RESEARCH ARTICLE



Estimating Ground-Level Hourly PM_{2.5} Concentrations Over North China Plain with Deep Neural Networks

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Abstract

Fine particulate matter ($PM_{2.5}$) has a considerable impact on the environment, climate change, and human health. Herein, we introduce a deep neural network model for deriving ground-level, hourly $PM_{2.5}$ concentrations by Himawari-8 aerosol optical depth, meteorological variables, and land cover information. A total of 151,726 records were collected from 313 ground-level $PM_{2.5}$ monitoring stations (spread across the North China Plain) to calibrate and test the proposed model. The sample- and site-based cross-validation yielded satisfactory performance, with correlation coefficients > 0.8 (R = 0.86 and 0.83, respectively). Furthermore, the variation in mean ground-level hourly $PM_{2.5}$ concentrations, using 2017 data, showed that the proposed method could be applied for spatiotemporal continuous $PM_{2.5}$ monitoring. This study will serve as a reference for the application of geostationary meteorological satellite to perform ground-level $PM_{2.5}$ estimation and the utilization in atmospheric monitoring.

Keywords Fine particulate matter · Deep neural networks · North China Plain · Himawari-8 · Aerosol optical depth

Introduction

Fine particulate matter ($PM_{2.5}$), which consists of particles with aerodynamic diameters < 2.5 µm, has attracted considerable scientific attention (Pope & Dockery, 2006). Previous studies have indicated that prolonged exposure to $PM_{2.5}$ is affiliated with many human health issues including respiratory problems, cardiovascular disease, cancer, and infectious diseases (Bartell et al., 2013; Brauer et al., 2012; Chen et al., 2017; Crouse et al., 2012; Dominici et al., 2006; Gent et al., 2009; Guo et al., 2016; Lao et al., 2019; Pope, 2000; Zhang et al., 2020). Generally, ground

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monitoring sites can provide accurate $PM_{2.5}$ measurements, but there are many regions for which measurements are unavailable as there are no monitoring networks. Thus, the sparse distribution of ground sites limits our capability to estimate the impacts of human exposure to $PM_{2.5}$, with data on local meteorological effects and emission sources absent. Consequently, it is important that models that can accurately predict the broader spatiotemporal distribution of ground-level $PM_{2.5}$ concentrations are developed.

Satellite has been applied to monitor ground-level $PM_{2.5}$ emissions to fill in spatial gaps in ground measurement coverage (Chu et al., 2016; Hu et al., 2014; Kloog et al., 2012; Ma et al., 2014). Several studies were conducted for estimating $PM_{2.5}$ concentrations from the aerosol optical depth (AOD), derived by satellite remote sensing, including multiple linear regression (Chu et al., 2016; Gupta & Christopher, 2008, 2009; Kacenelenbogen et al., 2006; Liu et al., 2005; Paciorek et al., 2008; Schaap et al., 2009; Wang, 2003; Yao et al. 2018), mixed-effect models (Just et al. 2015; Kloog et al. 2011, 2012, 2014; Lee et al. 2012; Zheng et al. 2016), geographically weighted regressions (Bai et al., 2016; Guo et al., 2017; He & Huang, 2018a, b; Hu, 2009; Ma et al., 2014; You et al., 2015; Zou et al., 2016), and chemical transport models (Crouse et al., 2016).

2012, 2016; Hystad et al., 2012; Liu et al., 2004; van Donkelaar et al., 2006; Wang & Chen, 2016). To improve the model performance, an increasing number of predictors, including meteorological information, land cover, and aerosol properties, were integrated. Thus, machine learning models, which are capable of complex nonlinear relationships fitting, have been applied to get $PM_{2.5}$ concentrations from satellite observations. For example, random forests (Chen et al., 2018; Hu et al., 2017), deep belief networks (DBNs) (Li et al., 2018; Liu et al., 2018), deep neural networks (DNNs) (Wang & Sun, 2019), and machine learning models with high-dimensional expansion (Xue et al., 2019) have been used, and they have delivered superior prediction accuracy and applicability.

