

ONE DAY AHEAD PREDICTION OF PM_{2.5} SPATIAL DISTRIBUTION USING MODIS 3 KM AOD AND SPATIOTEMPORAL MODEL OVER BEIJING-TIANJIN-HEBEI, CHINA

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Commission III, WG III/8

KEY WORDS: MODIS AOD, PM_{2.5}, PM_{2.5} spatiotemporal distribution, Spatiotemporal autoregressive model, Machine learning model.

ABSTRACT:

Accurate prediction of PM_{2.5} concentration is the premise and guarantees to effectively control PM_{2.5} concentration and avoid the adverse effects of high PM_{2.5} concentration on human health. However, given the existing statistical models can only predict the pollutant concentration at the monitoring sites, the spatial distribution of PM_{2.5} concentration cannot be predicted, which greatly limits the application of the model in PM_{2.5} concentration prediction. This study combined the PM_{2.5} spatial distribution data predicted using the Moderate Resolution Imaging Spectroradiometer 3 km aerosol optical depth (AOD) and meteorological factors into a spatiotemporal autoregressive (STAR) model to predict the regional PM_{2.5} concentration and quantify the short-term spatial distribution change of PM_{2.5} in Beijing–Tianjin–Hebei region (JingJinJi) one day in advance. Five simulation functions were used to simulate the STAR model, and the 2014 data of JingJinJi were used to verify its accuracy. Results showed that the STAR model had the best prediction performance when gradient boosting decision tree was used as the simulation function compared with other simulation functions. The coefficient of determination (R^2), root mean square prediction error (RMSE), index of agreement (IA), and mean absolute error (MAE) of the STAR model were 0.85, 27.08 $\mu\text{g}/\text{m}^3$, 0.96, and 20 $\mu\text{g}/\text{m}^3$, respectively. The spatial distribution prediction results of PM_{2.5} showed that the +1-day PM_{2.5} spatial distribution prediction results were in good agreement with the PM_{2.5} spatial distribution results predicted by AOD to provide accurate spatiotemporal distribution data for reducing air pollution and air pollution early warning.

1. INTRODUCTION

Air quality refers to the chemical state of the atmosphere at a specific time and place and reflects the degree of air pollution. The concentration of pollutants in the atmosphere will have adverse effects on human health, such as damage to immune and nervous systems and premature death, when it exceeds a certain boundary (Zhang et al., 2012). Among the many atmospheric pollutants, PM_{2.5} is the most harmful to human health because it contains toxic and harmful substances and can directly enter the alveoli (Belleudi et al., 2010; Crouse et al., 2012; Dominici et al., 2006; Pope III et al., 2002). With the rapid economic development and intensified anthropogenic emissions annually, China has suffered from serious air pollution, especially in northern China (Wang et al., 2019; Zheng et al., 2016). To effectively control PM_{2.5} concentration and avoid its adverse effects on human health, the government should conduct precautionary measures in advance (such as closing the main emission sources and vehicle restrictions) to reduce air pollution and issue air pollution warning for providing guidance for public travel (Zhang et al., 2012). Therefore, real-time air quality information should be obtained and the temporal and spatial change trends of PM_{2.5} concentration should be predicted (Chen et al., 2013).

Prediction methods of air pollution concentration can be mainly divided into two types, namely, statistical and deterministic models. Considering that meteorological and air pollutant concentration variables are statistically related, statistical models use different functions to simulate the relationship of measured pollutant variables and various selected predictors for predicting pollutant concentration (Hx, et al., 2021; Pak, et al., 2020; Wen et al., 2019; Cobourn 2007; Elangasinghe et al., 2014; Kurt and Oktay 2010; Nieto et al., 2013; Li et al., 2016; Sánchez et al., 2013; Qi et al., 2019; Soh et al., 2018). Statistical models have better prediction accuracy. However, the existing statistical models can only predict the pollutant concentration at the monitoring site and cannot be extended to other regions with different meteorological conditions or without monitoring sites (Cortina Januchs et al., 2015; Elangasinghe et al., 2014; Hooyberghs et al., 2005), that is, the existing statistical models cannot predict the regional PM_{2.5} concentration.

The deterministic model simulates pollutant discharge, diffusion, and disappearance in a model-driven manner (Li et al., 2016), thus enabling the prediction of pollutant concentration in areas without monitoring sites (Cortina Januchs et al., 2015). During simulation, pollutant discharge volume, chemical composition of pollution gas, and physical processes of the atmosphere should be fully understood, however, these key knowledge are often insufficient (Hrust et al., 2009). In addition, the model is

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simplified during prediction because of its incomplete theoretical basis and calculation complexity, thereby leading to low prediction accuracy (Feng et al., 2015).

