



Article

Superior PM_{2.5} Estimation by Integrating Aerosol Fine Mode Data from the Himawari-8 Satellite in Deep and Classical Machine Learning Models

Zhou Zang ¹, Dan Li ¹, Yushan Guo ¹, Wenzhong Shi ² and Xing Yan ^{1,*}

- State Key Laboratory of Remote Sensing Science, College of Global Change and Earth System Science, Beijing Normal University, Beijing 100875, China; 201921490029@mail.bnu.edu.cn (Z.Z.); 202021490031@mail.bnu.edu.cn (D.L.); 202021490028@mail.bnu.edu.cn (Y.G.)
- Department of Land Surveying and Geo-Informatics, The Hong Kong Polytechnic University, Hong Kong, China; lswzshi@polyu.edu.hk
- * Correspondence: yanxing@bnu.edu.cn

Abstract: Artificial intelligence is widely applied to estimate ground-level fine particulate matter (PM_{2.5}) from satellite data by constructing the relationship between the aerosol optical thickness (AOT) and the surface PM_{2.5} concentration. However, aerosol size properties, such as the fine mode fraction (FMF), are rarely considered in satellite-based PM_{2.5} modeling, especially in machine learning models. This study investigated the linear and non-linear relationships between fine mode AOT (fAOT) and PM_{2.5} over five AERONET stations in China (Beijing, Baotou, Taihu, Xianghe, and Xuzhou) using AERONET fAOT and 5-year (2015–2019) ground-level PM_{2.5} data. Results showed that the fAOT separated by the FMF (fAOT = AOT × FMF) had significant linear and non-linear relationships with surface PM_{2.5}. Then, the Himawari-8 V3.0 and V2.1 FMF and AOT (FMF&AOT-PM_{2.5}) data were tested as input to a deep learning model and four classical machine learning models. The results showed that FMF&AOT-PM_{2.5} performed better than AOT (AOT-PM_{2.5}) in modelling $PM_{2.5}$ estimations. The FMF was then applied in satellite-based $PM_{2.5}$ retrieval over China during 2020, and FMF&AOT-PM2.5 was found to have a better agreement with ground-level PM2.5 than AOT-PM_{2.5} on dust and haze days. The better linear correlation between PM_{2.5} and fAOT on both haze and dust days (dust days: R = 0.82; haze days: R = 0.56) compared to AOT (dust days: R = 0.72; haze days: R = 0.52) partly contributed to the superior accuracy of FMF&AOT-PM_{2.5}. This study demonstrates the importance of including the FMF to improve PM_{2.5} estimations and emphasizes the need for a more accurate FMF product that enables superior PM_{2.5} retrieval.

Keywords: AOT; fine mode aerosol; Himawari-8; PM_{2.5} estimation



Citation: Zang, Z.; Li, D.; Guo, Y.; Shi, W.; Yan, X. Superior PM_{2.5} Estimation by Integrating Aerosol Fine Mode Data from the Himawari-8 Satellite in Deep and Classical Machine Learning Models. *Remote* Sens. 2021, 13, 2779. https:// doi.org/10.3390/rs13142779

Academic Editor: Hanlim Lee

Received: 5 June 2021 Accepted: 12 July 2021 Published: 15 July 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/).

1. Introduction

Accurate monitoring of particulate matter that has a diameter of less than 2.5 μ m (PM_{2.5}) is vital to the atmospheric environment and human health [1,2]. Ground-based PM_{2.5} monitoring sites have limited connectivity and thus lack extensive spatial coverage; this in turn restricts investigations of spatial dynamics of PM_{2.5} and its impact on human health. To overcome this issue, satellite-based remote sensing has been widely used to obtain spatially continuous ground-level PM_{2.5} values [3]. Given their significant linear correlation, traditional satellite-based PM_{2.5} estimations mostly rely on building models between the aerosol optical thickness (AOT) and PM_{2.5} (Figure 1) [4]. Such models include empirical statistical models [5,6], chemical transport models [7], and physical models [8]. AOT products can be commonly obtained at various spatial and temporal resolutions by many satellites, such as the Moderate Resolution Imaging Spectroradiometer (MODIS) [9], the Ozone Monitoring Instrument (OMI) [10], the Visible Infrared Imaging Radiometer Suite (VIIRS) [11], and the Advanced Himawari Imager (AHI) onboard Himawari-8 [12].

