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Spatio-Temporal Pattern Estimation of PM_{2.5} in Beijing-Tianjin-Hebei Region Based on MODIS AOD and Meteorological Data Using the Back Propagation Neural Network

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Abstract: With the economic growth and increasing urbanization in the last three decades, the air quality over China has continuously degraded, which poses a great threat to human health. The concentration of fine particulate matter ($PM_{2.5}$) directly affects the mortality of people living in the polluted areas where air quality is poor. The Beijing-Tianjin-Hebei (BTH) region, one of the well organized urban regions in northern China, has suffered with poor air quality and atmospheric pollution due to recent growth of the industrial sector and vehicle emissions. In the present study, we used the back propagation neural network model approach to estimate the spatial distribution of $PM_{2.5}$ concentration in the BTH region for the period January 2014–December 2016, combining the satellite-derived aerosol optical depth (S-DAOD) and meteorological data. The results were validated using the ground $PM_{2.5}$ data. The general method including all $PM_{2.5}$ training data and 10-fold cross-method have been used for validation for $PM_{2.5}$ estimation ($R^2 = 0.68$, RMSE = 20.99 for general validation; $R^2 = 0.54$, RMSE = 24.13 for cross-method validation). The study provides a new approach to monitoring the distribution of $PM_{2.5}$ concentration. The results discussed in the present paper will be of great help to government agencies in developing and implementing environmental conservation policy.

Keywords: aerosol optical depth; PM_{2.5}; MODIS; air pollution; artificial neural network; Beijing-Tianjin-Hebei (BTH) region; back propagation neural network

1. Introduction

The exposure of people to fine particulate matter ($PM_{2.5}$, particles with aerodynamic diameter less than 2.5 µm) is associated with cardiovascular suffering and respiratory problems [1–4]. The sources of $PM_{2.5}$ are both natural and anthropogenic emissions. Although it accounts for a small proportion of the particles in Earth's atmosphere, $PM_{2.5}$ degrades the air quality and enhances atmospheric photochemical reactions [5,6]. In recent years, with intensive economic development and urbanization, the concentration of $PM_{2.5}$ has increased in most cities, including Beijing, the capital of China [7]. Such increases in $PM_{2.5}$ degrades air quality, posing a serious threat to human health and affecting

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day-to-day weather conditions. High concentrations of PM_{2.5} with favorable meteorological conditions (relative humidity and air temperature) are responsible for the dense fog and haze conditions.

In the wake of poor air quality in major cities such as Beijing, the Chinese government has established ground-based monitoring stations in major cities that provide data on atmospheric pollution and air quality (including the $PM_{2.5}$ concentration). The routine ground monitor stations cannot provide the spatiotemporal concentration of $PM_{2.5}$. For the spatial distribution of $PM_{2.5}$, the satellite-derived aerosol optical depths (S-DAODs) have been used to estimate $PM_{2.5}$ concentration [8–12]. A number of studies have employed regression models of $AOD-PM_{2.5}$ to estimate the ground-level $PM_{2.5}$ concentration from S-DAOD data [10,13–17]. However, these statistical models still have a key problem, in that statistical approaches were limited to specific regions and times [18–21]. There are actually no effective statistical models to estimate $PM_{2.5}$ concentration with high precision in large regions [22,23]. In addition, earlier studies tended to obtain $PM_{2.5}$ concentration by using low spatial resolution AOD products (10 km), until the 3 km Moderate Resolution Imaging Spectroradiometer (MODIS)AOD product (Collection 6) was recently released [24]. Although there could be slightly higher errors over land in the 3 km MODIS AOD product compared to the 10 km product, the 3 km MODIS AOD product has more capabilities for estimating $PM_{2.5}$ concentration on finer scales.

Efforts have not been made to use any statistical model for estimating $PM_{2.5}$ concentration using the 3 km MODIS AOD product in the Beijing-Tianjin-Hebei (BTH) region. As an attempt, we developed a back propagation neural-network (BPNN) model to estimate $PM_{2.5}$ concentration in the BTH region by combining meteorological data and the 3 km MODIS AOD data. At the same time, the effectiveness of the BPNN model in estimating $PM_{2.5}$ concentration was validated using ground data.

2. Materials and Methods

2.1. Study Area

The BTH region is the one of the largest urban economic circles (UECs) in Northern China (Figure 1), and covers an area of 218,000 km² with total a population of 110 million (about 8% of China's population). The region consists of two municipalities (Beijing and Tianjin) and one province (Hebei), which includes eleven prefecture-level cities (Shijiazhuang, Baoding, Langfang, Tangshan, Zhangjiakou, Chengde, Qinhuangdao, Cangzhou, Hengshui, Xingtai, and Handan) [25–27].