All these studies were limited to the use of polar orbit satellites, however, geostationary satellites are still rarely used in the estimation of PM_{2.5}. These geostationary satellites are able to conduct more measurements and facilitate the capturing of atmospheric aerosol variation data hourly. In particular, with the launch and operation of next-generation geostationary meteorological satellitessuch as the Advanced Geosynchronous Radiation Imager (AGRI) on board FengYun-4A, the Advanced Himawari Imager (AHI) on board Himawari-8/9, and the Advanced Baseline Imager (ABI) on board GOES-R-abundant AOD datasets have become available. The quality of these data has been validated: for example, it has been reported that the expected uncertainty for the Himawari-8 AOD is \pm $(0.1 + 0.3 \times AOD)$ (Zhang et al., 2019), whereas the expected uncertainty for the MODIS (C6.1) 10 km AOD product is $\pm (0.05 + 0.15 \times AOD)$ (Aldabash et al., 2020).

The North China Plain (NCP), which is renowned for experiencing severe atmospheric pollution events, has experienced high $PM_{2.5}$ concentrations for decades owing to the rapid economic and population development that has taken place nearby. In this study, we applied the DNN methodology to estimate hourly ground-level $PM_{2.5}$ concentrations over the NCP using Himawari-8 AHI AOD data.

The balance of this paper has been laid out as follows: data sets and a detailed description of the methodology may be found in "Materials and Methods" section, whereas the results and discussion have been given in "Results and Discussion" section. The study has been concluded in "Summary and Conclusions" section.

Materials and Methods

Datasets

Ground-Level PM_{2.5} Measurements

Ground-level PM_{2.5} concentration dataset was obtained from the China Environmental Monitoring Center (CEMC). Hourly PM_{2.5} measurements from 313 air quality sites in the NCP (as shown in Fig. 1) were collated for 2017. These concentrations represented the hourly averages established at the stations by the tapered element oscillating microbalance (TEOM). The accuracy of TEOM is \pm 1.5 µg/m³ (You et al., 2016). The data are available at http://106.37.208.233:20035/.

Himawari-8 AOD

Himawari-8 was launched by the Japan Meteorological Agency on October 7, 2014. It is a next-generation geostationary meteorological satellite. The AHI on board Himawari-8 has 16 channels. Its spatial temporal resolution is 0.5–2 km and 5–10 min, respectively (Yumimoto et al., 2016; Zhang et al., 2019).

The AOD products are provided with three levels: "Level2" (L2), "Level3" (L3), and "Level4" (L4) (Kikuchi et al., 2018). The spatial and temporal resolution of L3 is 0.05° and 1 h, respectively. In this study, the AOD data of L3 Version 3.0, which can be received from https:// www.eorc.jaxa.jp/ptree/index.html, were collected to estimate hourly PM_{2.5} concentrations. It should be noted that a comprehensive AOD validation, as used in this study, can be found in our previous work (Zhang et al., 2019).

Meteorological and Land Cover Data

Meteorological data for 2017 were obtained from the second Modern-Era Retrospective analysis for Research and Applications (MERRA-2). It is the atmospheric product supported by National Aeronautics and Space Administration, with a spatial resolution of $0.5 \times 0.625^{\circ}$ (Gelaro et al., 2017; Rienecker et al., 2011). We extracted six hourly meteorological factors from this dataset: surface pressure (PS; as Pa), air temperature at 2 m (TMP; as K), E and N wind speed at 10 m above ground (EW and NW; as m/s), relative humidity (RH; as %), and planetary boundary layer height (PBLH; as m). The data can be downloaded from the website https://disc.gsfc.nasa.gov/datasets.

Landcover-related variables—surface albedo (ALBEDO; which is a unitless variable) and surface incoming shortwave flux (SWGDN; as W/m²)—were also extracted from the MERRA-2 data. Elevation (ELEV; as



Fig. 1 North China Plain elevation. Ground-level data for the study were acquired from the air quality sites (white dots) (color figure online)

m) was terrain data at 1 km, whereas the normalized difference vegetation index (NDVI) was derived from MOD13A3, a monthly 1-km resolution dataset.

