BPNN after training is tested and the test results are output.

Establishment of PSOBP Model

BP network Structure

As one of the most popular learning algorithms, BPNN is a multi-layered feed-forward neural network with one input layer, one or more hidden layers and one output layer. In general, a three-layer BP network with one hidden layer could approximate any nonlinear function [25]. The BP network structure in this paper has three layers, and the number of neurons in input layer $I=4$; the number of neurons in the output layer $O=1$; the number of neurons in the hidden layer $H=50$.

PSO Strategy Improvement

PSO is a population stochastic optimization algorithm based on the principle of social psychology proposed by J. Kennedy et al. [29]. Unlike evolutionary algorithms such as GA, PSO does not use complex operations such as selection and crossover, which makes PSO converge faster and has fewer parameters. In PSO, each particle is an individual in the search space, and the current position of the particle can be considered as a feasible solution to the corresponding optimization problem. According to the individual extreme value of the particle and the change of the global extreme value of the population, the velocity and position of the particle can be adjusted [30].

Inertial Weighting Strategy. Y. Shi et al. [31] improved the particle velocity update formula by introducing the inertial weight factor $\omega$. The improved particle velocity update formula is as follows:

\[
v_{id}^{t+1} = \omega \times v_{id}^t + c_1 \times r_1 \times (g_{id}^t - x_{id}^t) + c_2 \times r_2 \times (z_{id}^t - x_{id}^t)
\]  

(1)
Among them, \( r_1 \) and \( r_2 \) are random numbers evenly distributed in the interval \((0, 1)\). \( c_1 \) and \( c_2 \) are positive learning factors. \( \omega \) determines the influence of the flying speed of the generation of particles on the flying speed of the contemporary particles. When \( \omega \) value is large, it is advantageous to global search; on the contrary, it is advantageous to local search. In the common linear inertia weight strategy, the linear descent of \( \omega \) value is fixed [32]. However, for specific practical problems, the decreasing range of \( \omega \) value is different in each iteration. If it is difficult to find the optimal value at the beginning of iteration, then with the decreasing of \( \omega \) value, it is likely that because the decreasing range is too large or too small, the local optimal value will appear. Therefore, in order to balance the local and global search ability of PSO and overcome the shortcomings of linear descending inertia weight strategy, a non-linear dynamic inertia weight strategy [33], whose inertia weight automatically changes with the value of particle fitness function, is introduced in this paper. Its expression is as follows:

\[
\omega = \begin{cases} 
\omega_{\text{min}} - \frac{(\omega_{\text{max}} - \omega_{\text{min}}) \times (f_{i,t} - f_{1,\text{min}})}{f_i - f_{1,\text{min}}}, & f_{i,t} \leq f_i \\
\omega_{\text{max}}, & f_{i,t} > f_i
\end{cases}
\]

(2)

Among them, \( \omega_{\text{max}} \) and \( \omega_{\text{min}} \) are the maximum and minimum values of inertia weight respectively, \( f_{i,t} \) is expressed as the fitness function value of the \( i \)-th particle of the \( t \)-th generation, \( f_i \) is expressed as the average of the fitness function of all particles of the \( t \)-th generation, \( f_{1,\text{min}} \) is expressed as the minimum fitness value of the \( t \)-th generation particle.

This strategy can make the particle approach the optimal search space better, because when the fitness function value of the particle is less than the average fitness function value, it means that such an example has approached the global optimal solution, and appropriately reducing its inertia weight can enhance its local search ability. While for particles whose fitness function value is larger than fitness function value, increasing their inertia weights can make them have better global search ability, thus effectively avoiding local optimum values.

**Learning Factor Strategy.** In the PSO algorithm, the learning factors \( c_1 \) and \( c_2 \) can be understood as the recall of the particle's own historical experience and the overall historical experience, reflecting the tendency of the particle to approach the individual optimal position and the global optimal position [30]. The standard learning factor strategy is usually used, i.e. \( c_1 = c_2 \). However, for specific problems, the optimal solution does not necessarily appear when \( c_1 = c_2 \). Therefore, a Synchronous Learning Factor Strategy [34], which changes with the number of iterations \( t \), is adopted. And its formula is as follows:

\[
c_1 = c_2 = \frac{c_{\text{max}} - c_{\text{min}}}{G_{\text{max}}} \times t
\]

(3)

Among them, \( c_{\text{max}} \) is the maximum learning factor and \( c_{\text{min}} \) is the minimum learning factor.