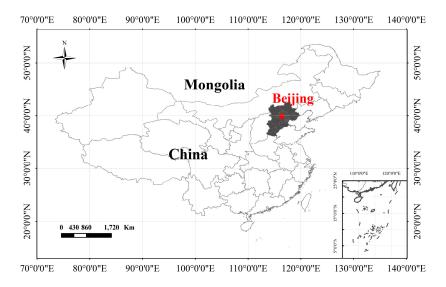


Figure 1. *Cont.*

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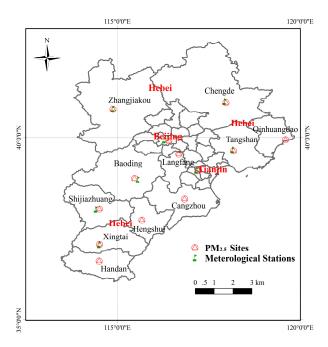


Figure 1. Study area. PM_{2.5}: particulate matter with aerodynamic diameter less than $2.5 \mu m$.

Due to various factors (including huge population, high-speed urbanization, industrial processes, transportation, coal consumption for winter heating, etc.), the BTH region suffers from serious air pollution. During the past several years, the PM_{2.5} concentrations in the BTH region have reached an alarming level. The annual average PM_{2.5} concentration in some cities of the BTH region was five times higher than the national standard (15 μ g/m³) and eight times higher than the WHO guidelines (10 μ g/m³) [27].

2.2. Data

The data used in the present study mainly include ground-measured $PM_{2.5}$, satellite data, and meteorological data (details are given in Table 1).

Data Type	Data	Acquired Time	Spatial Resolution	Source
Ground-level PM _{2.5}	$PM_{2.5} (\mu g/m^3)$	2014.1–2016.12	N/A	Tianqihoubao
Satellite Data	Aqua MODIS AOD products	2014.1–2016.12	3 km × 3 km	National Aeronautics and Space Administration (NASA), MODIS Team
Meteorological Data	Temperature (°C) Surface Pressure (pa) Relative humidity (%) Precipitation (mm) Visibility (km) Wind speed (m/s)	2014.1–2016.12		Global climate data

Table 1. Data sets used in this study. AOD: aerosol optical depth.

2.2.1. Ground PM_{2.5} Measurements

The Ministry of Environmental Protection of the People's Republic of China (MEPCN) has set up more than 900 air-quality monitoring sites in China for the purpose of monitoring air quality ($PM_{2.5}$ and PM_{10} concentration); hourly and 24 h average (daily-mean) $PM_{2.5}$ data are available

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through the national urban air quality real-time publishing platform [28]. Figure 1 shows the locations of 79 ground $PM_{2.5}$ monitoring stations. We have used the daily-mean $PM_{2.5}$ concentration data to validate the model estimate of $PM_{2.5}$.

2.2.2. Meteorological Data

The meteorological parameters (precipitation, air temperature, surface wind speed, relative humidity, surface pressure, and average visibility) were used in the present study together with satellite data. The meteorological parameters (annual averages, monthly averages, and daily averages) were downloaded from the global climate data (GCD) [29] which provide historical climate data based on more than 9000 stations distributed globally since 1929. In the BTH region, daily meteorological data from eight stations have been used in the present study for the period 2014–2016. In order to generate the gridded maps of variables from these stations, the ordinary kriging method has been used to interpolate meteorological parameters [30–32].

2.2.3. Satellite AOD Dataset

There are two types of MODIS AOD products with 10 km and 3 km spatial resolution. The 10 km MODIS AOD product is important to study local estimate of climate and its dynamics. However, for local climate study, fine resolution data are required [33]. The MODIS collection 6 (C6) with 3 km spatial resolution were released in the year 2013 [34,35]. The latest version of AOD product (C6) [36] have been validated using AOD observations [37]. In spite of a limitation that expected errors over land, we considered the 3 km \times 3 km MODIS AOD product for the period 2014–2016 compared to the 10 km MODIS AOD product. The 3 km data product provides finer information that provides effective supplements for the existing 10 km product in estimating PM_{2.5} [24].

2.3. Methodology

The approach used in the present study contains two modules: data pre-processing and model construction (flow chart, Figure 2). The model construction module consists of the artificial neural network (ANN) model construction and model validation.