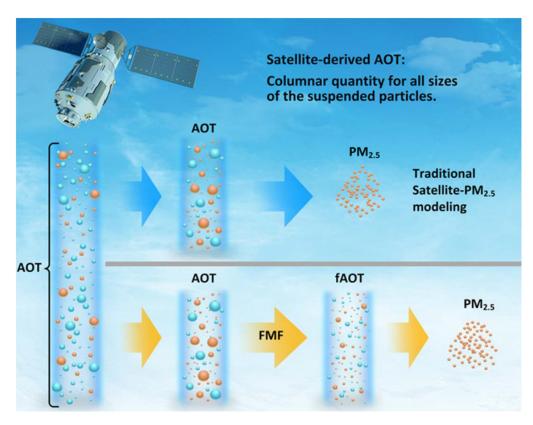


Figure 1. Schematic diagram showing traditional AOT-based and new fAOT-based $PM_{2.5}$ modeling based on satellite data.

AOT is an assembled optical parameter that associates with the columnar quantity of all sizes of suspended particles, as well as their composition, mixing state, density, vertical distribution, and so on, while $PM_{2.5}$ is the near-surface concentration of small-sized particulate matter with an aerodynamic diameter of less than 2.5 μ m. Therefore, it is difficult to find a general and uniform expression that directly converts AOT to $PM_{2.5}$, and this issue has been widely ignored in previous estimations of $PM_{2.5}$ [13]. The impact of fine mode fraction (FMF) on the correlation between $PM_{2.5}$ and AOT is non-negligible [14], and studies have used FMF to separate the contribution of fine particles from AOT [15]. In this respect, Yan et al. [16] used ground-based experimental data of a one-month duration and found that the linear correlation between fAOT and $PM_{2.5}$ (R = 0.74) was higher than the correlation between AOT and $PM_{2.5}$ (R = 0.49); this result provides evidence that fAOT is more suitable for use in estimating $PM_{2.5}$.

In recent years, machine learning models have been extensively applied in $PM_{2.5}$ estimations [17,18] because of their ability to capture the nonlinear relationship between $PM_{2.5}$ and AOT [19,20]. However, to our knowledge, in over 100 studies based on machine learning retrieved $PM_{2.5}$ (Table S1) during 2014–2021, most employed the AOT for $PM_{2.5}$ estimations. Only a limited number of studies have considered utilizing aerosol size information, such as the FMF, as the input parameter for the model. Therefore, the role of FMF in machine learning-based $PM_{2.5}$ retrieval models requires further intensive investigation.

Unfortunately, the reliability and accuracy of FMF data hinders its application in modeling PM_{2.5}. Only a limited number of satellites, such as the MODIS, Himawari-8, the Geostationary Ocean Color Imager (GOCI), and Polarization and Directionality of Earth's Reflectance (POLDER) provide FMF or fAOT products, albeit with poor accuracy. Levy et al. [21] reported that the MODIS-retrieved FMF over land remained highly uncertain, and it was then deleted in the MODIS Collection 6 global aerosol dataset (MOD08 and MYD08). For Himawari-8, Yang et al. [22] found that its V2.1 FMF data had a low accuracy (with a high RMSE of 0.30). Furthermore, Choi et al. [23] evaluated the GOCI FMF with

Remote Sens. 2021, 13, 2779 3 of 20

AERONET FMF for AERONET AOD > 0.3, and the results showed a mediocre RMSE of 0.264. Therefore, the lack of satellite-based FMF data accuracy makes it difficult to explore the role of aerosol size information in estimating $PM_{2.5}$. POLDER/Generalized Retrieval of Aerosol and Surface Properties (GRASP) FMF has substantially improved agreement with ground measurements compared with MODIS FMF [24,25], with an RMSE of 0.170 in China. However, the POLDER/FMF provided global coverage every two days, which results in a coarse temporal resolution compared to MODIS [26].

Nevertheless, Himawari-8, which was launched on 7 October 2014, is a promising geostationary satellite in this respect. It contains a state-of-the-art imager, the Advanced Himawari Imager (AHI), with 16 spectral bands from visible to infrared at high spatial (0.5–1.0 km at nadir for the visible and near-infrared bands, and 2 km at nadir for the infrared bands) and temporal (10 min for full disk coverage) resolutions [12]. This unparalleled spatiotemporal resolution enables detailed observations of aerosol properties to be made, and AOT and aerosol size information (the AE (Ångström exponent) and FMF) can be obtained over Asia and Oceania [27]. Himawai-8 updated its aerosol products from V2.1 to V3.0 on 30 October 2020, providing a valuable opportunity for investigating the impact of FMF on the accuracy of PM_{2.5} estimations in machine learning modeling.