Based on the AOD, meteorological and land cover, there are 11 predictors were used to derive hourly $PM_{2.5}$ concentrations over the NCP. That is AOD, surface pressure, air temperature, wind speed (*E* and *N*), PBLH, RH, ALBEDO, SWGDN, ELEV, and NDVI. Statistics for these datasets and predictors are listed in Table 1.

Methods

Data Integration

Firstly, because the original data involved various coordinate systems and spatial resolutions, all independent variables were recalibrated into the WGS84 coordinate system. Meteorological variables and land cover data were also recalibrated to, in this case, 0.05° resolution to ensure consistency. After these processes, the 11 predictors were matched with ground $PM_{2.5}$ in a co-location procedure. The predictors were collected into a station-centered pixel. These selection process eventually gave rise to a dataset consisting of 151,726 records.

DNN Model

The concentrations of ground-level $PM_{2.5}$ were affected by multiple factors, such as aerosol, meteorological, and surface cover. This complex relationship is difficult to describe accurately with a simple linear model, and so deep learning, which has been widely used in fitting complex, nonlinear relationships, was used to estimate ground-level $PM_{2.5}$ concentrations. Thus, a DNN model (Hinton et al., 2012) was fitted using Eq. (1):

 $PM_{2.5} = f(AOD, PS, TMP, EW, NW, PBLH, RH,$ ALBEDO, SWGDN, ELEV, NDVI),

Table 1Dataset informationand statistics

Datasets	Predictors ^a	Units	Spatial resolution	Temporal resolution	Factors
Himawari-8	AOD	_	0.05°	Hourly	Aerosol
MERRA-2	PS	Ра	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	TMP	Κ	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	EW	m/s	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	NW	m/s	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	PBLH	m	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	RH	%	$0.5 \times 0.625^{\circ}$	Hourly	Meteorological
	ALBEDO	-	$0.5 \times 0.625^{\circ}$	Hourly	Land cover
	SWGDN	W/m ²	$0.5 \times 0.625^{\circ}$	Hourly	Land cover
GMTED2010	ELEV	m	1 km	_	Land cover
MOD13A3	NDVI	_	1 km	Monthly	Land cover

^aThe meaning of each item is explained in text

where $f(\cdot)$ describes the prediction function. The meaning of each predictor has been described above.

Figure 2 shows the structure of the DNN model, where it can be seen that the model contained five hidden layers (which contained 60, 40, 30, 20, and 10 neurons), one input layer (which contained the 11 neurons shown in Eq. (1), and one output layer (which consisted of $PM_{2.5}$ concentration estimates). This gave the proposed DNN model a structure of 11-60-40-30-20-10-1. It should be noted that the numbers of layers and neurons were chosen by increasing the numbers of neurons until the best estimation results were derived.

Figure 3 illustrates the workflow used to estimate ground-level, hourly $PM_{2.5}$. The process can be described as follows:

(1) Conduct data integration, as described in "Data Integration" section. The derived AOD, meteorological variables, and land cover, which were consistent in time and space, were treated as model training and validation samples.

- (2) Perform DNN model fitting. To this end, all the 151,726 records (belonging to 313 sites) were first used to train the model, after which sample- and sitebased tenfold cross-validation (CV) was carried out to evaluate the performance. CV was conducted as follows:
 - (a) For sample-based CV, the samples were randomly divided into ten sets, with each set accounting for approximately 10% of the records. For each CV process, nine sets were used for training samples, with the tenth used to make predictions. Then, we repeated ten times until the predictions from each set were established;
 - (b) Site-based CV was conducted to examine model sensitivity with respect to the number of ground stations and performance with respect to spatial variations. The 313 sites were randomly split into ten sets, with each set accounting for approximately 10% of the sites. As for the sample-based CV, nine sets were



Fig. 2 Structure of the DNN model used for $PM_{2.5}$ estimation



used to fit the model, with the tenth used to make predictions. $PM_{2.5}$ concentration predictions were finally obtained by completing ten CV cycles;

- (c) Finally, to evaluate the levels of agreement, linear fit statistics for model predictions vs observations were performed. The statistical indicators include the correlation coefficient (*R*), slope, *y* intercept, and prediction root mean squared error (RMSE).
- (3) Finally, the prediction data (locations with no ground $PM_{2.5}$ observations) were input into the derived DNN model to obtain spatial distributions of hourly $PM_{2.5}$ concentrations over the NCP.