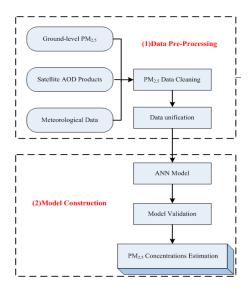


Figure 2. Flow chart showing approach for the estimation of the PM_{2.5}. ANN: artificial neural network.

2.3.1. Data Pre-Processing

We considered the World Geodetic System 1984 geographical coordinate system. The meteorological dataset was interpolated to 3 km resolution using an ordinary kriging

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method to generate the daily gridded maps [30]. For the $PM_{2.5}$ concentration, we considered daily-average $PM_{2.5}$ concentration, meteorological parameters (precipitation, air temperature, surface wind speed, relative humidity, surface pressure, and average visibility), and AOD data collocated in time and space. Sometimes, satellite-derived AOD are missing due to coverage and cloudy conditions, so validation with ground observed $PM_{2.5}$ may not be valid.

2.3.2. ANN Model

We used the artificial neural network (ANN) algorithm to model $PM_{2.5}$ concentration based on the meteorological variables and satellite-derived AOD data. The ANN algorithms are black-box models of artificial intelligence [38]. There have been more than 30 different neural network models that were developed and widely used [39,40]. We used a back-propagation neural network (BPNN) algorithm to build the $PM_{2.5}$ estimation model for predicting the $PM_{2.5}$ concentration [41]. The estimation of the $PM_{2.5}$ concentration model consists of seven neurons in the input layer, seven neurons in the hidden layer, and one neuron in the output layer. The seven parameters in the input layer include precipitation, air temperature, surface pressure, wind speed, relative humidity, average visibility, and MODIS AOD products. The neuron in the output layer is $PM_{2.5}$ concentration. Figure 3 shows the schematic diagram of the ANN model used in the present study.

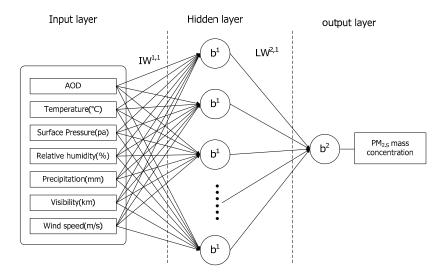


Figure 3. Topological structure of the back propagation neural-network (BPNN) model. IW is the weight matrix of the input layer to the hidden layer; LW is the weight matrix between the hidden layer and the output layer; b is the threshold vector. 1 means the first hidden layer; 2 is the output layer.

2.3.3. Model Evaluation

To assess the performance of the model, the ground $PM_{2.5}$ measured data were used for validation. We computed correlation coefficients, mean absolute percentage prediction error (APE), and root-mean-square error (RMSE). In addition, the 10-fold cross-validation method was used and it was found that the model over-estimated $PM_{2.5}$ concentrations [42]. The whole dataset was split into ten, and approximately 90% of the total dataset datasets were used for model training and only 10% of the datasets for the validation of $PM_{2.5}$ concentration.

3. Results and Discussion

3.1. Descriptive Statistics

Table 2 shows details of $PM_{2.5}$ and the model inputs. The annual mean and standard deviation of MODIS AOD were 0.64 and 0.60, respectively, in the study region. The annual mean value and

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the standard deviation (SD) of ground-level $PM_{2.5}$ concentration, respectively, were $81.33~\mu g/m^3$ and $53.19~\mu g/m^3$. The annual mean visibility values varied in the range 0.30–29.9~km, and surface air temperature varied in the range -10.10~C to 38.10~C. The annual mean precipitation was 2.52~mm, and relative humidity was 55.04%, which implies relatively dry atmospheric conditions. The wind speed varied in the range 1.50–39.60~m/s.

Parameters	Mean	SD	Min	Max
$PM_{2.5} (\mu g/m^3)$	81.33	53.19	3.00	739.00
MODIS AOD	0.64	0.60	0.03	4.49
Temperature (°C)	17.94	11.50	-10.10	38.10
Surface Pressure (pa)	1017.25	10.71	994.60	1054.40
Relative Humidity (%)	55.04	20.35	10.00	100.00
Precipitation (mm)	2.52	11.86	0.00	311.60
Visibility (km)	15.24	8.78	0.30	29.90
Wind Speed (m/s)	9.53	4.03	1.50	39.60

Table 2. The details of PM_{2.5} measurements and the model input parameters.