Therefore, this study aimed to determine the relationships between fAOT and $PM_{2.5}$ using the FMF, and then test the use of the FMF in the $PM_{2.5}$ retrieval ability of deep learning and classical machine models. Applying FMF in these models has rarely been considered in previous studies. By comparing the V2.1 and V3.0 Himawari-8 aerosol products (AE and FMF), we ascertained whether the improved FMF results enabled highly accurate $PM_{2.5}$ estimations. This study not only enhances our understanding of the use of aerosol size information and the FMF in satellite-based $PM_{2.5}$ retrieval by machine learning models, but also emphasizes the importance of a more accurate FMF product in $PM_{2.5}$ retrieval.

2. Data and Methods

2.1. Study Area and Himawari-8 V2.1 & V3.0 Aerosol Products

Himawari-8 hovers over the equator at 140E longitude and has an observation range of 80E–160W and 60S–60N. Figure S1 shows the geographical domain of Himawari-8 covering East Asia, Southeast Asia, Oceania, and the western Pacific Ocean. China is one of the largest developing countries within its domain, and it has experienced severe air pollution in recent years [28].

Himawari-8/AHI aerosol products were derived based on the methods of Fukuda et al. [29] and Yoshida et al. [30]. V2.1 has now been upgraded to V3.0, and the improvements include the use of canonical correlation analysis and a model forecast to enable an a priori estimate of retrieval. Himawari-8 V3.0 provides products that include AE at 440–675 nm and FMF over land and ocean, with spatial and temporal resolutions of 0.05° and 10 min, respectively; therefore, Himawari-8 V3.0 products can provide sufficient samples and detailed information about daily variations in aerosols [31]. The Himawari-8 V3.0 dataset also includes the Quality Assurance Flags of four values ("very good," "good," "marginal," "no confidence"); only "very good" products were considered in this study.

2.2. AERONET V3.0 Level 1.5 and Level 2.0

In this study, AERONET data were used to explore the role of FMF in estimating PM_{2.5}. AERONET is a globally distributed network of sun/sky radiometers that provide data with a low uncertainty and high temporal resolution (15 min) for all sites [32]. AERONET data were provided in different quality levels: level 1.0 (unscreened), level 1.5 (L1.5, cloud-screened and quality controlled) and L2 (cloud-screened and quality assured). In this study, the newly updated version 3 (V3.0) level 2 (L2) spectral deconvolution algorithm (SDA) data, including AOT [33], AE, and FMF [34], were selected when available. Although L1.5 data have comparatively higher uncertainty than L2 data, L1.5 were used when L2 data

Remote Sens. 2021, 13, 2779 4 of 20

were inadequate or unavailable. The distribution of the selected 89 AERONET stations is shown in Figure S1, and detailed information is given in Table S2.

It should be noted that AERONET SDA FMF is assumed as the weighting between one fine mode and one coarse mode, separating by spectral fashion [34]. While the fine and coarse mode in Himawari-8 is regarded as a monomodal lognormal volume size distribution with a defined radius cutoff for fine (0.143 μ m) and coarse (2.834 μ m) mode [30], for MODIS and VIIRS, FMF is defined as the contribution of fine-dominated aerosol to AOT, where the fine-dominated aerosol actually contains a coarse mode [35,36]. Therefore, these satellite FMF products and SDA FMF are not physically identical. However, AERONET SDA FMF is still considered comparable to satellite FMF products [35,37] and is widely used in FMF validation [22,38], thus, we use the AERONET SDA FMF as the ground truth in this study. Moreover, in satellite retrievals, the equation of fAOT = AOT \times FMF is based on the assumption of single scattering approximation, which is suitable over the ocean. While over land, this could be problematic when AOT is high [39].

