

## Article

# Prediction of PM<sub>2.5</sub> Concentration in Ningxia Hui Autonomous Region Based on PCA-Attention-LSTM

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**Abstract:** The problem of air pollution has attracted more and more attention. PM<sub>2.5</sub> is a key factor affecting air quality. In order to improve the prediction accuracy of PM<sub>2.5</sub> concentration and make people effectively control the generation and propagation of atmospheric pollutants, in this paper, a long short-term memory neural network (LSTM) model based on principal component analysis (PCA) and attention mechanism (attention) is constructed, which first uses PCA to reduce the dimension of data, eliminate the correlation effect between indicators, and reduce model complexity, and then uses the extracted principal components to establish a PCA-attention-LSTM model. Simulation experiments were conducted on the air pollutant data, meteorological element data, and working day data of five cities in Ningxia from 2018 to 2020 to predict the PM<sub>2.5</sub> concentration. The PCA-attention-LSTM model is compared with the support vector regression model (SVR), AdaBoost model, random forest model (RF), BP neural network model (BPNN), and long short-term memory neural network (LSTM). The results show that the PCA-attention-LSTM model is optimal; the correlation coefficients of the PCA-attention-LSTM model in Wuzhong, Yinchuan, Zhongwei, Shizuishan, and Guyuan are 0.91, 0.93, 0.91, 0.91, and 0.90, respectively, and the SVR model is the worst. The addition of variables such as a week, precipitation, and temperature can better predict PM<sub>2.5</sub> concentration. The concentration of PM<sub>2.5</sub> was significantly correlated with the geographical location of the municipal area, and the overall air quality of the southern mountainous area was better than that in the northern Yellow River irrigation area. PM<sub>2.5</sub> concentration shows a clear seasonal change trend, with the lowest in summer and the highest in winter, which is closely related to the climate environment of Ningxia.

**Keywords:** PCA-attention-LSTM; machine learning; PM<sub>2.5</sub>; prediction; meteorological elements



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## 1. Introduction

Air quality in China has been growing worse in recent years. Urban residents need to burn a lot of coal in their lives, especially in winter; rural residents burn the straw of crops; people's car exhaust produces a large number of atmospheric pollutants. According to statistics, China's coal use in 2020 will reach 3.9 billion tons, and coal combustion will produce a large number of atmosphere pollutants. Atmosphere pollutants will not only make the Earth's environment worse and worse but also seriously affect human health. Because of their small diameter, PM<sub>2.5</sub> particles of atmosphere pollutants easily enter the deep respiratory tract of the human body and even penetrate deep into the bronchi and alveoli, which reduces the body's immunity and forms chronic lung diseases, lung cancer, and cardiovascular diseases [1–4]. In recent years, the country and the people have paid more and more attention to the problem of air pollution, and the demand for fast, real-time, and accurate prediction of PM<sub>2.5</sub> concentration is increasing [5,6]. The prediction results of PM<sub>2.5</sub> concentration can better realize environmental management and formulate more effective decision-making plans. The model with high prediction accuracy is also conducive to the prediction of extreme events, thus further contributing to the prevention, preparation, and treatment of extreme air pollution events. The results of this paper provide feasible methods for global climate change and environmental degradation issues mentioned in the

World Summit on Sustainable Development “RIO + 10” held in Johannesburg, and effectively predict the concentration of atmospheric pollutants, which has important guiding significance for global implementation policies and human life orientation.

At present, the methods of predicting PM<sub>2.5</sub> concentration mainly include numerical model forecasting methods based on atmospheric circulation forms and statistical forecasting methods based on machine learning models. The numerical model forecasting method fully takes into account the physicochemical reactions to various atmosphere pollutants and meteorological factors in the form of atmospheric circulation, and mainly uses various meteorological data and emission source data [7–9]. Due to the uncertainty of the emission inventory and the complex response of the pattern, it is difficult for humans to accurately quantify the physical and chemical reactions between various data, and the model is susceptible to the influence of the terrain of the study area, so the prediction error of PM<sub>2.5</sub> concentration is large.

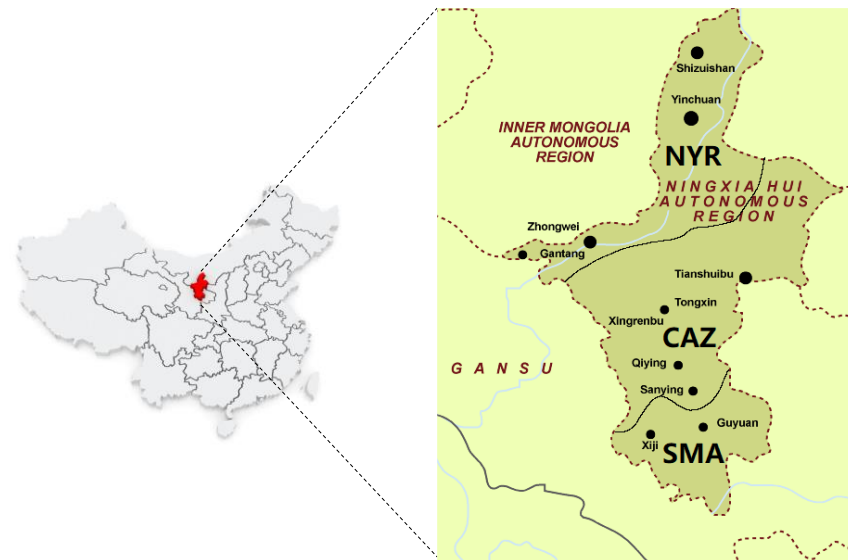
The statistical forecasting method based on machine learning models uses the real-time measurement data for each air monitoring station and meteorological monitoring station, which can predict the pollutant concentration in the study area [10–13]. In recent years, many researchers have begun to study the problem of PM<sub>2.5</sub> concentration prediction based on statistical and machine learning models. Brokamp et al. used satellite, meteorological, atmospheric, and land-use data to train a random forest model to predict daily urban fine particulate matter concentrations, and the model performed well, with overall cross-validation  $R^2 = 0.91$  [14]. Zhao et al. used multiple linear regression models to predict the PM<sub>2.5</sub> concentration in Beijing, China, and the results showed that the regression model based on annual data had goodness-of-fit ( $R^2 = 0.766$ ) and ( $R^2 = 0.875$ ) cross-validity. Regression models based on spring and winter seasonal data were more efficient, reaching goodness-of-fit of 0.852 and 0.874, respectively [15].

Deep learning is a new research direction in the field of machine learning that has risen rapidly since 2006, making significant advances in artificial-intelligence-related technologies. The motivation for deep learning is to build neural networks that simulate the human brain for analytical learning. Compared with traditional machine learning methods, it is more cutting-edge, the model is more complex, and the model understands the data more deeply. Akbal et al. used the hybrid deep learning method to model PM<sub>2.5</sub> in the Turkish capital Ankara, and compared the results with those of random forest regression and multiple linear regression ensemble machine learning methods. The results showed that the proposed hybrid model had the best prediction performance, and the model also performed well in classification tasks, with an accuracy rate of 94% [16]. Therefore, this paper uses a long-term short-term memory neural network (LSTM) based on deep learning to predict PM<sub>2.5</sub> concentration, but due to the complex structure of LSTM, after the correlation analysis of the data, it is found that there is a strong correlation between some input variables, and the information is hypertrophic, which increases the complexity of the model. Therefore, this paper constructs a long short-term memory neural network (PCA-attention-LSTM) model based on principal component analysis (PCA) and attention mechanism, and uses PCA to remove excess information, eliminate the correlation effect between indicators, and reduce the complexity of the model. After statistical analysis of the data, it is found that working days and non-working days also have a certain impact on PM<sub>2.5</sub> concentrations, and this paper combines the daily meteorological element data, air pollutant data, and weekday data of Ningxia Hui Autonomous Region from 2018 to 2020 to build a model. In order to compare the PCA-attention-LSTM model with the traditional machine learning models, this paper uses the SVR model, AdaBoost model, RF model, BPNN model, and LSTM model to predict the concentration of PM<sub>2.5</sub>, and compares them with the PCA-attention-LSTM model, so as to establish a machine learning model with good prediction effect of PM<sub>2.5</sub> concentration. The final results show that the PCA-attention-LSTM proposed in this paper has the best prediction results compared with the basic machine learning models, and the correlation coefficient of the model is between 0.90 and 0.93.

