

Study on prediction and spatial variation of PM_{2.5} pollution by using improved BP artificial neural network model of computer technology and GIS

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Abstract

Atmospheric pollutant PM_{2.5} seriously harm to human health, to accurately predict its pollution condition, can avoid or reduce the risk of pollution events. In this study, we used the different algorithms and number of hidden layer neurons to improve BP artificial neural network model of computer technology, coupling GIS to evaluate the impact of different algorithms on the prediction and spatial variation of PM_{2.5}, the results showed that, mean relative error and correlation coefficient of monitoring and predictive value by the six different algorithms and three different number of hidden layer neurons, were 14.02% and 0.97, respectively, indicating that improved BP artificial neural network model can be used to predict PM_{2.5} pollution. Optimization algorithm of trainrp and trainlm had the highest prediction accuracy while the number of neurons in the hidden layer is 20. In contrast, the same algorithm, different number of hidden layer neurons had a greater influence on the simulation of PM_{2.5}. Spatial variation of PM_{2.5} by different algorithms and Inverse Distance Weighted interpolation method has various degrees of difference from that of the observed, although the simulation of north-central high risk area and southeast low risk region are basically consistent to interpolation analysis of monitoring data.

Keywords: artificial neural network model, computer technology, PM_{2.5}, prediction, spatial analysis

1 Introduction

Air Pollution is critically damage to human health and the environment, is important for the sustainable development of social, economic and environmental challenges [1,2]. Accurate prediction of atmospheric pollutant concentrations are people ahead of preparedness and be the basis of control, therefore, to accurately predict the concentration of atmospheric particulate matter has a very important significance.

PM_{2.5} refers to a diameter less than or equal to 2.5 micron in atmospheric particles, often referred to as particulate matter into the lungs or fine particles [3]. Due to small size, easy with toxic and hazardous substances, stay in the atmosphere for a long time, transmission distance and other characteristics, leading to lung cancer and other respiratory diseases and human health damage [4], environmental damage [5], has become the focus of international air pollution prevention and control [6]. Around the distribution of PM_{2.5} pollution monitoring system [7], pollution analysis [8], influence factors [9], modeling and forecasting [10], and other aspects of human health risks, is

one of the hot atmosphere of international environmental studies.

PM_{2.5} is a primary pollutant affecting the air quality in China, the accurate prediction of PM_{2.5} concentrations, can make the people take necessary protective measures to the possible pollution in time, avoid or reduce the dangerous pollution events, has the important means for protecting human health and the environment science and social economy development. Currently PM_{2.5} air pollution forecasting methods are time-series model [11], gene expression programming algorithm [12], gray theoretical models [13,14], empirical coefficient method, multivariate statistical analysis and forecasting models [15], chaos theory and Back Propagation artificial neural network model [16] to study different forecasting methods will be applied to PM_{2.5} research, comparative analysis of the predictive accuracy of each method. BP artificial neural network model due to the uncertainty, multi-input, complex nonlinear problems with good mapping ability to create very complex nonlinear model in the field of atmospheric pollution prediction has a strong advantage. BP artificial neural network model was mainly used to time

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series prediction by most studies [17]. However, there is less study on the prediction of PM_{2.5} by using different algorithms and the number of neurons in the hidden layer, and the spatial interpolation analysis by coupling GIS and BP artificial neural network model is also less.

In summary, this study coupling GIS and BP artificial neural network model to evaluate the prediction accuracy of PM_{2.5} by different BP algorithms and hidden layer neurons, analyze the impact of different algorithms and the number of neurons in the hidden layer on simulation results of PM_{2.5}, application of Inverse Distance Weighted method to reveal spatial variation of PM_{2.5}, improving the prediction accuracy and spatial interpolation analysis of PM_{2.5} simulation, provide a scientific basis for prevention and control of PM_{2.5} pollution.

2 The study area

Xi 'an is located in the middle of Weihe river basin in the Guanzhong basin (E107°40' - E109°49', N34°42' - 34°45'33'), is the capital of Shaanxi province, the politics, economy, culture and science and education center, the world famous historical and cultural city. Annual average temperature was 13.0°C - 13.7°C (Figure 1).