3.2. Model Validation

We used PM_{2.5} concentration data from 79 ground stations to build the BPNN model and validated the estimated PM_{2.5} values with the ground-observed data. Figure 4 shows the scatter plots between the model-derived PM_{2.5} predictions and the actual ground-measured PM_{2.5} concentration.

We considered two methods to validate the effectiveness of the $PM_{2.5}$ concentration model in the present study. Figure 4a shows the validation results by comparing all the $PM_{2.5}$ observations with corresponding predictions from the $PM_{2.5}$ model estimation. The results show a good estimate of $PM_{2.5}$ concentration ($R^2 = 0.68$, RMSE = 20.99, APE = 20.70%). The scatter plots are distributed around the 1.0 slope of the fitting values, showing good estimate of the ground-observed data. Figure 4b shows the 10-fold cross-validation results with R^2 0.54, RMSE 24.13, and APE 22.50%. The results obtained show that the $PM_{2.5}$ concentration estimated from the model provide a very close estimation with the observed data. By comparing the two validation methods of the model-estimated $PM_{2.5}$ concentration, the R^2 of 10-fold cross-validation results decrease by approximately 0.13, and RMSE increases by approximately 3.14, which suggests that the estimated $PM_{2.5}$ concentration is not substantially over-fitted. Finally, our results show that the BPNN $PM_{2.5}$ concentration estimation model provides an accurate estimate because of the relative lower prediction error [22].

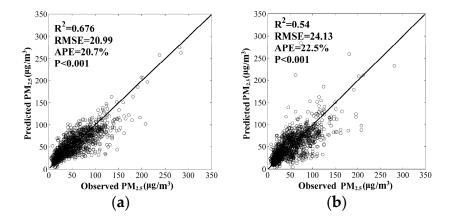


Figure 4. Comparison of model-derived satellite $PM_{2.5}$ with the ground measurements over 79 sites during 2014–2016. (a) The comparison results between all the observed $PM_{2.5}$ data and the corresponding predictions derived from the $PM_{2.5}$ estimation model trained using all surface measured $PM_{2.5}$ data; and (b) 10-fold cross-validation results.

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3.3. Estimation of PM_{2.5} Concentration

The PM_{2.5} estimating model input variables were gridded into the same spatial resolution with the 3 km MODIS AOD products. The spatial distributions of the daily PM_{2.5} concentration for the period January 2014 to December 2016 were obtained from the estimated PM_{2.5} model. Figure 5 shows the annual mean PM_{2.5} concentration in the BTH region. From the annual mean spatial distribution of PM_{2.5} concentration of the BTH region, we observed high concentrations of PM_{2.5} in central and southern BTH, especially in several cities and their surroundings (Beijing, Tianjin, Tangshan, Shijiazhuang, Baoding, Xingtai, etc.). The northern BTH region showed low PM_{2.5} concentration, especially in the Zhangjiakou and Chengde areas. The areal distribution of the PM_{2.5} concentration is controlled by the strong northerly wind in the northern parts of the BTH region during autumn and winter seasons that spreads fine particulate pollutants in the southern parts. At the same time, more population and industry cluster in central and southern parts of the BTH region, and are the main sources of pollution. In addition, the annual mean PM_{2.5} concentration for the years 2015 and 2016 were found to be lower compared to 2014 (Figure 5). Figure 6 shows changes in distribution of the annual mean PM_{2.5} concentration during 2014–2016. The results show that most of the BTH region exhibited a decrease in the annual mean PM_{2.5} concentration during 2015 and 2016 compared with 2014, while a small increase in concentration was observed in Zhangjiakou, Chengde, and other small areas in the BTH region.