Therefore, regional PM_{2.5} spatiotemporal distribution trend prediction with high precision should be explored to reduce the impacts of PM_{2.5} concentration on public health and provide guidance for public travel and government pollution prevention. The formation of PM_{2.5} is a dynamic system under the influence of meteorological and natural factors. The PM_{2.5} concentration at a certain location is related to its own and nearby PM_{2.5} concentration and meteorological factors. Therefore, PM_{2.5} has a strong spatiotemporal autocorrelation. A spatiotemporal autoregressive (STAR) model considers the temporal evolution of adjacent spatial grid points. In the STAR model, each target pixel value is simulated as a weighted sum of neighboring available raster pixel values (Zhang et al., 2009), thus, the model is frequently used for remote sensing images prediction (Cheng et al., 2017; Crespo et al., 2007; Das and Ghosh 2016). This study introduced the daily complete PM_{2.5} spatial distribution (raster

image) data obtained by Moderate Resolution Imaging Spectroradiometer (MODIS) AOD and meteorological factors into the STAR model to predict the one day ahead spatiotemporal distribution trend of PM_{2.5} and provide guidance for public travel and government pollution prevention. The rest of this paper is organized as follows. Section 2 introduces the study area, input data, and model structure. Section 3 presents the model's validation results, PM_{2.5} spatiotemporal distribution, and feasibility analysis. Section 4 provides the conclusions.

2. MATERIALS AND METHOD

2.1 Study area

The study area includes Beijing, Tianjin, and Hebei (JingJinJi) (Figure 1(a)). Excessive emissions, unfavorable terrain and meteorological conditions make JingJinJi a typical heavily polluted area in China. Therefore, this area is selected as the research area of this paper.

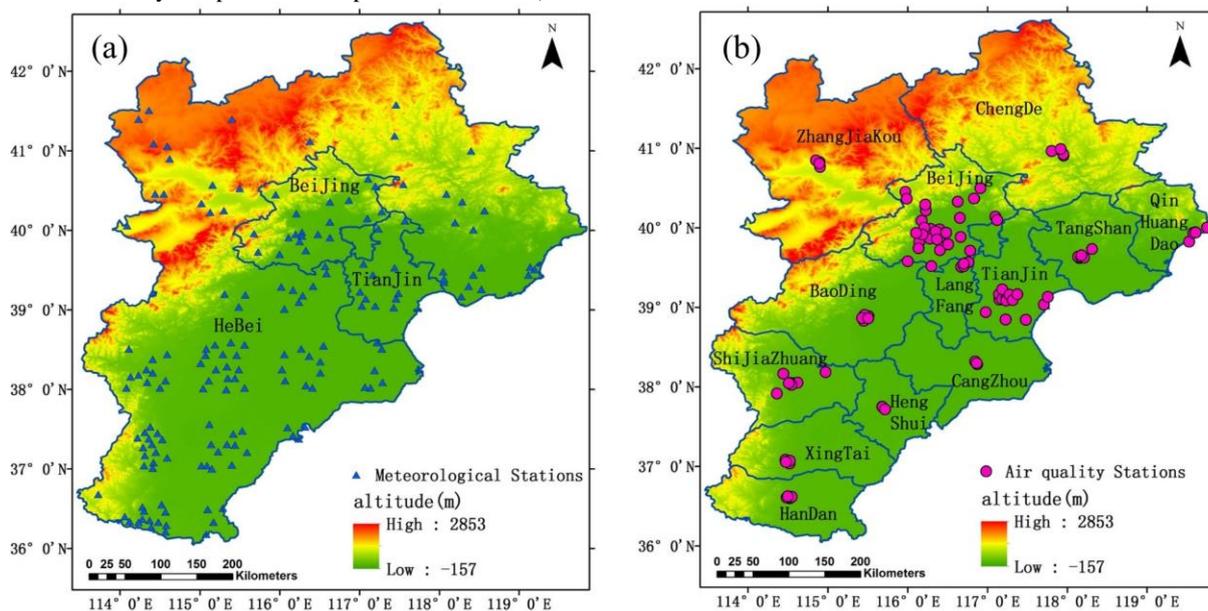


Figure 1. Schematic diagram of study area.

2.2 MODIS AOD Data

The Dark Target algorithm Collection 6 MODIS Aqua AOD data of 2014 were downloaded from the NASA official website (Yang et al., 2019), and the AOD resolution used in this study was 3 km.