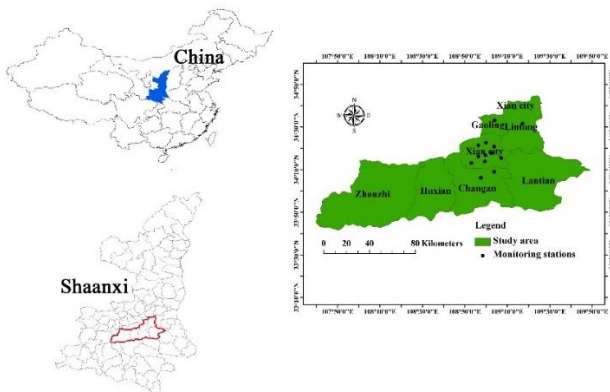


FIGURE 1 The study area of Xi'an in Shaanxi province, China

3 Materials and methods

3.1 BP ARTIFICIAL NEURAL NETWORK MODEL

BP artificial neural network model can automatically inductive rules from the known data, obtained the data of the inherent law, and have a strong nonlinear mapping ability. BP network is multilayer feed forward neural network based on error back propagation algorithm, each neuron connection, no layer coupling and feedback coupling. BP neural network for an output samples, after the weights and thresholds, and transfer function after operation, get an output, then compared with the desired samples, if there is deviation, starting from the output back propagation the deviation for weights and thresholds adjustment, so that network output is consistent with the hope output gradually.

3.2 DIFFERENT ALGORITHMS OF BP ARTIFICIAL NEURAL NETWORK MODEL AND HIDDEN LAYER NEURONS SETTINGS

3.2.1 Traingdm

Additional momentum gradient descent method. The method is based on the back propagation method, the weights change with each value of a ratio of the weight change in the previous and the change from the reverse spread to generate new weight values:

$$dX = mc \times dX_{prev} + lr \times (1 - mc) \times dperf / dX, \tag{1}$$

where *Prev* is the argument round learning, *mc* is momentum.

3.2.2 Traingda

Adaptive learning step method. Learning step can be adjusted based on the error performance function can be solved in the standard BP learning step the problem of improper selection.

$$mse(k + 1) < mse(k), lr = lr_inc \times lr \uparrow, \tag{2}$$

$$mse(k + 1) > 1.04 \times mse(k), lr = lr_dec \times lr \downarrow, \tag{3}$$

$$mse(k) < mse(k + 1) < 1.04 \times mse(k), lr, \tag{4}$$

where *mse* is the mean square error, *lr* is learning step.

3.2.3 Trainrpf

Flexible BP algorithm. This method eliminates the harmful effects of the size of the partial derivative of weights, using only symbols right direction derivative update, regardless of the size of the derivative.

$$dX = deltaX .* sign(gX), \tag{5}$$

where *gX* is the gradient, *deltaX* is updated weights value will be corrected in accordance with *gX* and symbols that appear repeatedly similarities and differences.

3.2.4 Trainscg

Trainscg conjugate gradient method. The method converges faster than ordinary gradient descent is much faster. Does not require a linear search more than the number of iterations required for the first three methods, but the amount of calculation for each iteration is much smaller.

3.2.5 Trainlm

Trainlm is the Levenberg-Marquardt optimization algorithm, this method of learning very fast, for medium-sized networks, is the best kind of training algorithm:

$$dX = -(jX^T \times jX + I \times mu)^{-1} jX^T \times E, \tag{6}$$

where *jX* is differential weights for the error on the Jacobian matrix, *E* is the error vector, *mu* for the adjustment amount.

3.2.6 Trainoss

Step secant method. As a compromise gradient and Newton's method conjugate:

$$dX = -gX + Ac \times X_step + Bc \times dgX, \tag{7}$$

where dgX is the latest iteration of the gradient, Ac and Bc is a new adjustment parameter search direction.

3.2.7 Hidden layer neurons settings

The number of hidden layer neurons is an important factor affecting the accuracy of the $PM_{2.5}$ prediction, help simulate more stable and accelerate convergence in the training. Based on existing research and many experiments, the number of neurons in the hidden layer was selected 5, 10 and 20 in this study.

3.3 INVERSE DISTANCE WEIGHTED INTERPOLATION METHODS

The principle of Inverse Distance Weighted method is each sampling on the result of interpolation weakened with the increase of distance, therefore, the right distance from the target point near the samples given greater weight. It is a global interpolation method, that is, all samples are estimated to be involved in a point estimate of Z values. Calculated as follows:

$$v_e = \sum_{j=1}^n w_j v_j, \tag{8}$$

where v_e ($j = 1, \dots, n$) is the point (x_j, y_j) of variable value, w_j is the weight corresponding to the coefficients.

3.4 EVALUATION OF PREDICTION ACCURACY

In order to evaluate the prediction accuracy of $PM_{2.5}$ of different algorithms and number of hidden layer neurons by using the BP artificial neural network model, the relative error and correlation coefficients were used in this study, each index is calculated as follows:

$$\Delta = \frac{1}{n} \sum_{i=1}^n \left(\frac{|S_i - O_i|}{O_i} \right) \times 100\%, \tag{9}$$

$$r = \frac{\sum_{i=1}^n (S_i - \bar{S}) \times (O_i - \bar{O})}{\sqrt{\sum_{i=1}^n (S_i - \bar{S})^2 \times \sum_{i=1}^n (O_i - \bar{O})^2}}, \tag{10}$$

where S_i is the simulated data, O_i is the observed data.