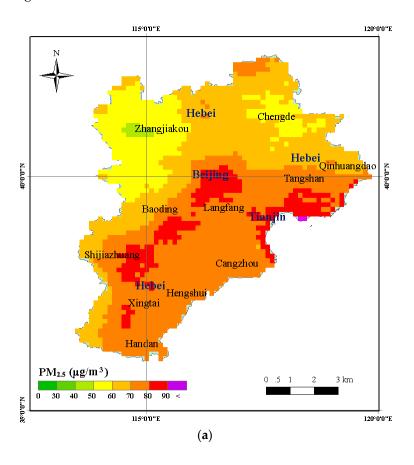


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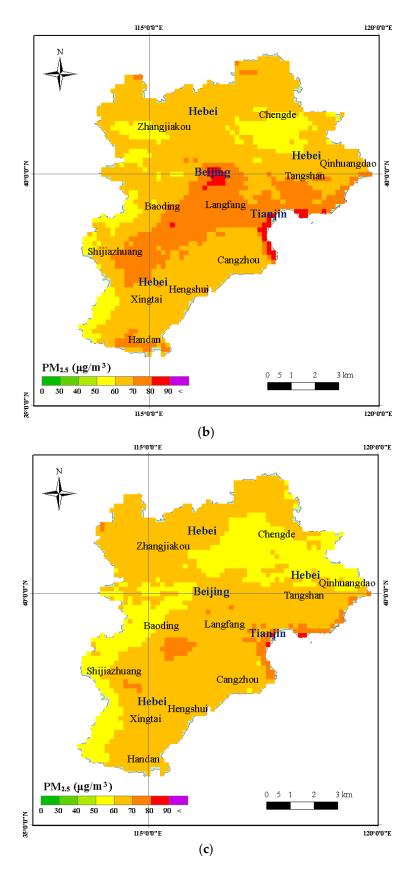


Figure 5. The spatial distribution of the annual mean $PM_{2.5}$ concentration in the Beijing-Tianjin-Hebei (BTH) region. (a) Annual mean $PM_{2.5}$ concentration in 2014; (b) Annual mean $PM_{2.5}$ concentration in 2015; (c) Annual mean $PM_{2.5}$ concentration in 2016.

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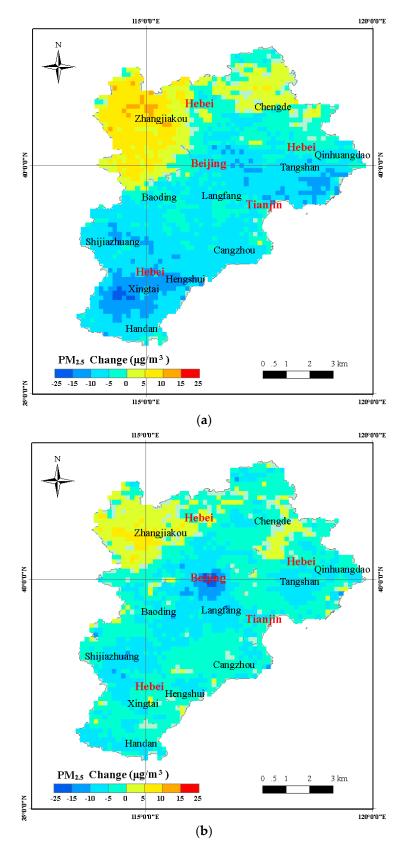


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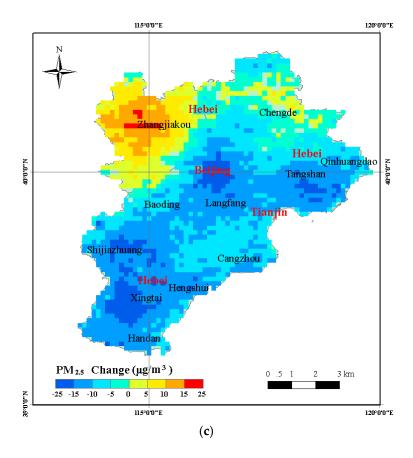


Figure 6. Changes in the annual mean $PM_{2.5}$ concentration from 2014 to 2016 in the BTH region. (a) Difference in spatial concentration of $PM_{2.5}$ in the BTH region during 2014 and 2015; (b) Difference in spatial concentration of $PM_{2.5}$ in the BTH region during 2015 and 2016; (c) Difference in spatial concentration of $PM_{2.5}$ in the BTH region during 2014 and 2016.

By comparing the annual mean $PM_{2.5}$ concentration of 2014 with 2016 (Figure 6c), we observed a decline in concentration in the cities having high concentration (average values greater than $10.00~\mu g/m^3$). In several major cities (Beijing, Tangshan, Shijiazhuang, and Xingtai), $PM_{2.5}$ varied in the range $15.00-25.00~\mu g/m^3$. However, Zhangjiakou city and outskirts showed higher $PM_{2.5}$ values (> $5.00~\mu g/m^3$), and in the center of the Zhangjiakou city $PM_{2.5}$ varied by up to $25.00~\mu g/m^3$. A declining trend in the annual mean $PM_{2.5}$ concentration was observed from 2014 to 2016 in most areas of the BTH region. In order to further evaluate the estimation of $PM_{2.5}$ concentration, we validated the change in trend of $PM_{2.5}$ concentration by using the ground-observed data. Figure 7 shows the change in yearly average trend of 12 cities from the actual ground-measured data and model estimation. Similar trends between ground-measured $PM_{2.5}$ and model estimation are clearly seen in Figure 7. A decreasing trend occurred in 10 cities of the BTH region, including Baoding, Beijing, Shijiazhuang, Tangshan, Tianjin, Xingtai, Cangzhou, Langfang, Hengshui, and Handan (Figure 7). A small increasing trend of $PM_{2.5}$ concentration in the Zhangjiakou region was observed. The evaluation result also demonstrated the accuracy of $PM_{2.5}$ concentration estimation.

