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Satellite-based mapping of daily high-resolution ground $PM_{2.5}$ in China via space-time regression modeling

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ABSTRACT

The use of satellite-retrieved aerosol optical depth (AOD) data and statistical modeling provides a promising approach to estimating $PM_{2.5}$ concentrations for a large region. However, few studies have conducted high spatial resolution assessments of ground-level $PM_{2.5}$ for China at the national scale, due to the limitations of high-resolution AOD products. To generate high-resolution $PM_{2.5}$ for the entirety of mainland China, a combined 3 km AOD dataset was produced by blending the newly released 3 km-resolution Moderate Resolution Imaging Spectroradiometer (MODIS) Dark Target AOD data with the 10 km-resolution MODIS Deep Blue AOD data. Using this dataset, surface $PM_{2.5}$ measurements, and ancillary information, a space-time regression model that is an improved geographically and temporally weighted regression (GTWR) with an interior point algorithm (IPA)-based efficient mechanism for selecting optimal parameter values, was developed to estimate a large set of daily $PM_{2.5}$ concentrations. Comparisons with the popular spatiotemporal models (daily geographically weighted regression and two-stage model) indicated that the proposed GTWR model, with an R^2 of 0.80 in cross-validation (CV), performs notably better than the two other models, which have an R^2 in CV of 0.71 and 0.72, respectively. The use of the combined 3-km high resolution AOD data was found not only to present detailed particle gradients, but also to enhance model performance (CV R^2 is only 0.32 for the non-combined AOD data). Furthermore, the GTWR's ability to predict $PM_{2.5}$ for days without $PM_{2.5}$-AOD paired samples and to generate historical $PM_{2.5}$ estimates was demonstrated. As a result, fine-scale $PM_{2.5}$ maps over China were generated, and several $PM_{2.5}$ hotspots were identified. Therefore, it becomes possible to generate daily high-resolution $PM_{2.5}$ estimates over a large area using GTWR, due to its synergy of spatial and temporal dimensions in the data and its ability to extend the temporal coverage of $PM_{2.5}$ observations.

1. Introduction

Fine particulate matter, a complex of solid and liquid particles suspended in the air with aerodynamic diameters of 2.5 μm or less ($PM_{2.5}$), has been associated with adverse effects on public health by many epidemiological studies (Kampa and Castanas, 2008; Madrigano et al., 2013; Pope and Dockery, 2006). The rapid urbanization and industrialization of China has led to $PM_{2.5}$ becoming a dominant factor in air pollution, especially over urban areas, and thus an unprecedented issue of public concern (Bi et al., 2014; Che et al., 2014; Guo et al., 2009). Given the advent of severe $PM_{2.5}$ levels in China, it is urgent to assess the health effects of $PM_{2.5}$ exposure across China, using $PM_{2.5}$ data with a high spatial resolution. However, currently, such an assessment is seriously hindered by the limited measurements available from the sparse network of surface monitoring stations.

Because satellite remote sensing has the capacity to provide data with large (even global) spatial coverage, satellite-derived aerosol optical depth (AOD) information is an alternative method of inferring ground-level $PM_{2.5}$ concentrations (Engel-Cox et al., 2004; Wang and Christopher, 2003). To better investigate $PM_{2.5}$ exposure for air pollution assessment and epidemiological research, satellite-derived $PM_{2.5}$ concentrations at high spatial resolution are needed. High-resolution studies in this research field have been increasingly carried out in North America using 1-km Multiangle Implementation of Atmospheric Correction (MAIAC) AOD (Hu et al., 2014; Kloog et al., 2014). However, equivalent studies for China are scarce, due to the lack of high-resolution satellite-derived AOD products. Studies on a national scale have only presented $PM_{2.5}$ variations with resolutions ranging from 10 to

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50 km, employing widely used AOD products, e.g., the Moderate Resolution Imaging Spectroradiometer (MODIS) Level 2 10 km AOD product and Multi-angle Imaging SpectroRadiometer (MISR) Level 2 17.6 km AOD product (Fang et al., 2016; Ma et al., 2014; Ma et al., 2016).

In early 2014, a 3-km aerosol product was included in the new MODIS Collection 6 (C6). It is the first daily global aerosol dataset with a relatively high spatial resolution (Remer et al., 2013). The fine aerosol gradients can benefit air quality applications, i.e., improve the performance of statistical models and provide details of spatial variation for fine particulate matter (Xie et al., 2015). However, the MODIS 3 km AOD data were retrieved using the Dark Target (DT) algorithm that derives AOD over dark surfaces, which may cause a large number of missing values in the daily AOD image, especially for a large area with a complex land surface (He et al., 2017). In other words, it is impossible to generate a daily $PM_{2.5}$ prediction at high spatial resolution for the entirety of China using only the MODIS 3 km AOD product as the primary predictor (Li et al., 2017; You et al., 2016). Thus, improving the daily coverage of the 3 km MODIS AOD for ground $PM_{2.5}$ estimation over a large area with multiple types of land cover is essential.