3.5 DATA COLLECTION

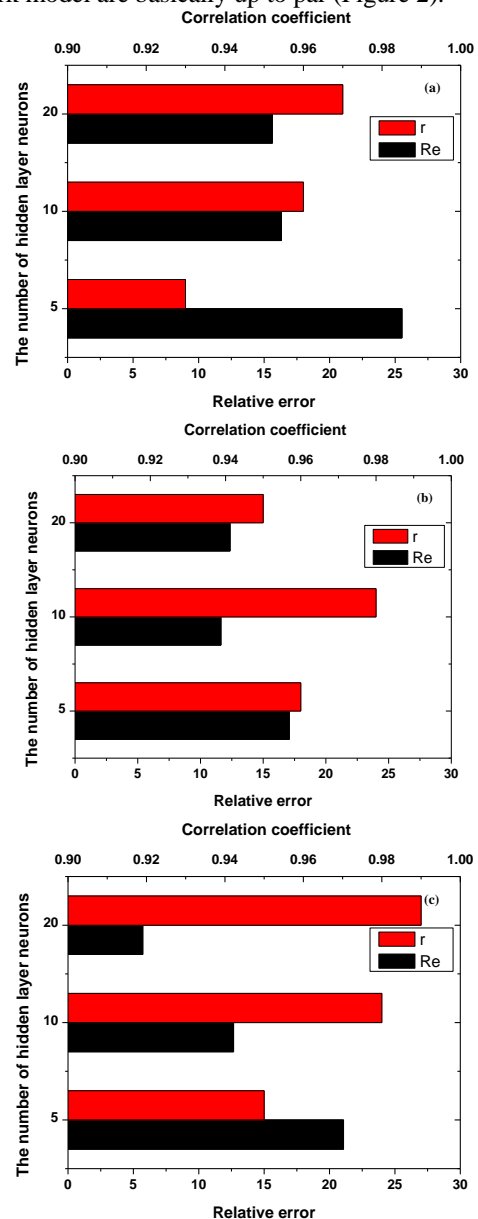
Research data including daily $PM_{2.5}$ monitoring data from January to December in 2013 and from January to June of 2014, including 13 monitoring stations, which are high-voltage switchgear plant, Xingqing district, the textile city,

hamlet, the people of the stadium, high-tech zone, Economic Development zone, Chang'an District, Yanliang District, Lintong District, Qujiang District, Guangyuntan and marsh. The spatial data of study area boundary, and latitude and longitude data of monitoring site.

4 Results and analysis

4.1 EVALUATION OF $PM_{2.5}$ PREDICTION ACCURACY BY DIFFERENT ALGORITHMS AND HIDDEN LAYER NEURONS

The Figure 2 shows that correlation coefficient of $PM_{2.5}$ value of prediction and observation by six different algorithms and three different number of hidden layer neurons, achieves 0.93 and above. The relative error is within 25.52%, prediction accuracy of different algorithms and the number of hidden layer neurons by BP artificial neural network model are basically up to par (Figure 2).



4.2 EFFECT OF DIFFERENT ALGORITHMS AND THE NUMBER OF HIDDEN LAYER NEURONS ON PM_{2.5} SIMULATION RESULTS

Different algorithms and the number of hidden layer neurons by BP artificial neural network model have different degrees of influence on PM_{2.5} simulation results. Overall, the Figure 3 shows that PM_{2.5} simulation effect by different algorithms and the number of hidden layer neurons is consistent with the observed value, but there are some differences. In contrast, the same algorithms, different number of hidden layer neurons had a greater influence on the simulation of PM_{2.5}, with the increase of the number of hidden layer neurons, PM_{2.5} prediction accuracy show the increasing trend. However, different algorithms, the same number of hidden layer neurons had a less effect on the PM_{2.5} prediction.