## 2. Data Presentation

### 2.1. Study Area Profiles

Ningxia is located in northwestern China. It is bordered by Shaanxi, Inner Mongolia, and Gansu. It has five prefecture-level cities, namely, Yinchuan, Shizuishan, Wuzhong, Guyuan, and Zhongwei. Ningxia is far from the ocean and is located inland, forming a more typical continental climate, with the characteristics of long winter coldness, short summer heat, warm spring, and early autumn; drought and little rainfall, sufficient sunshine, strong evaporation, wind, and sand; cool south and warm north, wet and dry south, and more meteorological disasters. The geographical location of the Ningxia Hui Autonomous Region on the map of China and the distribution of sites in the Ningxia area are shown in Figure 1. The red area on the left shows the geographical location of the Ningxia Hui Autonomous Region in China, and on the right is the distribution map of topographic and meteorological stations in the Ningxia Hui Autonomous Region. In the map, NYR represents the northern Yellow River, CAZ represents the central arid zone, and SMA represents the southern mountainous area. The three cities of Shizuishan, Yinchuan, and Zhongwei are distributed in NYR District, Wuzhong City is distributed in CAZ District, and Guyuan City is distributed in SMA District.



**Figure 1.** China Ningxia regional division and site distribution.

### 2.2. Sources and Data Presentation

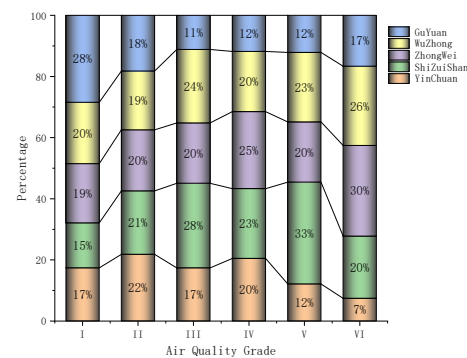
This article uses day-to-day data of  $PM_{2.5}$ ,  $PM_{10}$ ,  $NO_2$ ,  $SO_2$ ,  $O_3$ , and CO from 1 January 2018 to 31 December 2020 in five municipal districts of Ningxia from the website of the National Center for Environmental Information of the National Oceanic and Atmospheric Administration (NOAA—National Centers for Environmental Information, <https://www.ncei.noaa.gov/> (accessed on 5 April 2021)). Day-by-day data are the result of arithmetic averaging based on hourly data. Near-surface conventional meteorological data are derived from the Copernicus Atmosphere Monitoring Service (EAC4-Copernicus Atmosphere Monitoring Service, <https://ads.atmosphere.copernicus.eu/> (accessed on 10 April 2021)) global atmospheric composition reanalysis dataset, which includes the monitoring results of five stations in Ningxia, namely, Tongxin, Yinchuan, Zhongwei, Taole, and Guyuan. Table 1 shows the basic information of the five selected meteorological monitoring stations.

**Table 1.** Basic information of each monitoring station in Ningxia.

Site Number	Monitor the Site Name	Municipal Level	Longitude	Latitude	Elevation (m)
53614	Yinchuan	Yinchuan City	106°12′	38°28′	1110.9
53615	Taole	Shizuishan City	106°42′	38°48′	1101.6
53704	Zhongwei	Zhongwei City	105°11′	37°32′	1226.7
53810	Tongxin	Wuzhong City	105°54′	36°58′	1336.4
53817	Guyuan	Guyuan City	106°16′	36°00′	1752.8

### 2.2.1. Statistical Analysis of Data

According to the new air quality standard of the PM<sub>2.5</sub> testing network, the air quality is divided into six levels: excellent, good, light pollution, moderate pollution, heavy pollution, and serious pollution, by using the daily average concentration of PM<sub>2.5</sub>. The data were integrated, the proportion of air quality grades in five municipal areas were first counted, and the results shown in Figure 2 show that the concentration of Guyuan PM<sub>2.5</sub> in 0–35 accounted for the largest proportion of 28.47%, followed by Wuzhong accounting for 20.1%, Zhongwei accounting for 19%, Yinchuan accounting for 17%, and Shizuishan accounting for the smallest 14.7%. The PM<sub>2.5</sub> dataset was then statistically analyzed, and the results are shown in Table 2. The results showed that among the five cities, the average value of Shizuishan City was 40.26, followed by Wuzhong City at 35.39, Zhongwei City at 35.02, Yinchuan City at 33.90, and Guyuan City at 28.29; the minimum value of Guyuan City was 2, the maximum value was 169, and the standard deviation was 18.79. After a comprehensive comparison, the four statistical indicators of Guyuan City are significantly lower than those of the other four cities. In summary, the overall indicators of Guyuan are better than those of the other four cities, Shizuishan City is the worst, which has a clear correlation with the geographical location of the municipal area, and the overall air quality in the southern mountainous area is better than that in the northern Yellow River irrigation district.

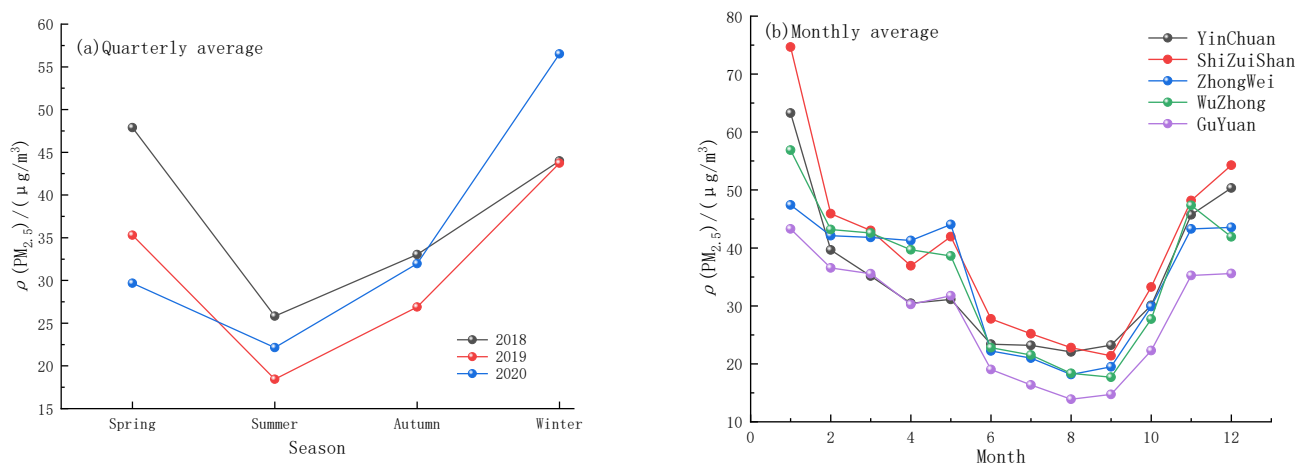
**Figure 2.** Five cities' AQI grade percentage stacked chart.**Table 2.** The main statistical indicators of PM<sub>2.5</sub> in air quality monitoring stations.

Statistical Indicators	Yinchuan	Shizuishan	Zhongwei	Wuzhong	Guyuan
Minimum ( $\mu\text{g m}^{-3}$ )	9	8	4	4	2
Maximum ( $\mu\text{g m}^{-3}$ )	240	207	217	239	169
average value ( $\mu\text{g m}^{-3}$ )	33.90	40.26	35.02	35.39	28.29
standard deviation	20.90	28.03	24.61	26.16	18.79

### 2.2.2. Time Dimension Analysis of PM<sub>2.5</sub> Concentration

Based on the dataset from 2018 to 2020, the three-year data of the five cities are divided according to the four seasons of spring, summer, autumn, and winter. The three-year PM<sub>2.5</sub> concentration data are divided into seasonal means and statistics, and the statistical results are shown in Figure 3a. It can be seen that PM<sub>2.5</sub> concentration is the lowest in summer and the highest in winter. This suggests that the concentration of PM<sub>2.5</sub> is affected by

seasonal changes and may have some correlation with meteorological elements. Therefore, the addition of meteorological factor data can better predict the concentration of PM<sub>2.5</sub>.