2.3. Ground-Based PM_{2.5}, Meteorological, and Radiosonde Data

To investigate the impact of aerosol size data on estimations over China, the ground-based hourly $PM_{2.5}$ data were collected from the National Urban Air Quality Real-Time Publishing Platform. 1701 $PM_{2.5}$ monitoring stations' data were obtained and their distributions showed in Figure S2a. The $PM_{2.5}$ data from 2015–2019 were used to explore the relationship between fAOT and $PM_{2.5}$, then the $PM_{2.5}$ data in 2020 were used to test the satellite-based $PM_{2.5}$ retrieval accuracy with or without aerosol size information. Meteorological factors are important for estimating $PM_{2.5}$ [40], and the in situ meteorological data were obtained from the National Center for Environment Information (NCEI). Via 405 meteorological stations over China (Figure S2c), temperature, dew point temperature, and wind speed data were obtained, and the relative humidity (RH) was further determined by temperature and dew point temperature. In addition, the data at 8:00 am (local time) for 95 radiosonde stations from Integrated Global Radiosonde Archive (IGRA) (Figure S2b) were collected, and the daytime boundary layer height (PBLH) was determined by the 'parcel method' [41,42], which is the height with the same virtual potential temperature as the surface one.

2.4. Classical Machine Learning Models

In this study, four traditional machine learning models were introduced to estimate PM_{2.5} when using different input variables, and schematic diagrams of these models are shown in Figure 2. The models used are described as follows and the detailed parameter settings for the four machine learning models is shown in Table S3:

- (1) Extratree is a supervised ensemble learning model that consists of the ensembles of unpruned classification or regression trees [43]. It uses a random value for the split of each node, which leads to more diversified trees and fewer splitters. Previous studies have used Extratree in both prediction [44] and classification [45].
- (2) Random Forest (RF) is a supervised ensemble learning model introduced by Ho [46], and its construction is based on the ensembles of unpruned classification or regression trees. It operates by selecting random features in the tree induction and bootstrap samples of the training data, and it splits each node in accordance with the largest information gain. RF has been widely applied in PM_{2.5} estimations in previous studies [17].
- (3) Extreme Gradient Boosting (XGBoost) is a machine learning algorithm based on the gradient boosting decision tree (GBDT) proposed by Chen and Guestrin [47]. It can conduct parallel computation efficiently, and it uses fewer computing resources than other methods. In XGBoost, each decision tree is split by a level-wise algorithm that is based on different independent variables. Pan [48] used XGBoost to forecast hourly PM_{2.5} in Tianjin based on data from air-monitoring stations.

Remote Sens. **2021**, 13, 2779 5 of 20

(4) LightGBM also has a GBDT framework. It grows trees using a leaf-wise algorithm and it only grows a leaf with the max delta loss. Compared to a level-wise algorithm, LightGBM shows higher loss reduction on the same leaf. Zhong et al. [49] utilized LightGBM to predict historical PM_{2.5} based on meteorological observations.

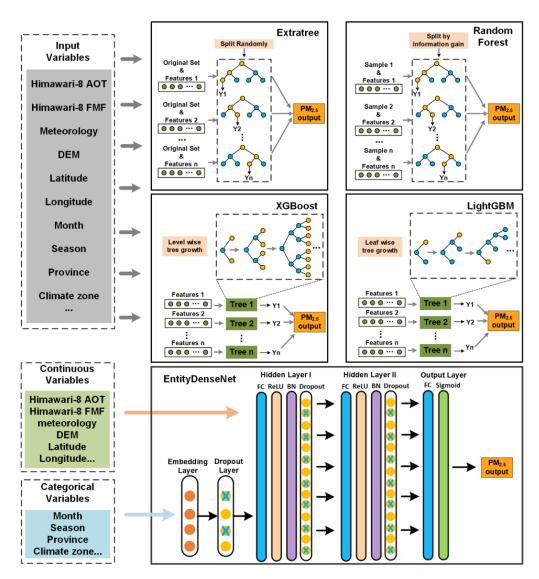


Figure 2. Schematic diagrams of the four traditional machine learning models (Extratree, Random Forest, XGBoost, and LightGBM) and the deep learning model (EntityDenseNet) used in this study.

2.5. Deep Learning Model EntityDenseNet

EntityDenseNet is a deep learning model that can reduce the overfitting problem, and it has a great capacity for capturing nonlinear relationships between variables [50]. As shown in Figure 2, it consists of one input layer, two hidden layers, and one output layer. Traditional neural network approaches (such as BPNN) cannot directly use categorical data, but EntityDenseNet uses an embedding layer to process categorical variables. This not only accelerates the training, but it also helps the neural network to learn about the intrinsic relationships between categorical variables [51]. Each hidden layer consists of one fully connected layer, a rectified linear unit (ReLU) layer, one Batch Normalization (BN) layer, and one dropout layer [52]. The ReLU layer is used as the activation function because it overcomes the saturated and vanishing gradient problem [53], and is faster than traditional activation functions, such as the sigmoid activation function [54]. The BN layer accelerates the training speed by equally distributing the data in each layer [54] and the dropout layer

Remote Sens. 2021, 13, 2779 6 of 20

reduces overfitting of the neural networks [55]. Further details about EntityDenseNet are found in the work of Yan et al. [50]. In this study, the optimal parameters (epochs = 40, hidden nodes = 256, dropout rate = 0.3, learning rate = 0.001, batch size = 128, weight decay = 0.0001) for EntityDenseNet were used by parameter tuning.