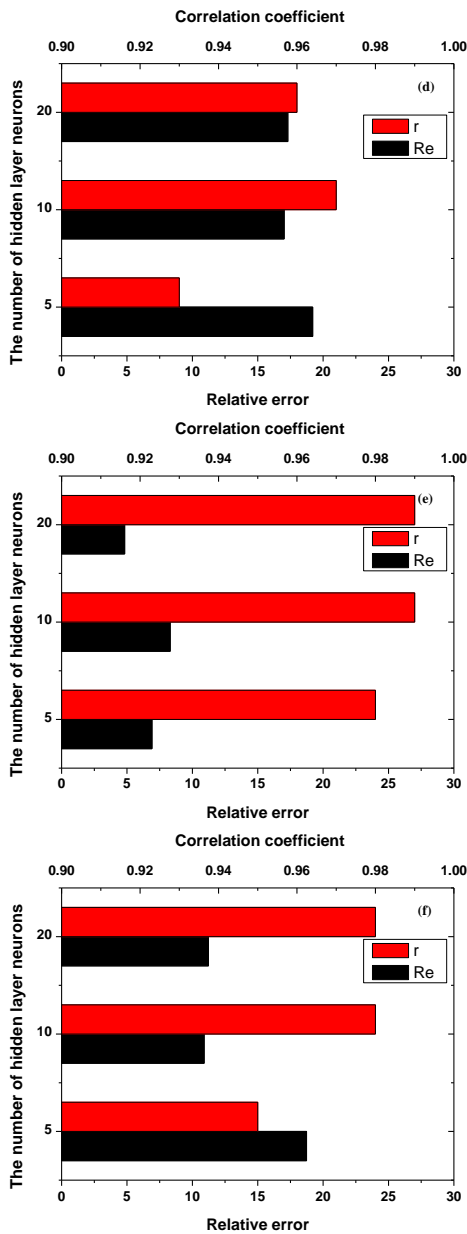
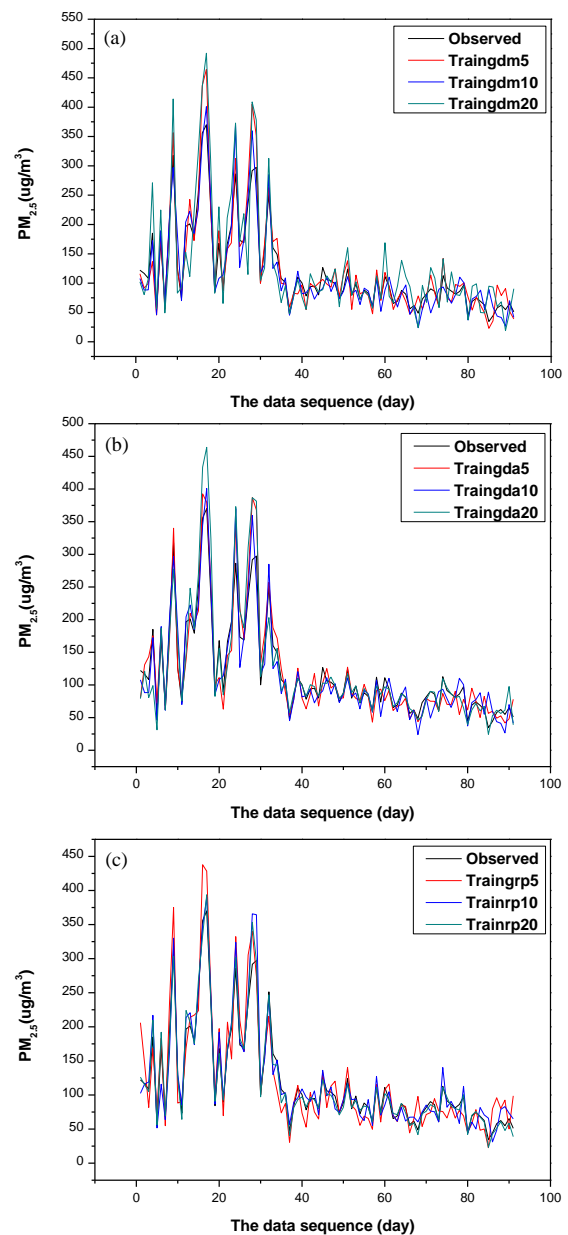


FIGURE 2 Relative error and correlation coefficient of PM_{2.5} predicted and observed value by different algorithms and the number of hidden layer neurons:

a) Traingdm, b) Traingda, c) Trainr, d) Trainscg, e) Trainlm, f) Trainoss

From the overall analysis, the relative error of trainlm algorithm was smallest while number of hidden layer neurons is 20, and the relative error is 4.82%, in contrast, the relative error of traingdm algorithm was biggest while number of the hidden layer neurons is 5, and the relative error is 25.52%. The correlation coefficient is 0.99, including that trainrp algorithm while number of neurons in the hidden layer is 20 and trainlm algorithm while number of hidden layer neurons is 10 and 20. The relative error is within 10%, consisting of trainrp algorithm while number of neurons in the hidden layer is 20 and trainlm algorithm while number of hidden layer neurons is 5, 10 and 20, respectively. The trainlm and trinrp algorithms have the highest prediction accuracy of PM_{2.5} while the number of neurons in the hidden layer is 20.