Various models have been developed to elucidate the quantitative association between satellite-based AOD and surface $PM_{2.5}$, ranging from a simple linear regression model (Engel-Cox et al., 2004; Wang and Christopher, 2003) to advanced statistical models such as the linear mixed effect (LME) model (Lee et al., 2011; Xie et al., 2015), land use regression model (Kloog et al., 2011; Kloog et al., 2012), and geographically weighted regression (GWR) model (Hu et al., 2013; Ma et al., 2014; Song et al., 2014; Zou et al., 2016). To date, two main spatial and temporal regression methods have been used to establish the $PM_{2.5}$-AOD relationship. One is the daily GWR model, which addresses the spatial variability between $PM_{2.5}$ and AOD for individual days and achieves reasonable results (Ma et al., 2014; Song et al., 2014). However, this model ignores the fact that the $PM_{2.5}$-AOD relationship could vary with time and may be dependent on previous days. Thus, daily GWR cannot make use of temporal autocorrelation existing in the data and fails to build a model for days with fewer $PM_{2.5}$-AOD samples. The other method is a two-stage model that can account for both spatial and temporal non-stationarities (Hu et al., 2014; Wu et al., 2016). However, this model calibrates the spatial and temporal $PM_{2.5}$-AOD relationship separately, i.e., using the LME model to account for its temporal variations in the first stage, and then the GWR model its spatial variations in the second stage. Consequently, this model does not simultaneously treat spatiotemporal variations of the $PM_{2.5}$-AOD relationship; it is thus not in a better position to predict $PM_{2.5}$ for days with insufficient or no $PM_{2.5}$ observations. As such, it becomes difficult to use the two methods to generate high-resolution $PM_{2.5}$ with high accuracy for a large area when there is a limited number of $PM_{2.5}$-AOD paired samples.

In recent years, the geographically and temporally weighted regression (GTWR) model proposed by Huang et al. (2010), which integrates spatial and temporal distance, has gained increasing popularity in environmental studies (Bai et al., 2016; Chu et al., 2015; Guo et al., 2017). Unlike the two spatiotemporal models already discussed, this space-time regression model can simultaneously incorporate temporal information from the estimation day or from previous days into the spatial variability through a spatial-temporal weighting mechanism. Nevertheless, the predictive power of GTWR for elucidating the relationship between $PM_{2.5}$ and AOD, especially for days without samples, has yet to be explored. Optimization of parameter values for GTWR is also required to reduce the computational cost for a large dataset. As a corollary, there are still considerable challenges confronting a space-time model, such as GTWR, in exploring the $PM_{2.5}$-AOD relationship, especially over an extensive area with a large but insufficient sample dataset.

The objective of this study is to overcome such challenges by predicting ground $PM_{2.5}$ at high spatial resolution on a daily basis for the entirety of mainland China, in the setting of a space-time regression model using the MODIS 3 km AOD as the major predictor, and meteorological and land use data as ancillary variables. A customized approach to filling in missing AOD values was devised to improve the availability of daily MODIS 3 km AOD. Subsequently, the GTWR model improved with the parameter optimization approach was developed to generate ground $PM_{2.5}$ concentrations at high resolution, and its inferring power also explored comprehensively. A daily GWR model and a two-stage (LME + GWR) model were also implemented as benchmarks to examine the extent to which GTWR's simultaneous spatial and temporal weighting established a reliable association between surface $PM_{2.5}$ and satellite AOD.

2. Data collection and preprocessing

2.1. Ground-level $PM_{2.5}$ observations

Daily average $PM_{2.5}$ observations from 1 January 2015 to 31 December 2015 were obtained from the China Environment Monitoring Center (http://106.37.208.233:20035/). Ground $PM_{2.5}$ mass concentrations of mainland China are measured by the tapered-element oscillating microbalance or beta-attenuation method, with calibration and quality control according to national standards GB3095-2012 (China's National Ambient Air Quality Standard, or CNAAQS) (China, 2012) and HJ 618-2011 (Determination of Atmospheric Articles PM_{10} and $PM_{2.5}$ in Ambient Air by Gravimetric Method, available at http://english.sepa.gov.cn/Resources/standards/Air_Environment/). At present, the observations come from 1456 monitoring stations in 329 cities (Fig. 1). Most are located in southeastern China, whereas the northwestern areas have little coverage.

2.2. MODIS AOD data

2.2.1. MODIS 3 km DT AOD products

MODIS is a sensor that has been on board NASA Terra since 1999 and Aqua since 2002, providing two daily observations of columnar aerosol properties at approximately 10:30 am (Terra) and 1:30 pm (Aqua) local time. The DT algorithm was originally developed to derive aerosol properties over dark surfaces (e.g., dense vegetated areas) at a 10 km spatial resolution. To satisfy an identified need for monitoring fine-resolution pollution, aerosol datasets with a 3 km resolution (MxD04_3K, x is O for Terra and Y for Aqua) were introduced in the most recently released MODIS C6 in addition to the standard 10 km Level 2 aerosol products (MxD04_L2). The 3 km DT aerosol retrievals use a similar protocol to the 10 km DT aerosol products, but organize 6 × 6 pixels into a retrieval box for inversion, rather than 20 × 20, after all undesirable ones, i.e., cloud and snow/ice pixels, have been screened out and discarded (Remer et al., 2013). MODIS 3 km AOD data at 550 nm (scientific dataset name: Optical_Depth_Land_And_Ocean) in 2015 (downloaded from https://ladsweb.nascom.nasa.gov/) were used to model the $PM_{2.5}$-AOD relationship. Data obtained before 2015 were used for calibration.

2.2.2. MODIS 10 km Deep Blue (DB) AOD products

The MODIS DB algorithm aims to generate AOD retrievals over bright land (e.g., deserts) to fill the gaps left by the DT algorithm (Hsu et al., 2013). Unlike the DT retrieval process, the DB algorithm first produces aerosol properties at a 1 km resolution and then averages the individual retrievals into a 10 × 10 km grid. As with the 3 km AOD data, we calibrated DB aerosol retrievals for 2015 using DB AOD products obtained before 2015, and filled in some gaps where the 3 km DT AOD values were missing with data obtained in 2015.

2.2.3. MODIS AOD combination

In MODIS Collection 6, the 3 km AOD data are retrieved using the DT algorithm, and the daily availability of 3 km AOD in the desert-like

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