2.3 Grounding Monitoring Data

The hourly meteorological data (including wind speed, wind direction, pressure, sea level pressure, water vapor pressure, temperature, and humidity) and pollutant monitoring data of 2014 were collected from the related official websites (<http://113.108.142.147:20035/emcpublish/>, <http://zx.bjmecm.com.cn/>).

2.4 Data Processing and Integration

The research results of Wang et al (2020) has showed that full-coverage and high-precision PM_{2.5} spatial distribution data in JingJinJi can be generated based on AOD, gaseous pollutants and meteorological factors. Details can be found in related article (Wang et al., 2020)). Therefore, the data processing results were

the 3 km resolution grid PM_{2.5} concentration values covering the entire JingJinJi obtained using MODIS 3 km Aqua AOD and the 3 km resolution grid meteorological data generated through Kriging interpolation.

During data integration, the grid PM_{2.5} concentration on day *t* was matched to the *t*-day grid meteorological data and *t*-1, *t*-2, *t*-3...day grid PM_{2.5} concentrations. Day of year (DOY, range 1–365) and grid position (GP, row number *m* and column number *n* of the 3 km resolution grid) were used as predictors to reflect the spatiotemporal heterogeneity.

2.5 Method

During prediction, the input variables of STAR model are the pixel values of the same and adjacent pixel positions, and the prediction result is the pixel values of each pixel (or window), as shown in Eq. (1). That is, the pixel value $p(x, y, t)$ of at GP (x, y) time *t* is the spatiotemporal function of the grid pixel value of the adjacent image.

$$p(x, y, t) = \varphi(p(x \pm \Delta x_i, y \pm \Delta y_i, t - \Delta t_i)), \quad (1)$$

where (x, y, t) is the location of raster cell at a given time, $(\Delta x_i, \Delta y_i, \Delta t_i)$ denotes the spatiotemporal structure of the adjacent raster cells, and ϕ denotes an simulation function that can be linear or nonlinear.

As shown in Figure 2, considering the PM2.5 concentration of the two previous days ($T=2$) adjacent to the $(\Delta x_i = \Delta y_i = 1)$ grid to predict PM2.5 concentration $p(m, n, t)$ of m -row and n -column grid at time t , Eq. (1) can be rewritten as follows:

$$p(m, n, t) = \sum_{i=1}^2 \left[\sum_{y=n-1}^{n+1} \sum_{x=m-1}^{m+1} (W_{xy}^i p(x, y, t-i)) + W_{mn}^t q(m, n, t) + \varepsilon(m, n, t) \right] \quad (2)$$

where $p(x, y, t - \Delta t_i)$ indicates the inversion results of Aqua AOD at position (x, y) and time $t - \Delta t_i$, $q(m, n, t)$ is the meteorological variable at position (m, n) and time t , W_{xy}^i and W_{mn}^t are the corresponding weight coefficients, and $\varepsilon(m, n, t)$ is the error term.

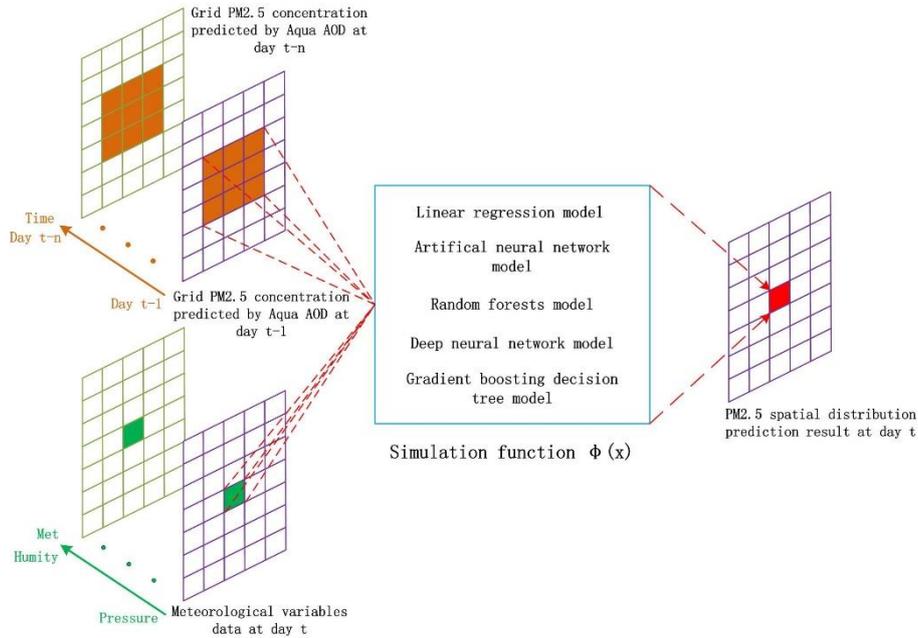


Figure 2. Schematic of the STAR model considering the influence of meteorological factors.