Results and Discussion

Descriptive Statistics

Variable histograms, covering all 151,726 samples, are presented in Fig. 4. The surface pressure (PS) was found to be almost exponentially distributed, whereas air temperature (TMP) was approximately bimodal in its distribution. The E wind speed, N wind speed, PBLH, surface albedo, surface incoming shortwave flux (SWGDN), RH, and NDVI were found to have approximately normal distributions. The other variables, including elevation, AOD, and PM_{2.5}, exhibited similar logarithmic distributions. The minimum, maximum, and mean PM_{2.5} concentrations were 1, 534, and 55.13 μ g/m³, respectively, whereas the minimum, maximum, and mean AOD were calculated to be 0, 2.99, and 0.4, respectively, with the high AOD and $PM_{2.5}$ maximums indicating that severe pollution was experienced over the NCP. Their standard deviations were calculated as 0.34 and 42.15 mg/m³, respectively, indicating



Fig. 4 Descriptive statistics for dependent and independent variables (minimums, maximums, means, and standard deviations). The meaning of each item is explained in text

that there had been significant fluctuations in the atmospheric particulate matter concentrations.

Variable Importance Analysis

To evaluate the potential effect of each predictor to the proposed DNN, we conducted a variable importance analysis. In Fig. 5, the variables for predicting $PM_{2.5}$ have been represented in the y axis, with the percentage RMSE increase without using the corresponding variable (%IncRMSE) shown on the x axis. The figure shows that AOD (55.07%) was the variable with the highest contribution, which would be attributable to its strong correlation with PM_{2.5} concentrations. The %IncRMSE calculated without using air temperature as a predictor was 45.92%, followed by PBLH (41.21%), SWGDN (35.07%), RH (34.86%), N wind speed (32.09%), surface pressure



Fig. 5 Variable importance analysis. The x axis indicates the percentage RMSE increase achieved without using the corresponding predictor (%IncRMSE)

(30.63%), E wind speed (24.22%), and surface albedo (24.01%).

Figure 5 also shows that elevation and NDVI were the weakest contributing variables for hourly $PM_{2.5}$ concentrations. These relatively low contributions may have been due to the small elevation variations over the NCP (shown in Fig. 4j). Furthermore, hourly $PM_{2.5}$ concentrations, usually with high frequency variations, were likely to be less affected by variables that varied only slowly over time, such as NDVI.

Model Performance and Validation

The scatter plot showing ground observed (*x* axis) and estimated (*y* axis) PM_{2.5} concentrations for sample- and site-based CVs is shown in Fig. 6a, b. The *R*, RMSE, slope, and y intercept of sample-based CVs were 0.86, 21.40 μ g/m³, 0.81, and 10.22 μ g/m³, respectively; with regard to the site-based CVs, the corresponding values were 0.83, 23.65 μ g/m³, 0.76, and 13.17 μ g/m³, respectively. This good level of consistency demonstrated that the proposed DNN model was capable of achieving satisfactory performance.

We noted that the site-based CV outcome was comparable with that of the sample-based CV, which indicated that the proposed model had good spatial prediction capability. In addition, both the regression linear fit slopes were < unity (0.81 and 0.76), which implied that the DNN model tended to develop results that were slightly underestimated in comparison with the observed PM_{2.5} concentration. This underestimation was confirmed by noting observed PM_{2.5} concentrations > 54 μ g/m³.

We deduced two possible reasons for the ground-observed $PM_{2.5}$ concentration underestimation by the model. Firstly, using spatially averaged AOD, meteorological, and land surface variables to estimate point ground-level $PM_{2.5}$ meant that it was difficult for meteorological parameters with relatively coarse spatial resolution ($0.5^{\circ} \times 0.625^{\circ}$) to characterize detailed spatial variations. The other reason was that a spatial average would lead to high values being averaged and low values being overwhelmed. Taken together, these points meant that when we compared spatially averaged estimations with ground measurements, low values appeared to be overestimated and high values underestimated.