**Results and Discussion**

In order to investigate the feasibility and reliability of the predicted results of the algorithm, the following three evaluation indicators are used: Mean Absolute Percentage Error (MAPE), Coefficient of Determination (\( R^2 \)) and Pearson correlation coefficient (\( r \)).

**Prediction Performance Analysis of BPNN Model**

The training sample data and test sample data are imported into the BPNN model (where the initial weights and thresholds in the BPNN model are randomly defined). After training, the test sample data were tested. Table 3 shows the results of 10 tests.

As can be seen from the above table, the prediction results of BPNN model are not ideal. On the one hand, the MAPE of the BPNN model varies greatly, ranging from 20% to 40%. The minimum
value was 12.701% in the 5th test. The maximum occurred in the 10th test, when the value exceeded 40%. On the other hand, it is known from the $R^2$ and $r$ obtained by the test that the fitting effect of the model is unsatisfactory. According to the statistical analysis of the predicted value of each model, it is found that it is feasible to take the average value of ten tests as the predicted value of the model. Because the predicted results have met the pre-set significance level of the study ($\alpha=0.05$).

| Testing times | $r$   | $R^2$  | MAPE (%) |
|---------------|-------|--------|-----------|
| 1             | 0.96148 | 0.92445 | 13.5784   |
| 2             | 0.9097  | 0.82755 | 24.8058   |
| 3             | 0.95874 | 0.91919 | 29.0441   |
| 4             | 0.94563 | 0.89421 | 20.8773   |
| 5             | 0.95826 | 0.91826 | 12.7003   |
| 6             | 0.84449 | 0.71316 | 14.8994   |
| 7             | 0.97419 | 0.94905 | 13.4712   |
| 8             | 0.97272 | 0.94619 | 20.7139   |
| 9             | 0.88148 | 0.777   | 33.9779   |
| 10            | 0.87599 | 0.76736 | 40.2744   |

Figure 2 shows the comparison between the average value and the real value of ten tests of BPNN model and the relative error between them. It can be seen from the graph that although there is sizeable slippage between the predicted value and the real value of the sample points, the NO\textsubscript{X} concentration curve predicted by BPNN model has the same trend as the true NO\textsubscript{X} concentration curve. Therefore, it is feasible to use BPNN model to predict NO\textsubscript{X} emission of diesel engine, although the predicted results are not so satisfactory.

**Predictive Performance Analysis of PSOBP Model**

By analyzing the prediction performance of BPNN model, it can be determined that the selection of initial weights and thresholds has a great impact on the prediction performance of BPNN model. Therefore, it is necessary to take appropriate methods to optimize the value of initial weights and thresholds.

In this paper, a PSOBP model using non-linear dynamic inertia weight strategy and synchronous learning factor strategy is established. In order to verify the superiority of the strategy adopted by the established PSOBP model, a set of comparison models is established, in which the PSO
algorithm adopts linear weighting strategy and learning factor strategy ($c_1 = c_2$), which is referred to as PSOBPC model. Table 4 shows the results of ten tests for these two models.

As can be seen from the above table, no matter what strategy PSO algorithm is adopted to optimize BPNN's initial weight and threshold model, the influence of initial weight and threshold on BPNN's performance can be reduced and the accuracy of model prediction can be improved. On the one hand, PSOBPC model and PSOBP model have high $r$ value and $R^2$ value, and the $r$ value and $R^2$ value of the two models are both higher than 0.98 and 0.96 respectively, which to some extent reflects the feasibility of using PSO algorithm to improve the performance of BPNN. On the other hand, compared with BPNN model, the MAPE values of the two models are improved greatly. For the PSOBPC model, its MAPE value range is less than 25% and the minimum value is 7.209%. For PSOBP model, the improvement effect is more obvious, its MAPE value ranges within 10% and around 8%, with a small variation range and more stable model performance.

Therefore, the PSOBP model is feasible to predict NO\textsubscript{X} emission of diesel engine, and its prediction results have certain reliability. Fig. 3 (a) and Fig. 3(b) respectively show the comparison and relative error between the average and the true values of the ten tests of the two models.