This study explored the effects of nonlinear functions, such as ANN, random forest (RF), deep NN (DNN), and gradient boosting decision tree (GBDT), on model accuracy.

2.6 Model Validation

During model validation, all the data were randomly divided into two groups, where 90% of the matching data were used for model fitting, and the remaining 10% were used for model validation. The coefficient of determination (R^2), root mean square prediction error (RMSE), index of agreement (IA), and mean absolute error (MAE) were used to estimate model performance and were defined as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^N (O_i - P_i)^2}{\sum_{i=1}^N (O_i - \bar{O})^2} \quad (3)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |O_i - P_i| \quad (4)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (O_i - P_i)^2} \quad (5)$$

$$IA = 1 - \frac{\sum_{i=1}^N (O_i - P_i)^2}{\sum_{i=1}^N (|O_i - \bar{O}| + |P_i - \bar{O}|)^2} \quad (6)$$

where N is the number of samples, O_i and P_i are the observation and prediction results, respectively, and \bar{O} is the average of the observations.

2.7 Parameters Settings

The machine learning models used in this study were all built using the “Keras” model in Python 3.6.0. The main parameter settings of each model are shown in Table 1.

Model	Parameters	Value
ANN	Activation function	‘relu’
	Hidden layer size	12
	Learning rate	‘constant’
RF	Max depth	8
	Random state	0
DNN	Activation function	‘relu’
	Loss function	‘mse’
	Hidden layers	6
	Hidden layers nodes	200
GBDT	Loss function	‘ls’
	Learning rate	0.1
	Boosting stages numbers	3000
	Max depth	4

Table 1. Parameter settings of machine learning models.

3. RESULTS AND DISCUSSIONS

3.1 Model Validation Results

Figure 3 shows the scatter plots of the STAR model with five simulation functions, namely, LR, ANN, DF, DNN, and GBDT.

(a1)–(e1) show the scatter plots comparing the predicted and AOD-based PM_{2.5} inversion results. (a2)–(e2) show the scatter plots comparing the predicted results and monitoring station PM_{2.5} concentration. As shown in (a1)–(e1), the STAR model had the best predictive performance when GBDT was used as the simulation function. The values of R², RMSE, IA, and MAE were 0.85, 27.08 μg/m³, 0.96, and 20 μg/m³, respectively. The R² using DNN reduced from 0.78 to 0.07 compared with GBDT. The model performance was the worst when the simulation function was LR. The R² and IA values were 0.68 and 0.88, respectively, and the RMSE and MAE values were 39.57 and 29.56 μg/m³, respectively, which may be because of the complex nonlinear relationship of PM_{2.5} and meteorological factors (Wang and Sun 2019; Elangasinghe et al., 2014; Kukkonen et al., 2003). As shown in (a2)–(e2), the model performance in terms of the prediction results of monitoring site PM_{2.5} was inferior to that compared with the AOD-based PM_{2.5} inversion results. In this case, the simulation function of the STAR model with the best

performance was GBDT, and its R², RMSE, IA, and MAE values were 0.75, 40.30 μg/m³, 0.92, and 30.04 μg/m³, respectively. Compared with the predicted performance of the model shown in Figure 1(e1), the R² and IA values decreased by 0.1 and 0.04, respectively, whereas the RMSE and MAE values increased by 13.22 and 10.04 μg/m³, respectively. The model performance decreased the most when DNN was used as the simulation function. The R² and IA values decreased by 0.15 and 0.06, respectively, whereas the RMSE and MAE values increased by 15.89 and 12.05 μg/m³, respectively. The performance degradation of the model was mainly because our data for +1-day PM_{2.5} prediction were the AOD-based PM_{2.5} inversion results. The inversion results had certain errors compared with the station monitoring results. Therefore, error propagation occurred during the +1-day PM_{2.5} spatial distribution prediction, resulting in degraded model performance.