2.6. Model Training and Validation

In this study, Himawari-8 and meteorological data for 2020 were used as modeling inputs. Ground-based PM_{2.5} data were provided on an hourly scale; therefore, the 10-min resolution satellite data were averaged on an hourly scale. In EntityDenseNet, we selected month, season, administrative divisions, and global climate zones (Figure S2d and Table S4) [56] as categorical variables, while AOT, FMF, digital elevation model (DEM), temperature, wind speed, RH, PBLH, longitude, and latitude were employed as continuous variables. In the four classical machine-learning methods, all variables were directly used as input data.

To integrate the input data with site-based $PM_{2.5}$ data, the meteorological data and DEM were interpolated into the same spatial resolution as Himawari-8 AOT and FMF (0.05°). Then, the pixels of input data closest to the $PM_{2.5}$ site were extracted and match the $PM_{2.5}$ value at the same hour. Therefore, the matched data is for retrieving hourly $PM_{2.5}$ at the spatial resolution of 0.05° .

Figure 3 shows the training process employed by all the models used in this study. The input data of 1650 stations were first separated into training, validation, and test data using the station-based method [57]. Specifically, we randomly selected input data from over 70% of the PM_{2.5} stations for training, from 20% of the PM_{2.5} stations for validation, and from 10% of the PM_{2.5} stations for testing. The training and validation data were then used to determine the hyperparameters in the models. EntityDenseNet was first initialized using the Xavier initialization scheme [58], which ensures that moderate weight values are used during the propagation of the network, and the hyperparameters were then determined using the validation data. The hyperparameters in the other machine learning models were directly determined using the validation data. Using the hyperparameters, the models were subsequently trained using the training data. Finally, the test dataset (41,836 samples) was used to evaluate the performances of the trained models. This station-based validation accurately reflects the spatial performance of each model and has been used in previous studies, such as that of Wang et al. [56].

3. Results

3.1. Linear and Non-Linear Relationships between fAOT and PM_{2.5}

To explore the relationship between fAOT and $PM_{2.5}$, data were collected from five AEROENT stations (in Beijing, Baotou, Taihu, Xianghe, Xuzhou) (Figure 4g) and $PM_{2.5}$ over stations located nearest to the AEROENT stations in mainland China during 2015–2019. Using FMF, the fAOT was separated from the AOT (fAOT = AOT \times FMF); this represents the AOT of fine mode particles with radii ranging from 0.439–0.992 μ m. Both linear and non-linear relationships between fAOT and $PM_{2.5}$ were investigated, and the results are shown in Figure 4. The linear relationships between fAOT and $PM_{2.5}$ show significant correlation values at the 95% significance level for the five stations, and the R of fAOT and $PM_{2.5}$ reached 0.48 on average. Of the five stations, Beijing showed the highest correlation between fAOT and $PM_{2.5}$ (R = 0.60), while other stations had correlation values ranging from 0.18 to 0.53. A significant linear relationship between fAOT and $PM_{2.5}$ was also reported by Zhang and Li [59] (with an R of 0.88) on haze days, and by Yan et al. [16] (with an R of 0.74) in Xingtai during May 2016.