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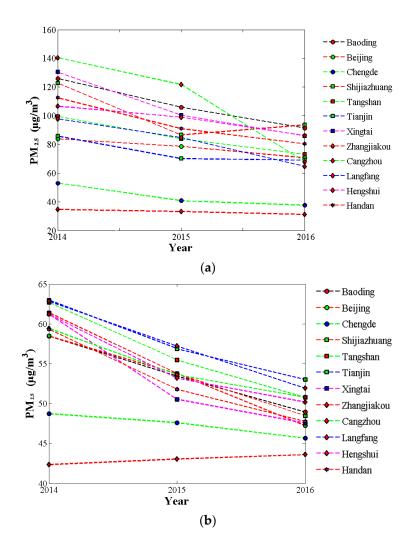


Figure 7. Changes trends in the annual mean $PM_{2.5}$ concentration from 2014 to 2016 in the BTH region. (a) The change trends of $PM_{2.5}$ concentration from the actual ground-measured data; (b) The change trends of $PM_{2.5}$ concentrations estimation.

4. Conclusions

In this study, we estimated the spatio-temporal distribution of $PM_{2.5}$ in the BTH region using the ANN model, with the inputs of MODIS AOD and meteorological data. The $PM_{2.5}$ estimation model using the BPNN approach was able to estimate $PM_{2.5}$ concentration with high accuracy. The model input variables—especially the 3 km AOD product—were used to estimate the spatial distribution of $PM_{2.5}$ concentration. The results provide a reasonably good estimate of $PM_{2.5}$, but we still have limitations and uncertainties in the estimation.

The surface measurements of $PM_{2.5}$ concentration are at the ground level, whereas the satellite AOD product accounts for pollution in the atmospheric column. The vertical profile of AOD or vertical profile of $PM_{2.5}$ concentration were not considered in the model; in the future, such consideration will improve the estimation of $PM_{2.5}$. In addition, the composition and concentration of $PM_{2.5}$ greatly vary due to different sources (natural and anthropogenic) in different regions, and concentrations vary in space and time. For example, the natural source mainly includes sea salt, dust, volcanic eruptions, forest fires, and grassland fires, and the anthropogenic sources mainly consist of fossil fuel combustion and industrial processes. At the same time, there are many uncertain sources which also seriously affect $PM_{2.5}$ concentration, and are not considered in the present study. In future studies,

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a more refined $PM_{2.5}$ estimation model will be conducted to account for seasonal variability and also different [43–45].

The approach based on a BPNN model for $PM_{2.5}$ concentration shows the feasibility of monitoring the $PM_{2.5}$ concentration in large-scale regions. In order to further improve the estimation of $PM_{2.5}$ concentration, we will make following efforts:

- Sometimes there are gaps in the area covered by the satellites; the higher temporal resolution will
 reduce the gaps in AOD data. Satellite remote sensing data from Terra MODIS AOD, Landsat 8,
 the Visible Infrared Imaging Radiometer Suite (VIIRS) onboard Suomi National Polar-Orbiting
 Partnership (Suomi NPP), and Environment and Disaster Monitoring Small Satellite (HJ-1) may
 provide better AOD data [46,47].
- Light detection and ranging (Lidar) data will be considered in the future to estimate the aerosol vertical profile and components, which would be helpful in understanding the vertical distribution and source of PM_{2.5} concentration [48]. In addition, the interpolation of meteorological data should also be studied to obtain the most accurate spatial distribution data, which can improve the estimation precision of the PM_{2.5} concentration distribution.

The method proposed in the present study can be extended to large areas, when the dense network of ground observing stations is expanded.

The estimate of PM_{2.5} over in China will be of great help in understanding the dynamics of pollutants, and will also help the government in making efforts to minimize atmospheric pollution and improve air quality, public health, and the climate—especially during the winter season.

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