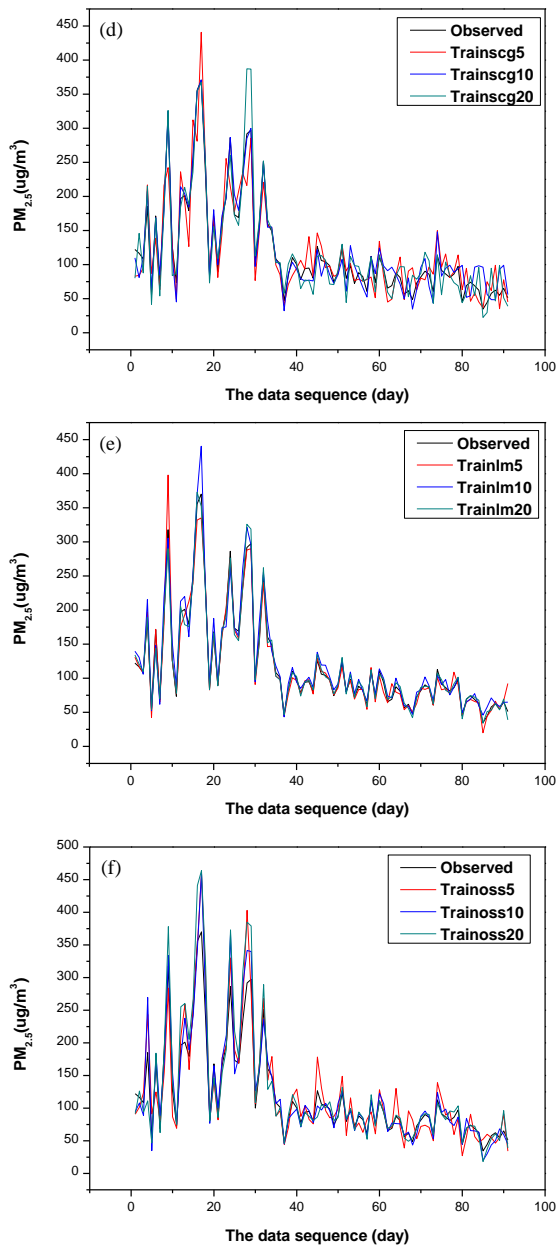


FIGURE 3 PM_{2.5} prediction results by different algorithms and the number of hidden layer neurons:

a) Traingdm, b) Traingda, c) Trainrp, d) Trainscg, e) Trainlm, f) Trainoss

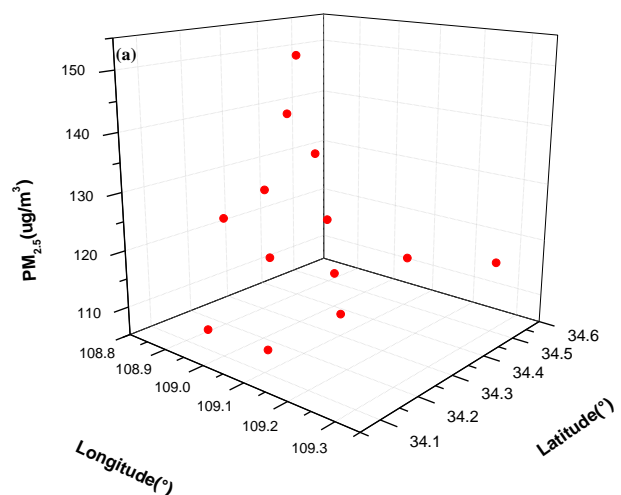
Specific analysis, comparison of simulated and observed values of PM_{2.5} by additional momentum gradient descent method traingdm while number of neurons in the hidden layer from 5 to 10, the absolute error showed declining trend, with the number of hidden layer neurons increasing from 10 to 20, traingdm algorithm performs further decreasing trend, PM_{2.5} simulation accuracy by traingdm algorithm presents increasing trend. Comparison of simulation and monitoring of PM_{2.5} values by adaptive learning traingda algorithm while number of hidden layer neurons from 5 to 10, the absolute error performs declining trend, traingda algorithm showed an increasing trend with the increase in the number of neurons in the hidden layer from 10 to 20, PM_{2.5} simulation accuracy by traingda

algorithm presented increase or decrease trend. Comparison of simulated and observed values of PM_{2.5} by flexible algorithm trainrp while number of hidden layer neurons from 5 to 10, the absolute error performs constantly decreasing trend, and trainrp algorithm presents further decreasing trend while number of neurons in the hidden layer from 10 to 20. The results show that with the increase in the number of hidden layer neurons, PM_{2.5} simulation accuracy by trainrp algorithm presents increasing trend.