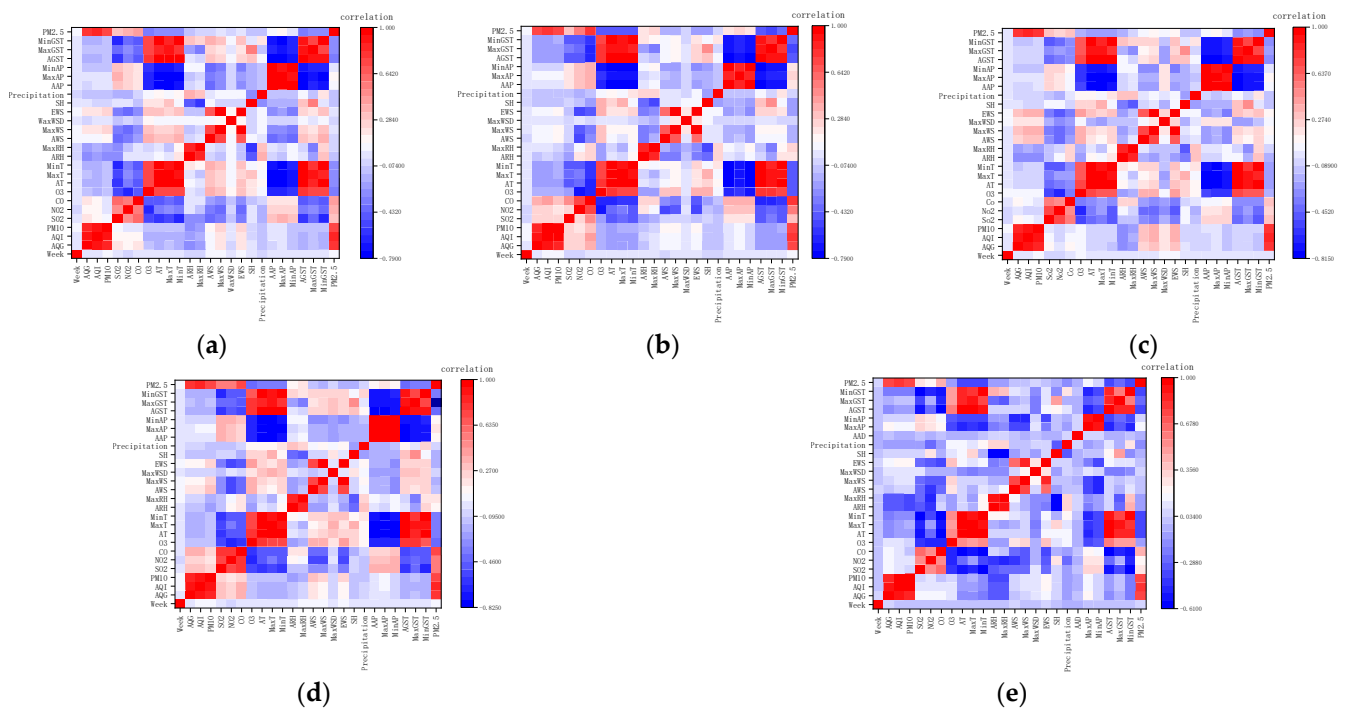


**Figure 3.** Statistics of seasonal and monthly mean value of PM<sub>2.5</sub> concentration. (a) Seasonal mean statistics of PM<sub>2.5</sub> concentration from 2018 to 2020; (b) Monthly mean statistics of PM<sub>2.5</sub> concentration in 5 cities.

The monthly statistics of PM<sub>2.5</sub> concentration data in five cities from 2018 to 2020 were carried out. The average value of PM<sub>2.5</sub> in each city in three years was calculated according to the month, and the statistical data were drawn as the line graph of Figure 3b. It was found that the monthly variation trend of PM<sub>2.5</sub> concentration was obvious. A monthly downward trend began in January until the lowest in June–September, followed by a monthly upward trend from September. It further illustrates the seasonal variation of PM<sub>2.5</sub> concentrations, with the lowest in summer and the highest in winter. First, since coal burning in winter is the main method of household heating and energy supply, this has a strong correlation with the soot emitted by coal and gas or fuel oil during the winter heating process in Ningxia. Secondly, the spring and winter periods in Ningxia have greater wind and sandstorms, and wind disasters and sandstorms are affected by the terrain; generally, there are more Yellow River irrigation areas in the north and fewer mountainous areas in the south. Wind and sand will increase the concentration of PM<sub>2.5</sub> in the atmosphere and make the air quality worse.

### 2.2.3. Variable Correlation Analysis

Variable correlation analysis was performed on the data of five municipal districts to obtain a heat map of the correlation coefficient shown in Figure 4. The results showed a strong positive correlation between air pollution level and PM<sub>2.5</sub> concentration, and the correlation coefficient was 0.78. Four atmospheric pollutants, PM<sub>10</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and CO, also had a strong positive correlation with PM<sub>2.5</sub> concentrations, with correlation coefficients of 0.37 to 0.74. O<sub>3</sub> was inversely correlated with PM<sub>2.5</sub> concentrations, with a correlation coefficient of −0.32. In addition, there was an obvious negative correlation between surface air temperature and PM<sub>2.5</sub> concentration among meteorological factors, and the correlation coefficient was −0.3~−0.35. There is a strong correlation between some input variables, and to eliminate the correlation effect between the variables, the experimental data need to be reduced by principal component analysis (PCA).



**Figure 4.** Correlation coefficient heat plot. (a) Wuzhong; (b) Yinchuan; (c) Zhongwei; (d) Shizuishan; (e) Guyuan.

### 2.3. Data Preprocessing

#### 2.3.1. Data Quality Control

The collected air pollutant data and meteorological factor data of the five cities are subjected to quality control; each feature is checked, and first of all, all data for that day need to be excluded for outliers that are not within the range of a feature value. Second, for the treatment of a feature missing value, it needs to be filled with the average of the two data values adjacent to the missing value. If the value adjacent to it does not exist, all data for that day need to be excluded. Through the quality control of the original 1095 days of data from 2018 to 2020 in five municipal areas, the data of 45 days were deleted and the remaining 1050 days of data were used for research. A total of 26 data on atmospheric pollutants and meteorological elements are available per day. Influencing factors are stated as follows: week, air quality grade (AQG), air quality index (AQI), average temperature (AT), maximum temperature (MaxT), minimum temperature (MinT), average relative humidity (ARH), maximum relative humidity (MaxRH), average wind speed (AWS), maximum wind speed (MaxWS), maximum wind speed (MaxWSD), maximum wind speed (EWS), hours of sunshine (SH), precipitation, average air pressure (AAP), maximum air pressure (MaxAP), minimum air pressure (MinAP), average surface temperature (AGST), maximum surface temperature (MaxGST), and minimum surface temperature (MinGST).