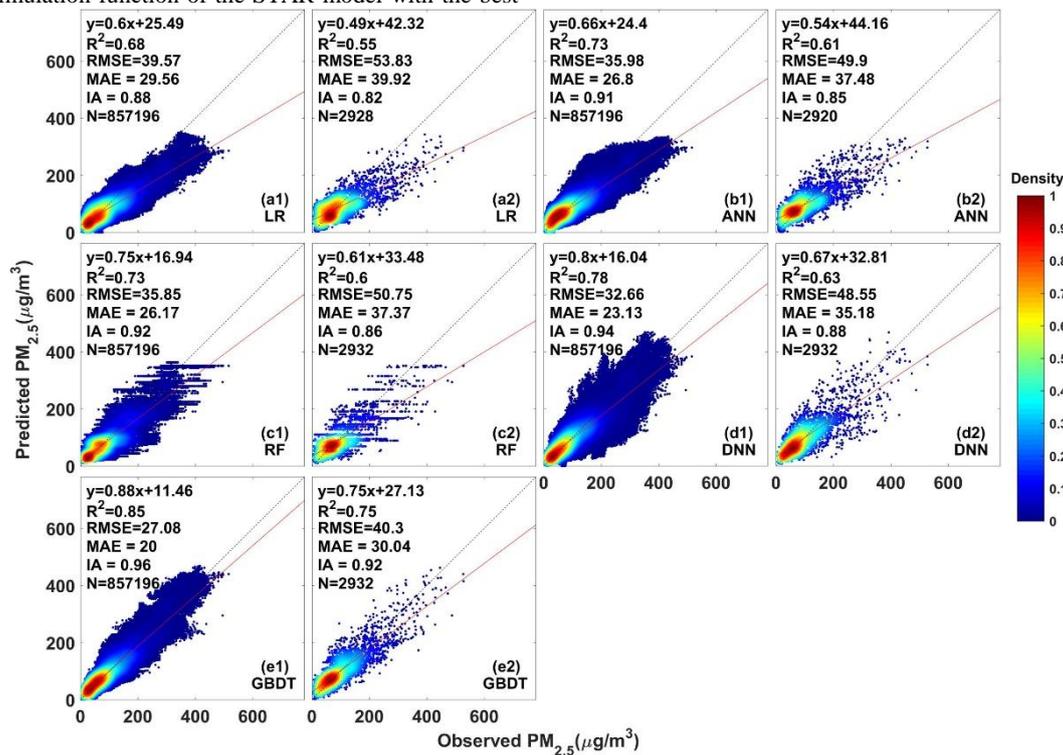


Figure 3. Scatter plots of the STAR model with five different functions. (a1)–(e1) show the scatter plots comparing the predicted and AOD-based PM_{2.5} inversion results. (a2)–(e2) show the scatter plots comparing the predicted results and monitoring station PM_{2.5} concentration.

Table 2 shows the STAR model performance statistics using different simulation functions and predictors. The STAR model under five simulation functions had similar prediction performance when the PM_{2.5} spatial distribution data of the previous day were used as predictors. This condition may be because the relationship of PM_{2.5} presented a linear relationship rather than a complex nonlinear relationship (Wang et al., 2019). The comparison experiments demonstrated that the introduction of DOY and GP immensely improve the performance of the

STAR model using a nonlinear simulation function. The model performance immensely improved with the introduction of DOY and GP as predictors and GBDT as the simulation function. The R² and IA values decreased by 0.14 and 0.05, respectively, whereas the RMSE and MAE values increased by 10.46 and 7.79 μg/m³, respectively, indicating that +1-day PM_{2.5} spatial distribution prediction results were immensely affected by time and location factors.

Model	Variables	R ²	RMSE(μg/m ³)	IA	MAE(μg/m ³)
LR	PM	0.62	42.91	0.85	31.02
	PM+MET	0.68	39.28	0.89	29.48
	PM+MET+GP	0.68	39.57	0.88	29.56
ANN	PM	0.62	42.9	0.85	31.02
	PM+MET	0.69	38.76	0.89	28.96

	PM+MET+GP	0.73	35.98	0.91	26.80
RF	PM	0.63	42.30	0.86	30.17
	PM+MET	0.68	39.18	0.9	28.32
	PM+MET+GP	0.74	35.85	0.92	26.16
	PM	0.61	43.31	0.85	30.57
DNN	PM+MET	0.60	43.95	0.89	31.62
	PM+MET+GP	0.78	32.66	0.94	23.13
GBDT	PM	0.63	42.32	0.86	30.13
	PM+MET	0.71	37.54	0.91	27.79
	PM+MET+GP	0.85	27.08	0.96	20.00

Table 2. Performance statistics of the STAR model under different simulation functions and predictors.