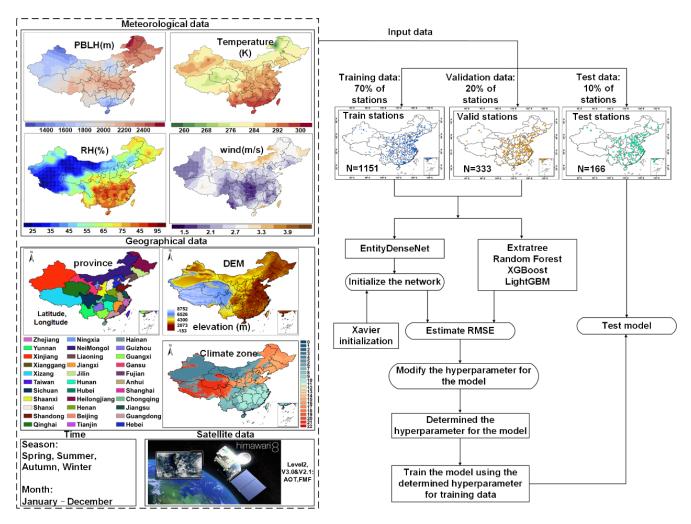


Figure 3. Flowchart of the entire training process for both EntityDenseNet and the four traditional machine learning models. The distributions of meteorological data were interpolated by the Kringing method using averaged values in 2020 over meteorology stations (for temperature, relative humidity (RH), and wind speed) and radiosonde stations (for the boundary layer height (PBLH)) in China.

The generalized additive model (GAM) was used to test the non-linear relationships between fAOT and PM_{2.5}, and the results showed that the non-linear relationships were significant at the 99% significance level (Figure 4h-l). In Beijing and Baotou, fAOT positively influenced PM_{2.5} when fAOT was less than 1 and 0.8, respectively, and PM_{2.5} had a negative influence on fAOT with a further increase in fAOT. This means that fine mode aerosols were not the only component in severe haze events in Beijing and Baotou, and the proportion of coarse mode aerosols was non-negligible [60]. The PM_{2.5} in Taihu and Xuzhou responded positively to fAOD when fAOD was less than approximately 1.7 and 2, but it was negatively correlated with a further increase in fAOD. This is partly related to the fact that although fine mode aerosols dominate local PM_{2.5} on severe pollution days, fine particles can absorb moisture and increase in size [61]. The dominant coarse-mode aerosols on severe pollution days caused this negative response between fAOT and PM_{2.5}. In Xianghe, there was a strong positive response between fAOT and PM_{2.5}, even when fAOT was greater than 3, which indicated that PM_{2.5} in Xianghe consisted mainly of fine mode particles on both clean and heavy pollution days [62]. Figure 4 shows the relationship between fAOT and PM_{2.5}, which indicates the importance of using aerosol size information when estimating $PM_{2.5}$.

Remote Sens. **2021**, 13, 2779 8 of 20

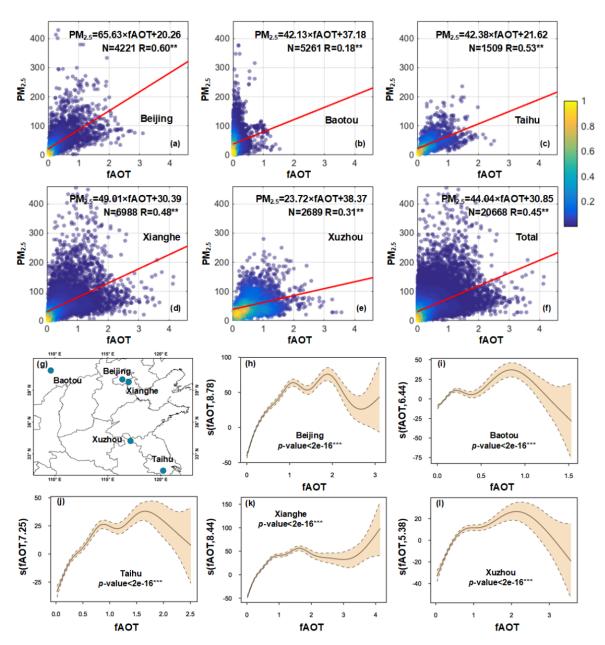


Figure 4. (a–f) The linear correlation of fAOT with PM_{2.5} over five stations (Beijing, Baotou, Taihu, Xianghe, Xuzhou) each and total in China during 2015–2019. The red lines represent fitting lines and the "**" after each R value represents the correlation significance > 95%, (g): the location of the 5 stations. (h–l): the GAM plots of fAOT and PM_{2.5} in five AERONET stations over China. The light brown shaded color represents the 95% confidence interval of fitting, and the y-axis represents the smooth fitted values with the degrees of freedom of fitting shows in the parentheses. The p-value attached with "***" means the significant GAM fitting at 99% significance level.