#### 2.3.2. Data Normalization and Data Segmentation

In order to avoid dimensional differences between various factors, this paper uses min–max normalization for data normalization, and the specific functions are as follows:

$$x_k = (x_k - x_{\min}) / (x_{\max} - x_{\min}) \quad (1)$$

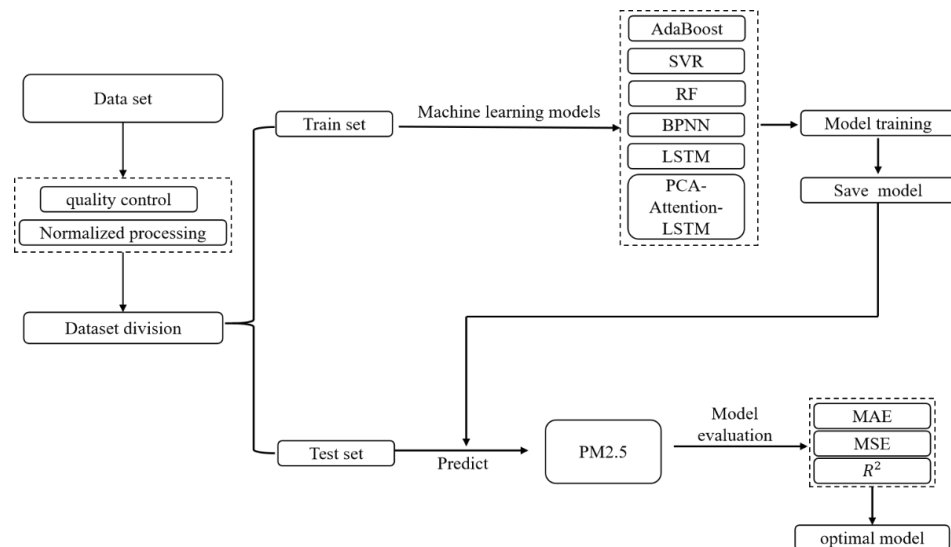
where  $x_{\max}$  is the maximum number in the data series and  $x_{\min}$  is the smallest number in the data series. The dataset is then divided into 850 days of data to train the model as a training set and 200 days of data to test the model as a test set.



### 3. Research Methodology

#### 3.1. Experimental Process and Evaluation Method

The experimental process of predicting PM<sub>2.5</sub> concentration is shown in Figure 5, including data preprocessing, model construction, model prediction, and analysis. Firstly, the experimental data are preprocessed and normalized, and the data are divided into training set and test set. Secondly, the training set is used to train multiple machine learning models and save them. Finally, the prediction values of each model for PM<sub>2.5</sub> concentration are obtained by the test set, and the experimental results are compared and analyzed by the evaluation method. The specific process is as follows:



**Figure 5.** Experimental flow chart.

In this paper, three model evaluation methods were adopted for the statistical testing index: correlation coefficient ( $R^2$ ), mean absolute error (MAE), and mean squared error (MSE). The calculation method of each indicator is as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (C_m - C_0)^2}{n \sum_{i=1}^n (C_m - \bar{C}_0)^2} \quad (2)$$

$$MAE = \frac{1}{n} \left( \sum_{i=1}^n (C_m - C_0)^2 \right) \quad (3)$$

$$MSE = \frac{1}{n} \left( \sum_{i=1}^n |C_m - C_0| \right) \quad (4)$$

where  $C_m$  is the simulated value,  $C_0$  is the observed value, and  $\bar{C}_0$  is the observed mean.

#### 3.2. Machine Learning Methods

The random forest model (RF) is a bagging method, which draws multiple samples from the dataset randomly placed back at a set feature ratio, then trains each sample by returning to the tree, and finally adopts a combined strategy for the prediction results obtained by each tree, then obtains the prediction results of the final random forest model [17–19].

The support vector machine (SVM) uses the SMO or gradient descent method to solve the parameters in the Lagrange dual function, and then finds the optimal classification decision boundary. Generalized support vector regression (SVR) models can be used to

solve regression problems; SVR models find a regression plane so that the data sample is closest to the regression plane, thereby obtaining the predicted value [20–23].

The AdaBoost model improves model accuracy by automatically adjusting the weights of each round. The model learns a weak classifier at a time by iterating and changing the weights of each data in each iteration. The weak classifiers are then linearly combined to obtain a strong classifier.

The BP neural network model (BPNN) is an iterative form, first using the forward propagation of the signal to obtain the results of the first training, and then, according to the error of the ideal and actual output, the signal is backpropagation, so that the process of learning and training is learned and trained through continuous propagation and adjustment of model parameters [24,25]. The input layer of the neural network in this paper is the air pollutant data and meteorological feature data, the activation function of the implicit layer is the sigmoid function, and the output layer is the predicted value of PM<sub>2.5</sub>.

### 3.3. PCA-Attention-LSTM

#### 3.3.1. Principal Component Analysis (PCA)

PCA transforms multiple indexes into several comprehensive indexes, and the transformed comprehensive indexes are transformed into principal components. The principal components are not correlated with each other, which simplifies the research problem and improves the analysis efficiency.

The total number of indicators studied in this paper is  $m = 26$ , which are represented by  $x_1, x_2, \dots, x_m$ , each prefecture-level city has  $n = 1050$  samples, and the  $j$ th indicator of the  $i$ th sample takes the value of  $x_{ij}$ , converting  $x_{ij}$  into a standardized indicator  $\tilde{x}_{ij}$ ,

$$\tilde{x}_{ij} = \frac{x_{ij} - \bar{x}_j}{s_j}, (i = 1, 2, \dots, n; j = 1, 2, \dots, m) \quad (5)$$

where  $\bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_{ij}$ ,  $s_j = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}$ , ( $j = 1, 2, \dots, m$ ), i.e.,  $\bar{x}_j$  and  $s_j$  are the sample mean and standard deviation of the  $j$ th indicator, respectively. Correspondingly,  $\tilde{x}_i = \frac{x_i - \bar{x}_i}{s_i}$ , ( $i = 1, 2, \dots, m$ ) is called a standardized indicator variable.

Correlation coefficient matrix  $R = (r_{ij})_{m \times m}$ ,  $r_{ij} = \frac{\sum_{k=1}^n \tilde{x}_{ki} \cdot \tilde{x}_{kj}}{n-1}$ , ( $i, j = 1, 2, \dots, m$ ), where  $r_{ij}$  is the correlation coefficient between the  $i$ th indicator and the  $j$ th indicator. We calculate the eigenvalue  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m \geq 0$  of the correlation coefficient matrix  $R$ , and the corresponding eigenvector  $u_1, u_2, \dots, u_m$ , where  $u_j = (u_{1j}, u_{2j}, \dots, u_{nj})^T$ , consists of a new indicator variable  $m$  by the eigenvectors

$$\begin{cases} y_1 = u_{11}\tilde{x}_1 + u_{21}\tilde{x}_2 + \dots + u_{n1}\tilde{x}_n, \\ y_2 = u_{12}\tilde{x}_1 + u_{22}\tilde{x}_2 + \dots + u_{n2}\tilde{x}_n, \\ \dots \\ y_m = u_{1m}\tilde{x}_1 + u_{2m}\tilde{x}_2 + \dots + u_{nm}\tilde{x}_n \end{cases} \quad (6)$$

where  $y_1$  is the 1st principal component,  $y_2$  is the 2nd principal component, and  $y_m$  is the  $m$  principal component. Calculate the information contribution rate and cumulative

contribution rate of the eigenvalue  $\lambda_j$  ( $j = 1, 2, \dots, m$ ).  $b_j = \frac{\lambda_j}{\sum_{k=1}^m \lambda_k}$  ( $j = 1, 2, \dots, m$ ) is the information contribution rate of the  $j$ th principal component;  $\alpha_p = \frac{\sum_{k=1}^p \lambda_k}{\sum_{k=1}^m \lambda_k}$  is the cumulative



contribution rate of the principal component  $y_1, y_2, \dots, y_p$ ,  $AP = 85\sim 90\%$  is selected, the number of  $p$  main components is selected, and the  $p$  comprehensive variable replaces the original  $m$  initial index. We bring  $p$  synthesis metrics into the BP neural network model. We bring  $p$  synthesis metrics into the long short-term memory neural networks that incorporate attention mechanisms.