Comparative speaking, absolute error of simulated and observed value showing declining trend by using the conjugate gradient method trainscg while number of neurons in the hidden layer from 5 to 10, trainscg algorithm showed an increasing trend with the increase in the number of neurons in the hidden from 10 to 20, PM_{2.5} simulation accuracy by trainscg algorithm presents increase or decrease trend. Comparison of simulation and monitoring of PM_{2.5} by using Levenberg-Marquardt optimization algorithm trainlm while number of hidden layer neurons from 5 to 10, the absolute error showed increasing trend, trainlm algorithm showing declining trend with the increase in the number of neurons in the hidden layer from 10 to 20, simulation accuracy by trainlm algorithm presents increase or decrease trend. Absolute error of simulated and observed value showing declining trend by using the step secant method trainoss while number of neurons in the hidden layer from 5 to 10, trainoss algorithm showed an increasing trend with the increase in the number of neurons in the hidden layer from 10 to 20, PM_{2.5} simulation accuracy by trainoss algorithm performs increasing trend.

4.3 PM_{2.5} DISTRIBUTION CHANGES OF DIFFERENT MONITORING SITES BY DIFFERENT ALGORITHMS

Figure 4 shows that daily average concentration of PM_{2.5} in different monitoring sites is relatively close, the same change trend, but there is a difference on the distribution.



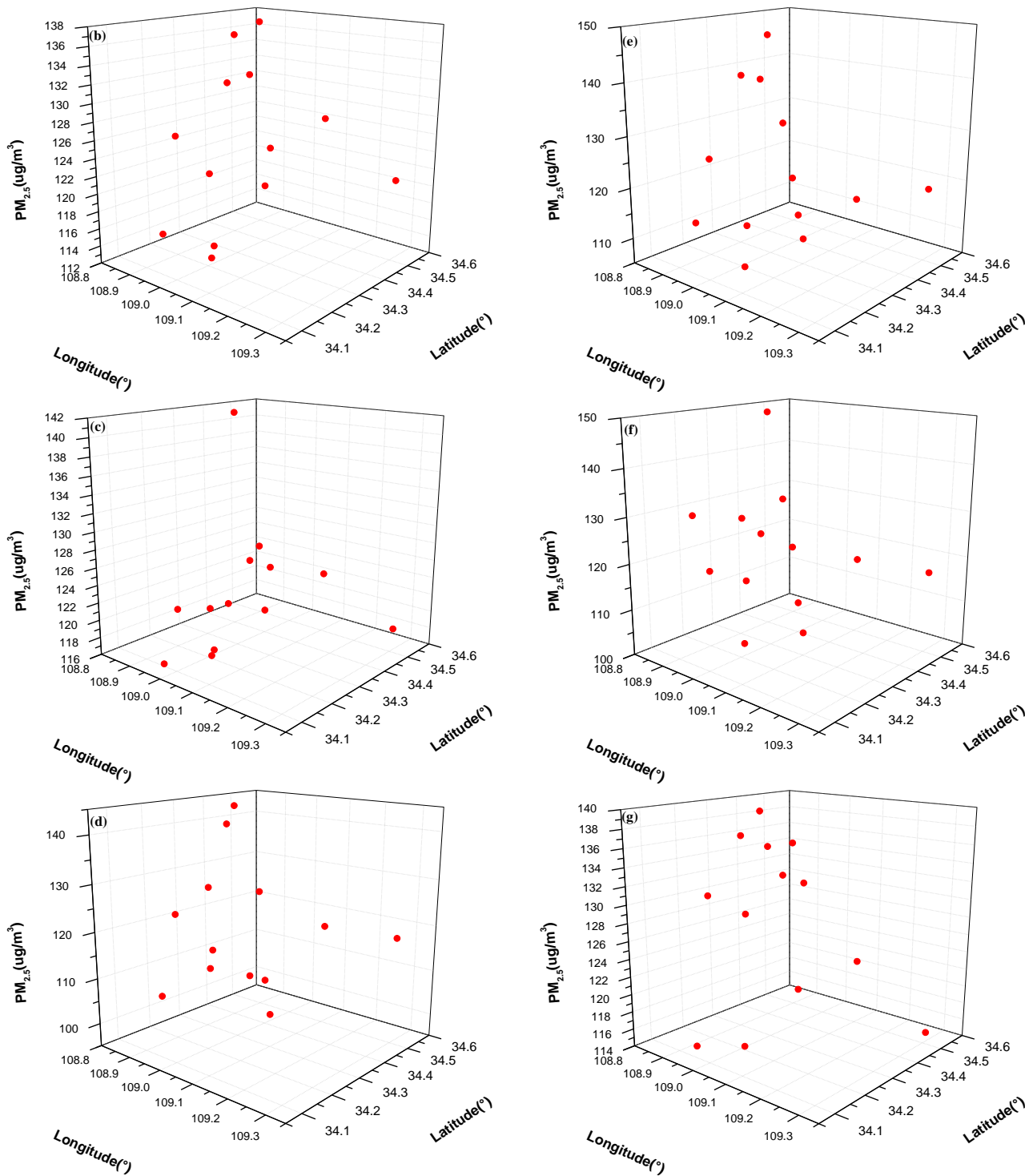


FIGURE 4 Daily average concentration of PM_{2.5} of different monitoring stations by different algorithms:
 a) Observed, b) Traingdm, c) Traingda, d) Trainrp, e) Trainscg, f) Trainlm, g) Trainoss