3.2. Evaluation of Himawari-8 V3.0 Aerosol Size Data and Its Performance in PM_{2.5} Retrievals

Figure 5 shows the overall evaluations of V3.0 and V2.1 AE (a,b), AE with quality assurance (AE QA) (c,d), and FMF (e,f). Both AE and AE QA were superior when using the V3.0 data compared to the V2.1 data, and a tighter clustering of points was seen around the 1:1 line. Specifically, there were improvements for AE in the correlation with AERONET for V3.0 (R = 0.20, RMSE 0.38) and V2.1 (R = 0.11 and RMSE = 0.56). After quality control, the data volume of AE QA decreased from 71,390 to 5371, while the performance of AE QA was superior to that of AE. In addition, V3.0 AE QA (R = 0.29, RMSE = 0.35) outperformed V2.1 AE QA (R = 0.19, RMSE = 0.48). For FMF, the V3.0 FMF (R = 0.33, RMSE = 0.26) also

Remote Sens. **2021**, 13, 2779 9 of 20

showed an overall better retrieval than V2.1 FMF (R = 0.28, RMSE = 0.37). In addition, the significant underestimation and overestimation phenomena of V2.1 FMF were reduced in V3.0 FMF, which provided a more reliable FMF product. The site-based validation results are shown in Figures S3–S5, where it is evident that V3.0 AE performed better than V2.1 AE before and after quality control, and that FMF was generally improved over the sites. The validations suggest that using FMF with the Himawari-8 L2 V3.0 AE provides an overall improvement compared with using FMF with V2.1 AE.

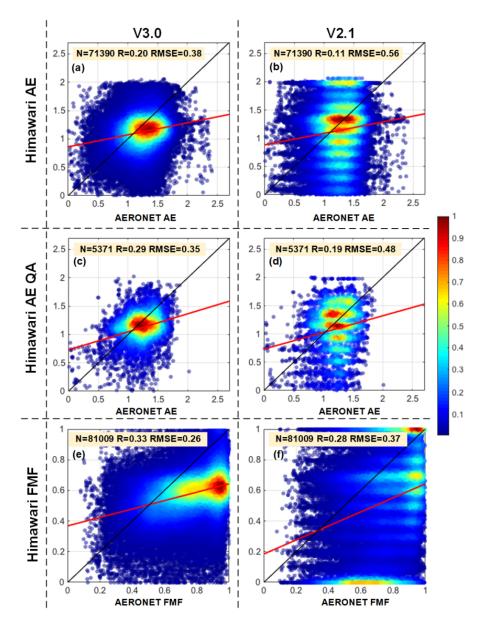


Figure 5. Density scatter plots of the Himawari-8 AE (**a**,**b**), Himawari AE after quality control (AE QA) (**c**,**d**), and Himawari FMF (**e**,**f**) with their ground-based AEROENT values for both V3.0 and V2.1 data. The black and red lines represent 1:1 and fitting lines, respectively.

To compare the spatial distribution of V3.0, V2.1 AE, and FMF, the annual means of V3.0, V2.1 AE, and FMF, and their differences (V3.0 minus V2.1) are shown in Figure 6. It is clear that for both V3.0 and V2.1 AE, high values (>1.1) were observed over southeastern Asia, northern India, northeastern China, and central Australia, and these corresponded to the dominance of fine mode aerosols due to biomass burning and anthropogenic emissions [63–66]. However, compared with V2.1 AE, the value of V3.0 AE was much lower over northeastern China and central Australia, where the difference exceeded -0.4. In

southeastern Asia, the values of V3.0 AE was much higher than that of V2.0 AE, with a difference greater than 0.2. The high values of both V3.0 and V2.1 FMF (>0.6) corresponded well with regions where there were fine mode aerosols, such as southeastern Asia, northern India, northeastern China, and central Australia. The difference between V3.0 and V2.1 FMF also showed a large positive value (>0.2) over southeastern Asia and a negative value over central Australia (>0.2).

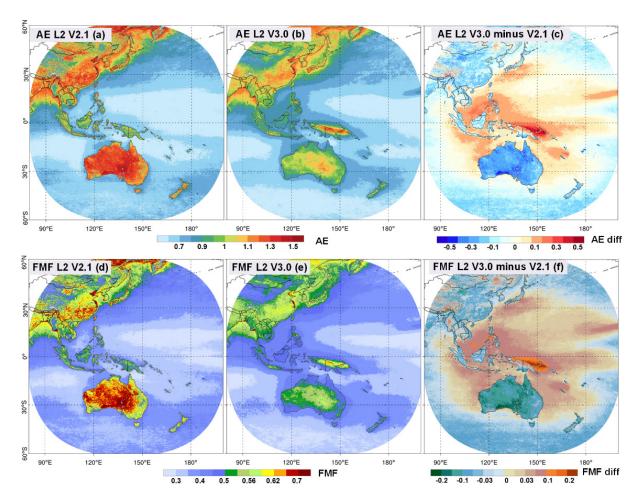


Figure 6. Spatial distribution of the averaged Himwari-8 L2 V2.1 AE (a)/FMF (d), the averaged Himwari-8 L2 V3.0 AE (b)/FMF (e), difference of the averaged V3.0 and V2.1 AE (c)/FMF (f) (V3.0 minus V2.1) in 2020.