### 3.3.2. Long Short-Term Memory Neural Network (LSTM)

Recurrent neural network (RNN) is a neural network for processing sequence data, and long short-term memory neural network (LSTM) is a special kind of RNN, mainly used to solve the gradient disappearance and gradient explosion problems in the long sequence training process. Compared to ordinary RNNs, in longer sequence, LSTM has better performance. On the basis of the original RNN, LSTM adds an additional unit that can save the long-term state in the hidden layer, and the internal structure of the LSTM unit is shown in Figure 6. LSTM and GRU are special RNN architectures used to solve the gradient vanishing problem. GRU can be considered a simplified version of LSTM. The performances of GRU and LSTM are indistinguishable in many tasks. The fewer GRU parameters make it easier to converge, but LSTM has better expression performance when the dataset is large. After comprehensive consideration, LSTM is selected as the main algorithm for predicting  $PM_{2.5}$  concentration in this paper. At the top of Figure 6 is a long-term memory C line that runs horizontally to achieve the purpose of sequence learning. Three neural network layers represent three doors.

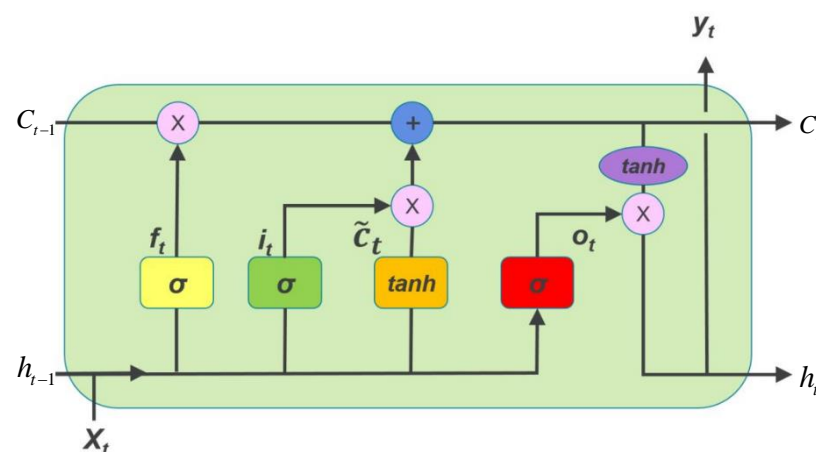


Figure 6. LSTM unit internal structure diagram.

The forgetting gate determines the retention of past information by judging the importance of the current input information, the gate reads  $h_{t-1}$ ,  $x_{t-1}$ , outputs a value between 0 and 1 to each number in the cell state  $C_{t-1}$ , 1 means complete retention, 0 means complete discard.

The input gate determines the retention of the input information by judging the importance of the current input information, which determines how much new information is added to the cell state, a sigmoid layer determines that the information needs to be updated, and a tanh layer generates a vector, that is, the alternative content used to update, merging the two parts to update the cell state. The output gate runs a sigmoid layer to determine the part of the cell state that will be exported, and then the cell state is processed by tanh to obtain a value between  $-1$  and  $1$ , and it is multiplied by the output of the sigmoid gate to obtain the output result. The symbols in the figure are calculated as follows:

$$f_t = \sigma(w_f \cdot [h_{t-1}, x_t] + b_f) \quad (7)$$

$$i_t = \sigma(w_i \cdot [h_{t-1}, x_t] + b_i) \quad (8)$$

$$\tilde{c}_t = \tanh(w_c \cdot [h_{t-1}, x_t] + b_c) \quad (9)$$

$$o_t = \sigma(w_o \cdot [h_{t-1}, x_t] + b_o) \quad (10)$$

$$h_t = o_t * \tanh(c_t) \quad (11)$$

$$c_t = f_t * c_{t-1} + i_t * \tilde{c}_t \quad (12)$$

where  $h_{t-1}$  represents the output of the previous cell;  $x_t$  represents the input of the current cell;  $\sigma$  represents sigmoid function;  $c_{t-1}$  is the output of the previous moment;  $c_t$  is the output of the current moment;  $f_t$  is the output of forgetting gate;  $o_t$  is the output of the output gate;  $\tilde{c}_t$  is an alternative content for updating;  $i_t$  is the update degree of input gate;  $h_t$  is the current cell output.

### 3.3.3. Attention Mechanism

The essence of the attention mechanism is the mental activity of the brain when people observe things. When the brain sees something important that often appears in one part of a scene, it will learn and then focus on this part when it sees a similar scene. In the actual application process, the standard LSTM cannot be handled well in the face of multidimensional and multivariable datasets, and some important time series information may be ignored during the model training process, which will affect the accuracy of the model. Therefore, attention mechanism is added on the basis of LSTM in order to better judge the importance of information at each input moment. Attention mechanism gives different weights to the input characteristics of LSTM, highlights the key influencing factors, and improves the prediction accuracy of the model without increasing the calculation and storage space of the model.

The attention model uses the attention mechanism to dynamically generate the weights of different connections between the input and output of the same layer of network to obtain the output model of the network. The self-attention model can be used as a layer of the neural network, it can also be used to replace the convolution layer or loop layer, or it can be cross-stacked with the convolution layer or loop layer. The mathematical formula is used to express the self-attention mechanism. Assuming that the input sequence in a nerve layer is  $X = [x_1, x_2, \dots, x_N] \in R^{d_1 \times N}$ , and the output sequence is  $H = [h_1, h_2, \dots, h_N] \in R^{d_2 \times N}$  with the same length, three groups of vector sequences are obtained through linear transformation.  $Q$  is the query vector sequence,  $K$  is the key vector sequence, and  $V$  is the value vector sequence.

$$Q = W_Q X \in R^{d_3 \times N} \quad (13)$$

$$K = W_K X \in R^{d_3 \times N} \quad (14)$$

$$V = W_V X \in R^{d_3 \times N} \quad (15)$$

where  $W_Q, W_K, W_V$  are learnable parameter matrices. We calculate the output vector:

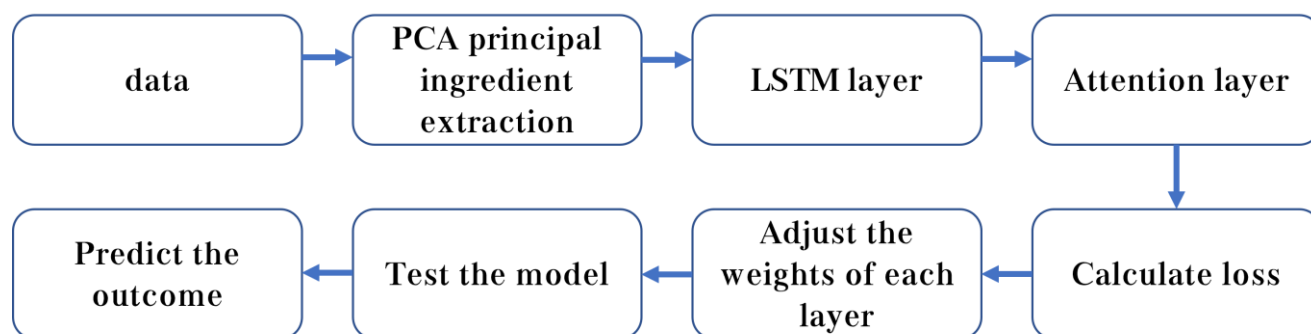
$$\begin{aligned} h_i &= \text{att}((K, V), q_i) = \sum_{j=1}^N \alpha_{ij} v_j \\ &= \sum_{j=1}^N \text{softmax}(s(k_j, q_i)) v_j \end{aligned} \quad (16)$$

where  $i, j \in [1, N]$  is the position of the output and input vector sequence, the connection weight  $\alpha_{ij}$  is dynamically generated by the attention mechanism.

### 3.3.4. PCA-Attention-LSTM Forecasting Model

LSTM solves the problem of gradient disappearance and gradient explosion during long sequence training very well. PCA is used to reduce the dimensionality of the data to speed up the training speed of the model with the smallest amount of lost information. Adding the attention mechanism can better capture important features of long time series data. The model adopts the keras deep learning framework architecture network model, integrates the three algorithms of PCA, attention mechanism, and LSTM, and establishes

an LSTM model based on PCA and attention mechanism; the model framework is shown in Figure 7.