Figure 4 shows the statistics of IA and MAE values of the STAR model under five simulation functions at different monitoring sites. As shown in Figure 4, the spatial distribution of MAE at each monitoring was regional. The areas with small MAE were mainly distributed in the northern areas, such as Chengde, Qinhuangdao, and Zhangjiakou, whereas the areas with large MAE were mainly concentrated in southern Beijing, Baoding, Shijiazhuang, Handan, and Tangshan. The two main reasons for this phenomenon were provided as follows: First, the PM_{2.5} concentration in different regions was different. MAE was high in areas with high PM_{2.5} concentration, whereas MAE was relatively low in areas with low PM_{2.5} concentration. Figure 5(a) shows the PM_{2.5} annual average concentration of each monitoring station in JingJinJi in 2014. The areas with high annual average PM_{2.5} concentration were concentrated in the south of Beijing, Baoding, Shijiazhuang, Handan, and Tangshan, which was consistent with high MAE areas of the prediction results. As shown in the scatter plot in Figure 3, underestimation was serious when the PM_{2.5} concentration was high, resulting in high MAE. Second, the regional MAE spatial distribution may be related to the AOD-based PM_{2.5} inversion performance. Figure 5(b) shows the AOD-based PM_{2.5} inversion performance statistics for each monitoring site. The areas with large RMSE were consistent with high MAE areas of the prediction results. As shown in Figure 4, the MAE of each monitoring site was significantly lower than those of the four other simulation functions when GBDT was used as the simulation function. From a regional perspective, the areas with large MAE improvement of GBDT were mainly the south of Beijing, Baoding, and Shijiazhuang. In the southern part of Beijing, the MAE of GBDT reduced by approximately 30 $\mu\text{g}/\text{m}^3$ compared with the other simulation functions. The above comparison experiments showed that the STAR model had the best predictive performance when GBDT was used to simulate the STAR model during the +1-day PM_{2.5} spatial distribution prediction. The experimental results based on GBDT are shown as follows.

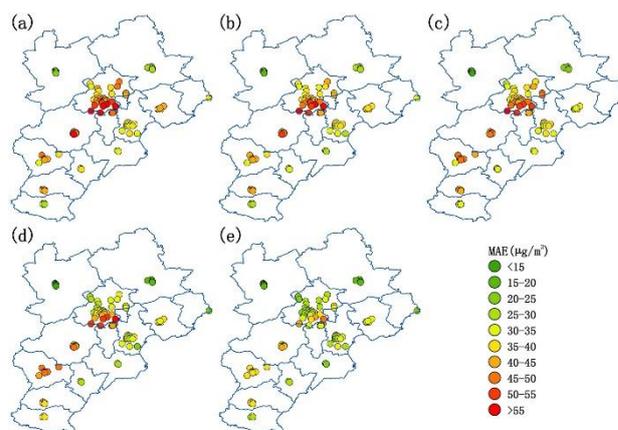


Figure 4. Spatial distribution of MAE of the STAR model at different monitoring sites using different simulation functions. (a)–(e) is LR, ANN, RF, DNN, and GBDT, respectively.

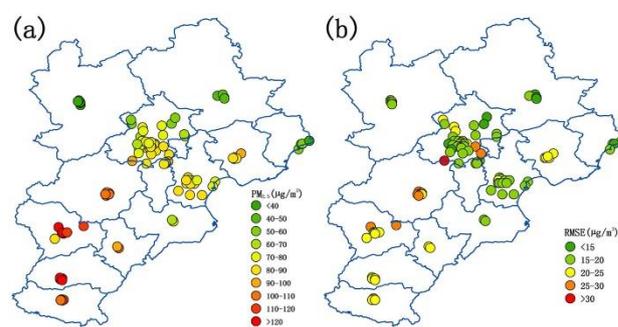


Figure 5. (a) PM_{2.5} annual average concentration of the monitoring sites in JingJinJi in 2014; (b) PM_{2.5} inversion performance statistics of each monitoring site.

3.2 Model Parameters Determination

Table 3 shows the performance statistics of the STAR model under different parameters using GBDT as the simulation function. As shown in Table 3, the model performance slightly changed with the increase in Δx_i and T. This condition may be because many prediction variables were introduced into the model with the increase in Δx_i or T. These variables were far from the destination grid and did not contribute to the model performance. Variables Δx_i and T were set to one for reducing the model complexity.