According to figure 3 (a), the trend of NO\textsubscript{X} curve of PSOBPC model and PSOBP model is basically consistent with the actual value of NO\textsubscript{X} curve, and the predicted value of the two models on a large number of points is basically consistent with the actual value.

| Testing times (-) | PSOBPC model | PSOBP model |
|-------------------|--------------|--------------|
|                   | $r$ (-)      | $R^2$ (%)    | MAPE (%) | $r$ (-)      | $R^2$ (%)    | MAPE (%) |
| 1                 | 0.982        | 0.965        | 12.669    | 0.988       | 0.976        | 8.905    |
| 2                 | 0.986        | 0.971        | 7.801     | 0.990       | 0.981        | 9.758    |
| 3                 | 0.985        | 0.970        | 12.605    | 0.984       | 0.968        | 8.802    |
| 4                 | 0.989        | 0.977        | 7.209     | 0.987       | 0.974        | 8.108    |
| 5                 | 0.982        | 0.964        | 13.290    | 0.990       | 0.981        | 7.249    |
| 6                 | 0.984        | 0.968        | 8.591     | 0.992       | 0.983        | 7.399    |
| 7                 | 0.980        | 0.959        | 12.948    | 0.990       | 0.980        | 8.760    |
| 8                 | 0.985        | 0.970        | 24.785    | 0.988       | 0.977        | 8.189    |
| 9                 | 0.986        | 0.973        | 9.760     | 0.988       | 0.975        | 8.789    |
| 10                | 0.987        | 0.974        | 10.253    | 0.984       | 0.968        | 8.079    |

It can be seen from figure 3 (b) that, compared with the BPNN model, the relative error range between the predicted value and the actual value of sample points in the PSOBPC model and the PSOBP model is greatly reduced. Among them, the decrease of PSOBP model is more obvious, and the relative error of most sample points is between 10%.
This clearly indicate that it is feasible to optimize the initial weight and threshold of BPNN by PSO algorithm, and establish the corresponding prediction model of NO\textsubscript{X} emission of diesel engine. Moreover, the non-linear weight strategy and learning factor strategy for PSO algorithm can make the prediction result of the model closer to the actual value.

**Performance Comparison of Three Models**

In this paper, the Sum of Squares for Errors (SSE), Mean Square Errors (MSE) and Root Mean Square Errors (RMSE) are used to show more intuitively the difference of the predictive performance of the three models, and the results are shown in Table 5. Although BPNN model can be used to predict NO\textsubscript{X} emission of diesel engine, its prediction results are not accurate due to the large influence of initial weight and threshold. By using PSO algorithm to optimize the initial weights and thresholds of BPNN model, the influence of initial weights and thresholds on the prediction results of BPNN model can be reduced to some extent, and the reliability of the prediction results can be improved. Among them, the PSOBP model using nonlinear dynamic weight strategy and synchronous learning factor strategy can improve the prediction performance of BPNN more obviously than the PSOBPC model using general linear weight strategy and learning factor strategy.

|             | BPNN  | PSOBPC | PSOBP  |
|-------------|-------|--------|--------|
| AAE         | 0.0650| 0.0629 | 0.0558 |
| MSE         | 0.1085| 0.0095 | 0.0055 |
| RMSE        | 0.3295| 0.0974 | 0.0739 |

**Conclusion**

In this paper, a PSOBP model for predicting NO\textsubscript{X} emission from diesel engine is established by taking four parameters as input: speed, load, and exhaust temperature and fuel-air ratio. Although the BPNN model can also predict the emission of NO\textsubscript{X}, the prediction effect of the model is not ideal due to the great influence of initial weights and thresholds on the performance of the BPNN model, and its MAPE value is between 10\%~40\%.

The study shows that the established PSOBP model can effectively reduce the influence of initial weights and thresholds on the prediction performance of BPNN. The test shows that the MAPE value of PSOBP model is floating around 8\%, and \( r \) and \( R^2 \) are above 0.98 and 0.96 respectively. Compared with traditional BPNN model, PSOBP model not only improves the accuracy of prediction results, but also makes the prediction results more stable. In addition, compared with the PSOBPC model, although the fitting effect of the PSOBP model is very similar to that of the PSOBPC model, but the PSOBP model has more reliable prediction accuracy, the AAE, MSE and RMSE values of PSOBP model were 0.0558, 0.0055 and 0.0739, respectively.

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