**Figure 7.** PCA-attention-LSTM model technical roadmap.

## 4. Experimental Results and Analysis

### 4.1. PCA-Attention-LSTM Model Building Results

According to the cumulative contribution rate of 85% to 90%, the number of principal components corresponding to the data of the five prefecture-level cities in Ningxia was determined, and the results are shown in Table 3. Wuzhong and Gu Yuan selected eight main components, and Yinchuan, Zhongwei, and Shizuishan selected seven main components. This turns the original 26 indicators into seven or eight comprehensive indicators, so that while eliminating the influence of correlation between variables, the complexity of the model can be reduced and the operation speed of the model can be improved. In the process of the simulation experiment, the principal components are input into the LSTM neural network based on the attention mechanism to build a PCA-attention-LSTM model. The number of principal components selected in the five regions of this paper is seven or eight, and the specific results are shown in Table 3.

### 4.2. Model Parameter Selection

Adaboost model parameters are `base_estimator = None`, `n_estimators = 56`, `learning_rate = 0.1`, `algorithm = SAMME.R`, `random_state = None`. SVR model parameters are `kernel = rbf`, `gamma = scale`, `tol = 0.001`, `C = 1.1`, `epsilon = 0.08`, `shrinking = True`, `cache_size = 200`, `verbose = False`, `max_iter = -1`. RF model parameters `estimator = rf`, `n_iter = 100`, `score = "neg_mean_absolute_error"`, `cv = 3`, `random_state = 42`, `n_jobs = -1`, `param_distribution = random_grid`. The parameters of BPNN model are `num_iterations = 1000`, `learning_rate = 0.01`, `n_h = 6`, `correct = 0.1`. LSTM model parameters are `time_step = 20`, `rnn_unit = 10`, `batch_size = 60`, `input_size = 26`, `output_size = 1`, `lr = 0.006`. In the PCA-attention-LSTM model, the LSTM layer activation function is sigmoid, full connection layer node number is 4, full connection layer node learning rate is 0.005, and full connection layer activation function is sigmoid.

### 4.3. Model Prediction Results and Comparisons

Experiments were conducted using data of the five municipal districts to obtain a line chart of the measured and predicted values of  $PM_{2.5}$  in the five municipal areas, as shown in Figure 8. Three model evaluation methods,  $R^2$ , MAE, and MSE, were used to analyze the prediction accuracy of the models. The results are shown in Table 4. The correlation coefficient ( $R^2$ ) values for the six models ranged from 0.75 to 0.93. The results showed that Wuzhong, Yinchuan, Zhongwei, Shizuishan, and Guyuan all adopted the PCA-attention-LSTM model as the best, and the correlation coefficients  $R^2$  were 0.91, 0.93, 0.91, 0.91, and 0.90, respectively, followed by the LSTM model, with the correlation coefficients  $R^2$  of 0.87, 0.91, 0.99, 0.99, 0.99, and 0.87, respectively, and the SVR model was the worst, with the correlation coefficients  $R^2$  of 0.75, 0.79, 0.83, and 0.79, respectively.

**Table 3.** Principal component analysis.

City	Principal Component	Eigenvalue	Contribution Rate %	Cumulative Contribution Rate %
Wuzhong	1	3.0824	0.3800	0.3800
	2	1.8978	0.1441	0.5241
	3	1.6590	0.1101	0.6342
	4	1.4086	0.0794	0.7136
	5	1.1236	0.0505	0.7640
	6	1.0012	0.0401	0.8041
	7	0.9901	0.0392	0.8434
	8	0.9293	0.0345	0.8779
Yinchuan	1	3.1003	0.3845	0.3845
	2	1.8770	0.1409	0.5254
	3	1.6928	0.1146	0.6400
	4	1.4783	0.0874	0.7274
	5	1.0550	0.0445	0.7720
	6	1.0200	0.0416	0.8136
	7	0.9766	0.0381	0.8518
	8	0.9270	0.0365	0.8883
Zhongwei	1	2.0319	0.1651	0.5317
	2	1.6637	0.1107	0.6424
	3	1.4807	0.0877	0.7301
	4	1.1071	0.0490	0.7791
	5	0.9926	0.0394	0.8185
	6	0.9313	0.0347	0.8532
	7	0.9313	0.0347	0.8879
	8	0.9313	0.0347	0.9226
Shizuishan	1	3.1661	0.4010	0.4010
	2	1.9037	0.1450	0.5460
	3	1.6964	0.1151	0.6611
	4	1.5811	0.1000	0.7610
	5	1.0097	0.0408	0.8018
	6	0.9549	0.0365	0.8383
	7	0.9472	0.0359	0.8742
	8	0.9472	0.0359	0.9101
Guyuan	1	2.7533	0.3032	0.3032
	2	1.9831	0.1573	0.4605
	3	1.8137	0.1316	0.5921
	4	1.4256	0.0813	0.6734
	5	1.1952	0.0571	0.7305
	6	1.0271	0.0422	0.7727
	7	1.0165	0.0413	0.8141
	8	0.9750	0.0380	0.8521

**Table 4.** Model evaluation results.

City	Evaluation Methods	BPNN	SVR	RF	AdaBoost	LSTM	PCA-Attention-LSTM
Wuzhong	$R^2$	0.81	0.75	0.78	0.77	0.87	0.91
	MAE	6.47	9.61	6.67	8.32	5.79	5.57
	MSE	140.61	181.92	157.82	167.86	97.17	78.49
Yinchuan	$R^2$	0.90	0.79	0.89	0.87	0.91	0.93
	MAE	4.85	8.12	5.10	6.50	4.35	4.07
	MSE	54.15	107.34	56.01	64.15	43.57	39.59
Zhongwei	$R^2$	0.88	0.81	0.84	0.84	0.89	0.91
	MAE	6.52	7.77	6.67	7.86	5.64	5.40
	MSE	96.12	111.58	97.41	93.45	68.02	54.64
Shizuishan	$R^2$	0.89	0.83	0.89	0.87	0.90	0.91
	MAE	5.98	8.11	6.08	6.95	5.28	4.92
	MSE	86.96	101.03	89.42	96.84	64.30	67.81
Guyuan	$R^2$	0.87	0.79	0.85	0.81	0.87	0.90
	MAE	5.23	6.35	5.29	7.05	4.89	4.72
	MSE	59.31	69.91	62.01	78.32	57.81	50.22