	$\Delta x_i=1$				$\Delta x_i=2$				$\Delta x_i=3$			
	R ²	RMSE	IA	MAE	R ²	RMSE	IA	MAE	R ²	RMSE	IA	MAE
T=1	0.85	27.08	0.96	20.00	0.84	27.88	0.96	20.51	0.85	27.29	0.96	20.22
T=2	0.85	27.24	0.96	20.25	0.85	27.09	0.96	19.95	0.85	27.13	0.96	20.08

T=3	0.85	27.18	0.96	20.22	0.85	27.10	0.96	19.98	0.85	27.01	0.96	19.90
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Table 3. Performance statistics of the STAR model under different parameters

3.3 Prediction Maps of PM2.5 Spatial Distribution

Figure 6 shows the prediction results of +1-day PM2.5 spatial distribution during heavy pollution from October 6, 2014 to October 12, 2014. The prediction results of the STAR model were consistent with the PM2.5 spatial distribution inversion and site monitoring results, thereby accurately reflecting the emergence, diffusion, and disappearance of PM2.5 during heavy

pollution and providing spatiotemporal distribution data for reducing air pollution and air pollution early warning. The PM2.5 spatial distribution prediction results in this study produced high-value underestimation (Figure 6(b1) and (b2)) and low-value overestimation (Figure 6(g1) and (g2)) with the change of PM2.5. Underestimation occurred when the pollution was serious (Figure 6(d1) and (d2)).

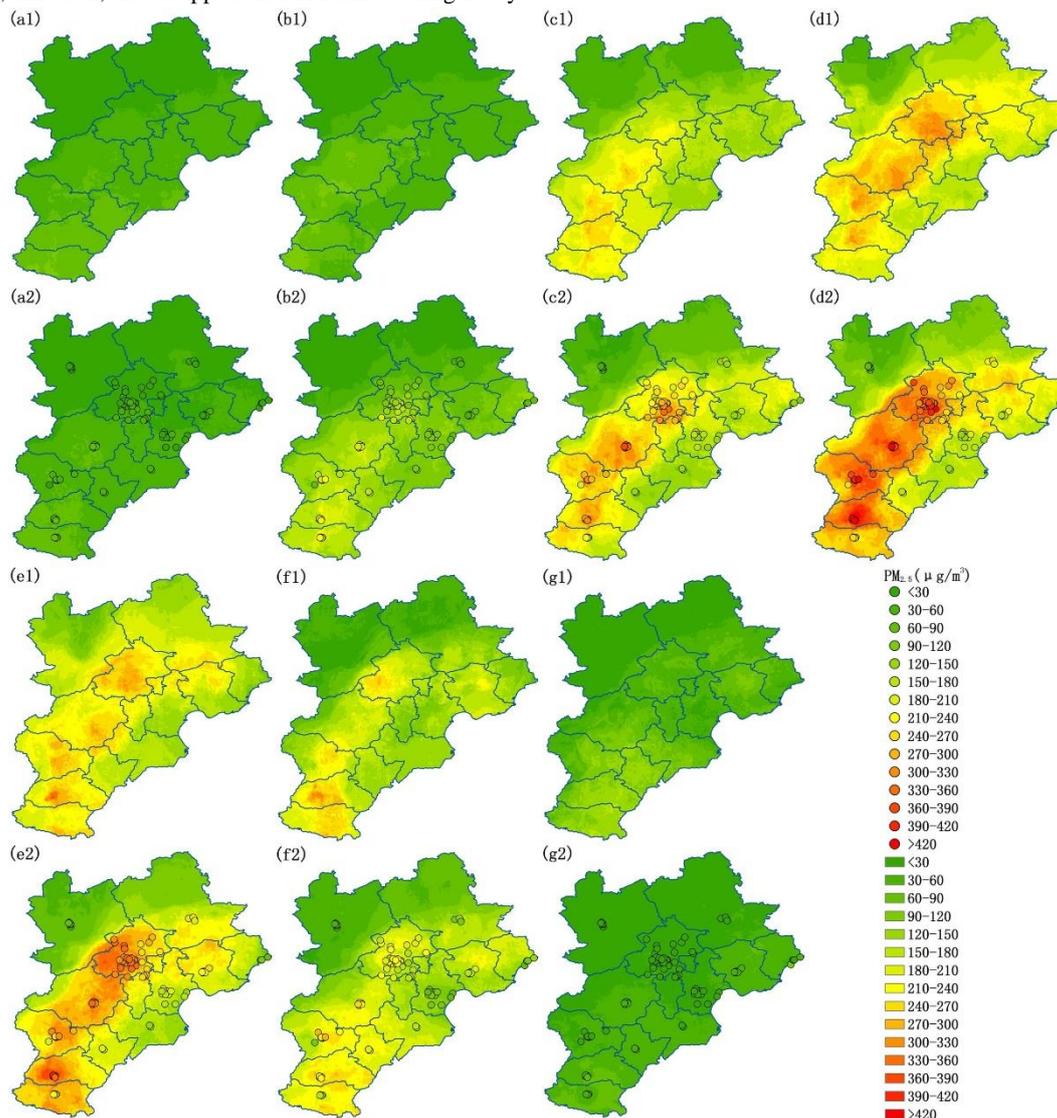


Figure 6. +1-day PM2.5 prediction results from October 6, 2014 to October 12, 2014. (a1)–(g1) show the +1-day PM2.5 prediction results; (a2)–(g2) show the PM2.5 inversion results and the site monitoring PM2.5 concentration.