The spatial performance of the sample-based CV is illustrated in Fig. 7, where it can be seen that both *R* and RMSE (Figs. 7a, b, respectively) exhibit spatial variations. The *R* ranged between 0.48 and 0.93, whereas the RMSE ranged between 13.33 and 45.63, with 81% of R > 0.75 (254 sites out of 313), and 68% of the RMSE < 25 µg/m³ (213 out of the 313 sites). With respect to geographic distribution, sites in Henan Province performed better, with the RMSE being lower in Anhui and Zhejiang.

Scatter plots for ground-observed (*x* axis) and estimated (*y* axis) daily and monthly PM_{2.5} concentrations are shown in Figs. 8a, b. The daily data *R* and RMSE were calculated to be 0.81 and 24.94 μ g/m³, whereas the corresponding estimates for the monthly data were 0.90 and 9.91 μ g/m³, respectively, showing that the model could accurately represent seasonal PM_{2.5} levels, with only small deviations.

Map of PM_{2.5} Estimation

The distributions of seasonal average $PM_{2.5}$ over NCP in 2017 are shown in Fig. 9; in Fig. 9a–d; the seasonal variations in $PM_{2.5}$ are clearly observable. The highest $PM_{2.5}$ estimations were in winter, followed by spring, and then autumn, with the lowest values appearing in summer. Mean $PM_{2.5}$ estimations for spring, summer, autumn, and winter



Fig. 6 Scatter plots for tenfold cross-validations (CVs): a sample-based CV; b site-based CV



Fig. 8 Model validation scatter plots: a daily data; b monthly averages

were 48.93, 39.85, 48.06, and 74.78 μ g/m³, respectively. The seasonal ground-level PM_{2.5} observations showed spatial distributions similar to those seen for the estimates, as shown in Figs. 9e–h. The *R* values of four seasons were 0.88, 0.86, 0.91, and 0.97, respectively (Figs. 9i–1), whereas the corresponding RMSEs were 4.53, 5.22, 4.83, and 5.80 μ g/m³, respectively.

Annual estimated $PM_{2.5}$ patterns for the NCP are plotted in Fig. 10. Generally, low AOD and $PM_{2.5}$ levels occurred in NW Hebei Province, with its low population density and few industries. These spatial AOD (Fig. 10a) and $PM_{2.5}$ (Fig. 10b) distribution results were not completely consistent, however, which indicated that their interrelationship

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was complex. Meanwhile, a heavily polluted region was revealed at the junction of the five provinces (Hebei, Henan, Anhui, Jiangsu, and Shandong). Scatter plots for annualized ground-level observations vs estimated $PM_{2.5}$ levels are shown in Fig. 10c, with the *R* and RMSE calculated to be 0.94 and 3.64 µg/m³ (Fig. 10d), respectively.

Annualized $PM_{2.5}$ estimate averages for ten hours (00:00–09:00 (Coordinated Universal Time, UTC)), in 2017, are shown in Fig. 11, whereas Fig. 12 shows the corresponding ground-level observation frequencies. Figure 11 proves that the proposed model can provide at least ten hourly $PM_{2.5}$ estimations in one day for any given area, i.e., it can provide $PM_{2.5}$ concentration information at high



Fig. 9 Spatial distributions for spring (March, April, and May), summer (June, July, and August), autumn (September, October, and November), and winter (December, January, and February) mean

 $PM_{2.5}$ concentrations: **a**-**d** estimates; **e**-**h** ground-observations; **i**-**l** ground observation versus estimates distribution scatter plots



Fig. 10 Spatial distribution for annual average $PM_{2.5}$ concentrations: **a** AOD; **b** estimates; **c** ground-level observations; **d** scatter plot for ground-level observations versus estimates

frequencies. In Fig. 12, we can see that the spatial distribution of ground-level measurements exhibited temporal variations, peaking at noon, local time (03:00 UTC), whereas the data volume gradually decreased in the mornings and afternoons. This could be explained by the fact that the ability of the satellite to capture aerosol signals

decreased as the solar zenith angle increased (Zhang et al., 2019).