Distributed simulation of PM_{2.5} by traingdm (Figure 4b) algorithm is basically in accordance with observed values in Figure 4a but the peak is less than the monitoring values. In contrast, traingda algorithm (Figure 4c) simulated the distribution of PM_{2.5} and monitoring values (Figure 4a) are quite different, uneven distribution and are mainly distributed in the region of peak and low value by traingda algorithm. Distributed simulation of PM_{2.5} by trainrp algorithm (Figure 4d) is more consistent with the monitoring

data (Figure 4a), but simulation of peak and low value are quite different. Trainscg (Figure 4e) and trainlm (Figure 4f) algorithms simulated the distribution of PM_{2.5} are basically in accordance with observed values (Figure 4a). The difference between trainoss algorithm (Figure 4g) and observed values (Figure 4a) are that, the peak is less than the monitoring values and are mainly distributed in the region of peak and low by trainoss algorithm.

4.4 SPATIAL DISTRIBUTION CHARACTERISTICS OF PM_{2.5} BY DIFFERENT BP ALGORITHMS BASED ON THE INVERSE DISTANCE WEIGHTED INTERPOLATION METHOD OF GIS

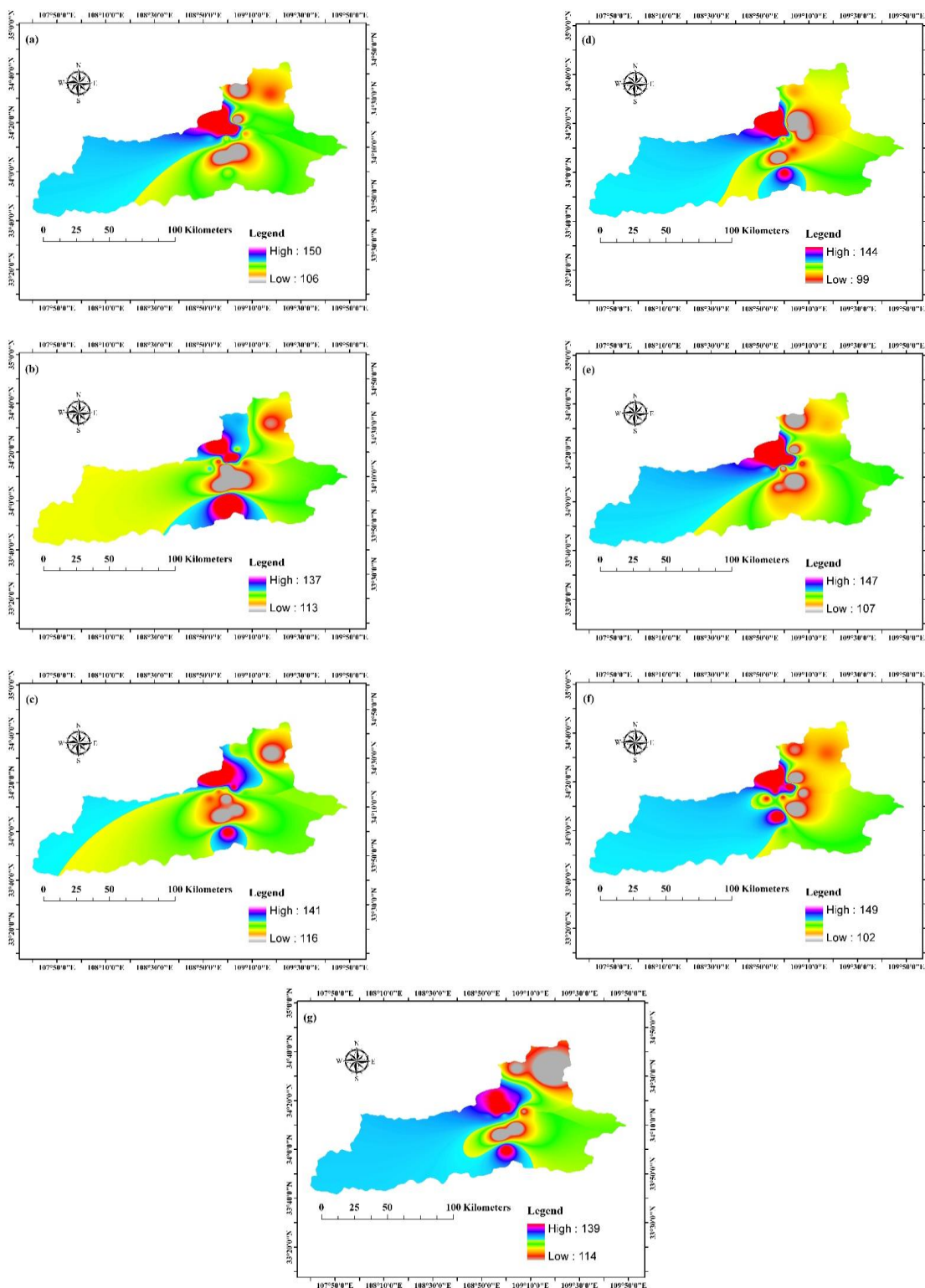


FIGURE 5 PM_{2.5} spatial distribution by different algorithms based on IDW interpolation method (Unit: $\mu\text{g}/\text{m}^3$): a) Observed, b) Traindm, c) Traingda, d) Trainrp, e) Trainscg, f) Trainlm, g) Trainoss

Spatial distribution of PM_{2.5} by different algorithms and IDW interpolation method as is shown in Figure 5.

From the analysis of spatial interpolation results, compared with the monitoring data, different algorithms have various degrees of difference from the spatial distribution of PM_{2.5}. The range of PM_{2.5} monitoring values is 106-150 µg/m³, high-risk areas are mainly located in central and northern, moderate-risk areas in the west and low risk areas in the eastern and south (Figure 5a). Additional momentum gradient descent method *trainngdm* simulated range of PM_{2.5} is 113-137 µg/m³, high-risk areas are mainly located in the central, southern and northeast, moderate-risk areas are mainly distributed in the western, low-risk areas located in the southeast (Figure 5b). The range of simulated PM_{2.5} by adaptive learning step method *trainngda* is 116-141 µg/m³, high-risk areas are mainly distributed in the central and northeastern, moderate risk areas are mainly located in the western, low-risk areas in the eastern and southwestern (Figure 5c).