3.4 Feasibility and Uncertainty Analysis

Previous studies have improved PM2.5 prediction accuracy by introducing the PM2.5 concentration from adjacent monitoring sites (Zheng et al., 2015; Kukkonen et al., 2003; Li et al., 2015; Wen et al., 2019), indicating that PM2.5 has a strong spatial-temporal autocorrelation. Based on this, we established the STAR model to realize the +1-day region PM2.5 spatial distribution prediction. The pollutant concentrations were cyclical because of the influence of time factors (Zhang et al.,

2012). Therefore, day of week and DOY were frequently used as predictors to improve the pollutant prediction performance ADDIN(Kurt and Oktay 2010; Qi et al., 2019; Feng et al., 2015). The PM2.5 spatial distribution maps showed that the PM2.5 spatial distribution was regional. Therefore, the introduction of DOY and GP improved the prediction accuracy of the model.

Scholars have conducted numerous studies on the prediction of PM2.5 in JingJinJi using statistical models (Soh et al., 2018; Feng et al., 2015; Li et al., 2016; Qi et al., 2019). Although these

studies have achieved high prediction accuracy, some limitations are found because they only predicted the PM_{2.5} concentration of monitoring sites. First, air quality is affected by complex factors, such as meteorological factors, transportation, and land use types, and immensely varies with time and location (Zheng et al., 2013). Therefore, single-site pollutant concentration prediction cannot effectively help people to make decisions. Different models are required in predicting the pollutant concentration at different stations (Zheng et al., 2015). Second, these studies can only predict the PM_{2.5} concentration in areas with monitoring stations. Taking the study area as an example, JingJinJi has few monitoring stations that are mainly concentrated in urban areas. Therefore, statistical models in previous studies cannot be used to predict the pollutant concentration in vast areas without monitoring sites. Other scholars used the deterministic models to simulate the PM_{2.5} concentration in eastern China (Zhou et al., 2017; Zheng et al., 2015). Although the regional PM_{2.5} concentration prediction can be achieved, the model accuracy is low with R² are 0.45 and 0.64, respectively. The model used in this study fully considered the spatial-temporal autocorrelation of PM_{2.5}, not only extended the PM_{2.5} concentration prediction to other areas without monitoring sites, but also achieve regional PM_{2.5} concentration prediction with high accuracy, thereby overcoming the limitations of statistical models and deterministic models to some extent.

The model prediction results in this study had underestimation problems. This condition was because the AOD-based PM_{2.5} inversion results had certain errors, thereby resulting in error propagation. Therefore, the accuracy of the STAR model can be enhanced to some extent by improving the AOD-based inversion accuracy. At the same time, some advanced statistical models, such as long-short memory DNN (Li et al., 2017), can be used to solve the underestimation of the model.

4. CONCLUSION

Statistical models can only predict the pollutant concentration at the monitoring sites and cannot be extended to other regions with different meteorological conditions and without monitoring sites. This study establish a STAR model based on the spatial distribution of PM_{2.5} predicted using MODIS AOD for predicting the one day ahead PM_{2.5} spatial distribution in JingJinJi. The results showed that the performance of the STAR model was relatively different compared with different simulation functions. The model performance was the best when GBDT was used as the simulation function. The R², RMSE, IA, and MAE values were 0.85, 27.08 µg/m³, 0.96, and 20 µg/m³, respectively. The introduction of DOY and GP immensely improved the model performance, and R² and IA decreased by 0.14 and 0.05, respectively, whereas RMSE and MAE increased by 10.46 and 7.79 µg/m³, respectively, indicating that the PM_{2.5} spatial distribution prediction results were immensely affected by time and location factors. The performance statistics of each monitoring station showed that the model performance distribution was regional. The regions with low PM_{2.5} concentration had better performance, whereas the regions with high PM_{2.5} concentration had poor performance. The PM_{2.5} prediction results of heavily polluted weather indicated that the model can accurately reflect the emergence, diffusion, and disappearance of PM_{2.5} during heavy pollution and provide spatiotemporal distribution data for reducing air pollution and air pollution early warning.

ACKNOWLEDGEMENTS

This work was supported by the Special Project of Science and Technology Basic Resources Survey, China Ministry of Science and Technology, under Grant 2019FY202503.

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