Variations in annual average hourly $PM_{2.5}$ estimations experienced by different cities are shown in Fig. 13. The cities were selected based on their distribution and representativeness for different regions. They displayed similar trends, i.e., over the period 00:00–09:00 (UTC), the $PM_{2.5}$



Fig. 11 Annualized PM2.5 estimate averages for different hours (as UTC) in 2017: a-j represent 00:00-09:00, respectively

levels peaked at certain times and then decreased. The peaks for Hefei (117.24, 31.84), Shijiazhuang (114.52, 38.03), Nanjing (118.80, 32.07), and Jinan (117.13, 36.64) appeared at either 02:00 or 03:00 (UTC), whereas Beijing (116.41, 39.90) and Zhengzhou (113.64, 34.75) peaked at 01:00. Minimum values were experienced by all cities at either 08:00 or 09:00 (UTC). Figure 13 shows that the proposed model could describe variety in $PM_{2.5}$ concentrations at a temporal resolution of 1 h.

Summary and Conclusions

It is still a challenge to derive high temporal ground-level $PM_{2.5}$ accurately using satellite-derived AOD data, especially for regions with higher particulate matter concentrations and complex compositions, such as the NCP, which has become heavily polluted with respect to $PM_{2.5}$. Herein, we presented a DNN model that was calibrated

using aerosol product (from a new-generation geostationary satellite Himawari-8), meteorological, and land cover information to estimate hourly ground-level PM2.5 concentrations of NCP. The estimated PM_{2.5} concentrations had a spatial and temporal resolution of 0.05° and 1 h, respectively, which can capture detailed variations in temporal PM_{2.5} distributions than would have been possible using polar orbit satellites such as MODIS. A total of 11 independent variables were used to fit the proposed model: AHI AOD, surface pressure, air temperature, E and N wind speeds, PBLH, RH, surface albedo, SWGDN, elevation, and NDVI. Through data integration, a total of 151,726 records related to 313 ground stations were collected. To validate the model performance, tenfold CV was conducted, and it was found that both sample-based RMSE = $21.40 \ \mu g/m^3$) (R = 0.86,and site-based $(R = 0.83, \text{RMSE} = 23.65 \text{ }\mu\text{g/m}^3)$ CVs exhibited satisfactory performances. R values were calculated to be 0.81 and



Fig. 12 Annualized frequencies for PM_{2.5} concentration estimates for different hours in 2017 (as UTC): a-j represent 00:00–09:00, respectively



Fig. 13 Annual mean variations in 2017 for hourly $\text{PM}_{2.5}$ concentrations in selected study area cities

0.90, respectively, for daily and monthly averaged $PM_{2.5}$ levels.

When mapped, the estimated $PM_{2.5}$ concentrations for the NCP showed clear seasonal variations, with the highest $PM_{2.5}$ concentrations appearing in winter, followed by spring, autumn, and summer. The annual patterns showed that low $PM_{2.5}$ concentration levels occurred in NW Hebei Province, whereas the area representing the junction of Hebei, Henan, Anhui, Jiangsu, and Shandong provinces was identified as being heavily polluted.

We also produced mapping, in which 2017 hourly data were used to generate annualized averages for ten hours (from 00:00 to 09:00 UTC). These results suggested that the proposed model could provide at least ten different hourly $PM_{2.5}$ estimations daily, and thus, it had the capability to reveal high levels of atmosphere variation over time. Such successful testing allowed us to conclude that new-generation geostationary satellites have the potential to be used as useful data sources for ground-level $PM_{2.5}$ estimation.

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Availability of Data and Material The ground PM_{2.5} measurements can be obtained from http://106.37.208.233:20035/. The Himawari-8 AOD can be obtained from https://www.eorc.jaxa.jp/ptree/index.html. The MERRA-2 data can be obtained from https://disc.gsfc.nasa.gov/ datasets.

Declarations

Conflicts of interest The authors declare no conflict of interest.

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