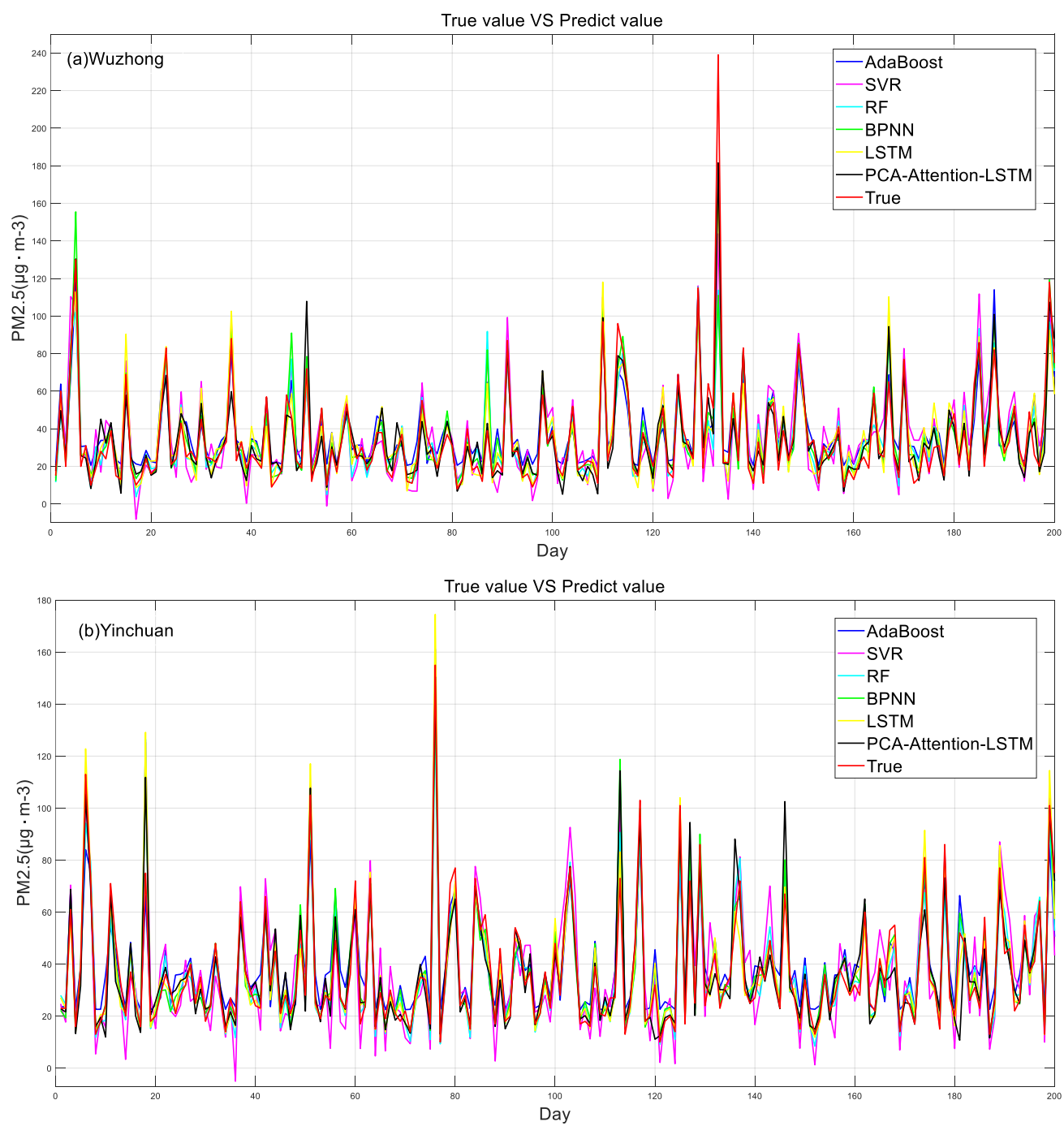


Figure 8. Cont.

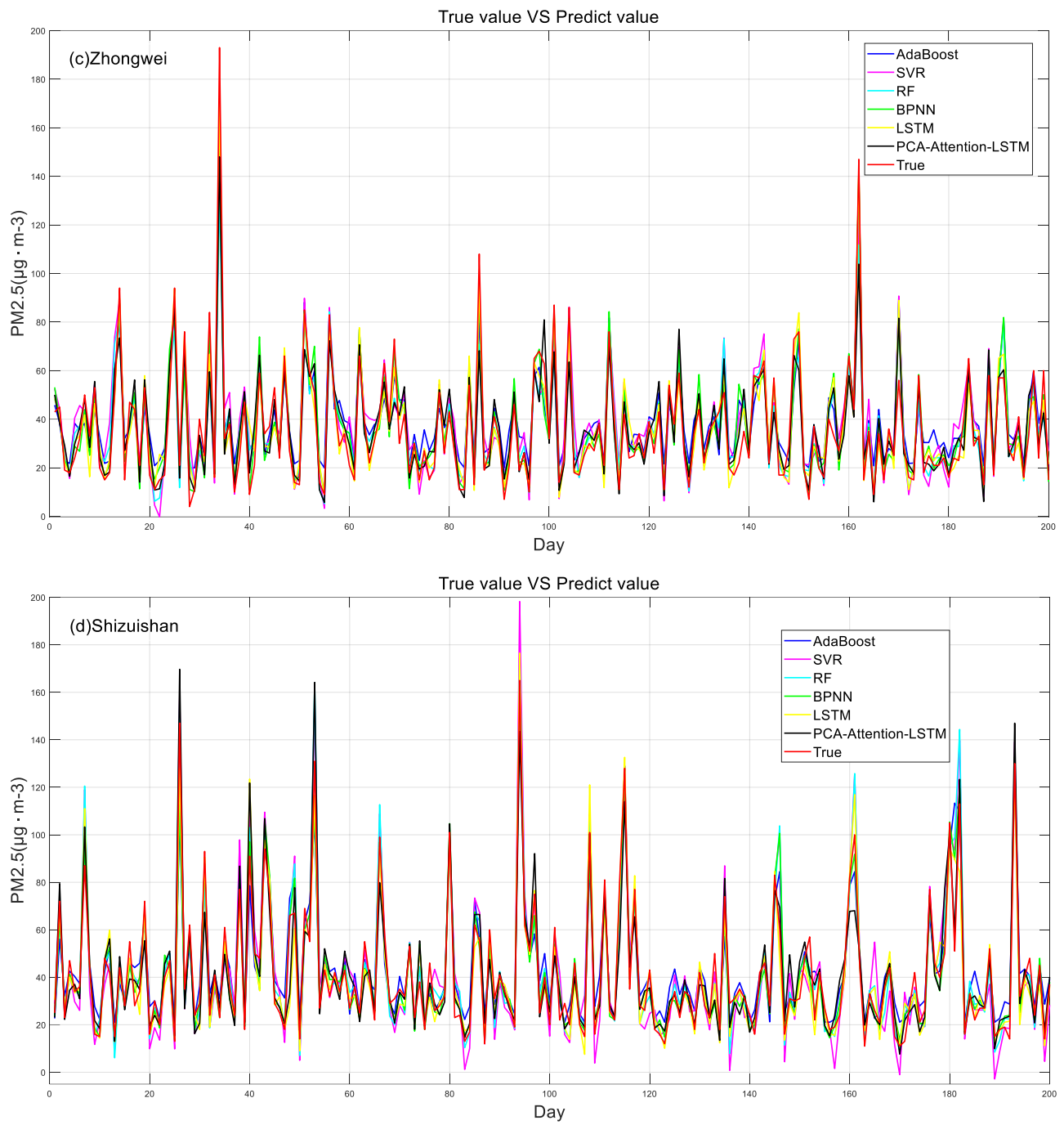
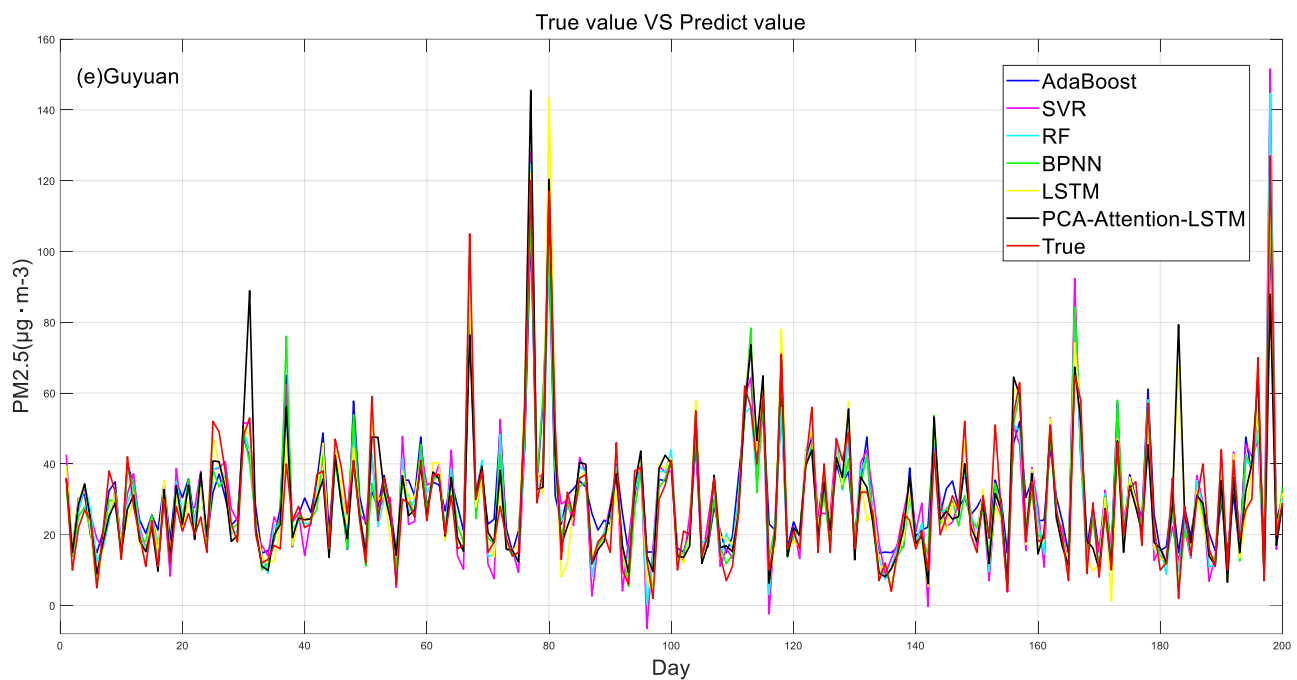