Comparative speaking, flexible BP algorithm *trainrp* simulated range of PM_{2.5} is 99-144 µg/m³, high-risk areas are mainly located in central and northern, moderate-risk areas are mainly distributed in the western, low-risk areas in the south and east (Figure 5d). Range of simulated PM_{2.5} by conjugate gradient method *trainscg* is 107-147 µg/m³, high-risk areas are mainly located in central and northern, moderate-risk areas are mainly distributed in the western, low-risk areas located in the east (Figure 5e). Levenberg-Marquardt optimization algorithm *trainlm* simulated range of PM_{2.5} is 102-149 µg/m³, high-risk areas are mainly located in central and northern, moderate-risk areas are mainly distributed in the western, low-risk areas in the eastern and south (Figure 5f). Range of simulated PM_{2.5} by step secant algorithm *trainoss* is 114-139 µg/m³, high-risk areas are mainly located in central and northern, moderate risk areas mainly in the west and south, the distribution of low-risk areas in the east (Figure 5g).

5 Conclusions

The paper coupled GIS and BP artificial neural network model to reveal the impacts of different algorithms and the

number of hidden layer neurons on simulation and prediction of PM_{2.5}, evaluation of PM_{2.5} spatial variation by different algorithms based on Inverse Distance Weighted method of GIS, the following main conclusions are reached:

(i) The correlation coefficient of train, validation and test samples of different algorithms by BP artificial neural network model on the whole is greater than 0.8, shows that the BP artificial neural network model in each sample meets the requirements in the process of simulation, can be used in the prediction research of PM_{2.5}. The correlation coefficient is 0.99 including that *trainrp* algorithm while number of hidden layer neurons is 20 and *trainlm* algorithm while that are 10 and 20. The relative error is within 10%, consisting of *trainrp* algorithm while number of neurons in the hidden layer is 20 and *trainlm* algorithm while that are 5, 10 and 20.

(ii) The different algorithms and hidden layer neurons by BP artificial neural network model have various degrees of impact on the PM_{2.5} simulation results. The same algorithm, different number of neurons in the hidden layer have greater impact on PM_{2.5} simulation, the difference is about 20%. Different algorithms, the same number of neurons have less effect on PM_{2.5} prediction, the difference is about 10%.

(iii) Spatial variation of PM_{2.5} by different algorithms based on BP artificial neural network model has various degrees of difference from the interpolation results of observed data, although the spatial distribution of the high and low risk area by different algorithms relatively consistent with the interpolation analysis of observed values.

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