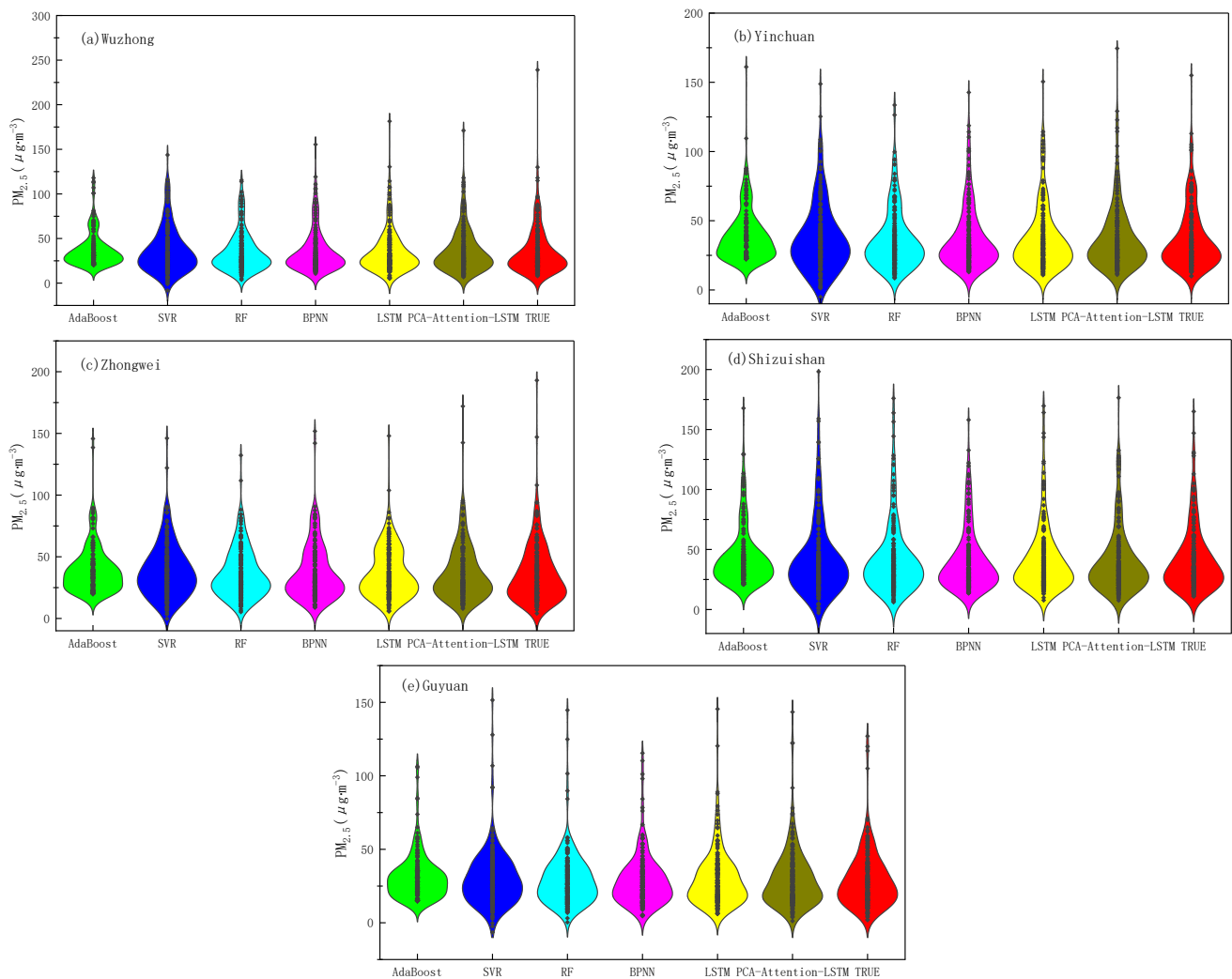
Figure 8. Cont.





**Figure 8.** True value versus predicted value.

In order to further compare the relationship between the predicted values and the measured values of the six models, Figure 9 compares the true values of  $PM_{2.5}$  concentrations in five municipal areas with the predicted values of the models. It can be seen from Figure 9 that the AdaBoost model in the Wuzhong area as a whole shows an overestimation phenomenon, SVR and RF show an underestimation phenomenon, and the distribution of the PCA-attention-LSTM model and true values is the closest, but the peak is underestimated. The AdaBoost model in Yinchuan showed an overall overestimation phenomenon, the SVR showed an underestimation phenomenon, and the PCA-attention-LSTM model and the LSTM model were close to the distribution of the measured values. The LSTM model, BPNN model, and AdaBoost model in Zhongwei area showed an overall overestimation phenomenon, the RF model showed an underestimation phenomenon, and the PCA-attention-LSTM model was close to the overall distribution of the measured values but the peak was underestimated. The Shizuishan area and the AdaBoost model as a whole showed an overestimation phenomenon, the SVR and RF models showed an underestimation phenomenon, and the range of predicted values became larger, and the PCA-attention-LSTM model and LSTM model were close to the overall distribution of the measured values. The AdaBoost model in the Guyuan area showed an overall overestimation phenomenon, and the PCA-attention-LSTM model was closest to the overall distribution of the measured values.



**Figure 9.** A plot of the distribution of predicted and true values.

## 5. Conclusions and Discussions

- (1) Statistical analysis of the data shows that the overall indicators of Guyuan are better than those of the other four cities, and the worst is Shizuishan City, which has a clear correlation with the geographical location of the municipal areas, and the overall air quality in the southern mountainous areas is better than that of the Yellow River irrigation area in the north.
- (2) The three-year data of five cities in Ningxia were integrated and divided into four seasons and month by month. The results showed that the  $PM_{2.5}$  concentration showed an obvious seasonal change trend, which was the lowest in summer and the highest in winter. This was mainly related to the dust emission from coal combustion and gas or fuel during winter heating in Ningxia.
- (3) Through the analysis of variable importance, the results show that  $PM_{10}$  is the most important, followed by air quality index, air quality grade, and CO having equal importance, and precipitation in meteorological elements is also a relatively important variable. For future studies of  $PM_{2.5}$  concentration prediction, the week can also be used as an input variable, indicating that  $PM_{2.5}$  concentration generation is also affected by weekdays and non-working days.

- (4) The concentration of PM<sub>2.5</sub> was predicted by using six models, and the results showed that the PCA-attention-LSTM model had the best prediction accuracy, and its correlation coefficient was 0.91~0.93. The prediction accuracy of the SVR model was poor, and its correlation coefficient was 0.75~0.83. The LSTM model and the BPNN model also predicted better results.
- (5) Experimental results show that the training evaluation results of the PCA-attention-LSTM model are better than those of the LSTM model, which shows that the cumulative variance contribution rate of the selected principal components reaches 85–90%, which reduces the data dimension and reduces the time complexity and spatial complexity of the model. At the same time, the attention mechanism can better capture important information.

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