Figure 7 shows the estimation of $PM_{2.5}$ obtained from the deep learning model (EntityDenseNet) and the four classical machine learning methods (Extratree, Random Forest, LightGBM, and XGBoost) using Himawari-8 V2.1 and V3.0. To ensure consistency in $PM_{2.5}$, we used the same training and test data for all the models. The results clearly show that for all models, $PM_{2.5}$ based on both FMF and AOT (FMF&AOT- $PM_{2.5}$) performed better than $PM_{2.5}$ based only on AOT (AOT- $PM_{2.5}$), which indicates the importance of using FMF to improve the estimation of $PM_{2.5}$. EntityDenseNet exhibited the best improvement of all models: R^2 increased by 0.11 (0.03) and RMSE decreased by 1.82 (0.88) $\mu g/m^3$ for V2.1 (V3.0) data.

MODIS daily Level-2 data (MOD04_L2) [36] and the Suomi National Polar-orbiting Partnership (SNPP) VIIRS L2 dark target products (AERDT_L2_VIIRS_SNP) [36,67] also provide the FMF over land at the spatial resolution of 10km and 6km, respectively. In this study, we further used MODIS and VIIRS FMF for comparison. Table S5 evaluated the MODIS, VIIRS, Himawari-8 V2.1, and Himawari-8 V3.0 FMF against the AERONET stations in mainland China during 2020. We can see that the MODIS and VIIRS FMF has significantly lower accuracy (RMSE > 0.50) compared to Himawari-8 V3.0 FMF (RMSE = 0.21). Because

Remote Sens. 2021, 13, 2779 11 of 20

MODIS and VIIRS are polar-orbiting satellites, they have smaller match-ups (N < 500) with AERONET data in comparison to Himawari-8 (N > 7000). Figure S6 shows the application of the four FMF products to estimate $PM_{2.5}$ over China. We found that the $PM_{2.5}$ estimated by MODIS and VIIRS FMF have a poorer performance than by the Himawari-8 V3.0 FMF.

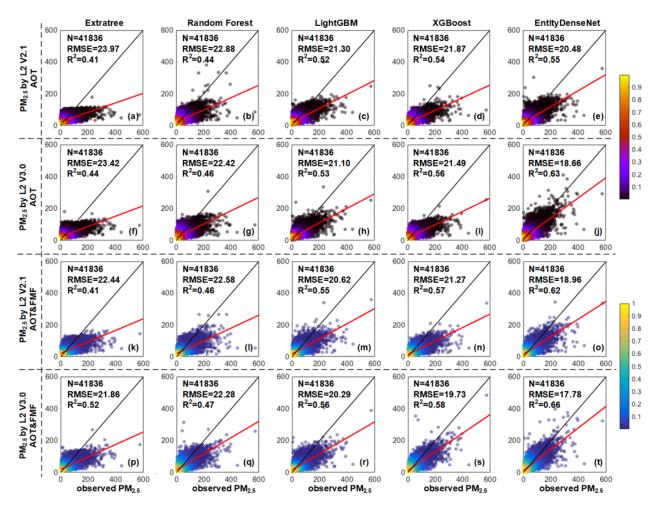


Figure 7. Density scatter plots of modeling results of ground-based PM_{2.5} retrieved by five models: Extratree (**a**,**f**,**k**,**p**), Random Forest (**b**,**g**,**i**,**q**), LightGBM (**c**,**h**,**m**,**r**), XGBoost (**d**,**i**,**n**,**s**) and EntityDenseNet (**e**,**j**,**o**,**t**), based on four different input data (V2.1 and V3.0 data and AOT and AOT&FMF data). The black and red lines represent 1:1 and fitting lines, respectively.

Previous studies have also shown improvements in $PM_{2.5}$ estimation accuracy with the addition of FMF. For example, Choi et al. [68] used a global chemical transport model (GEOS-Chem) and reported a considerable improvement in the results of $PM_{2.5}$, with regression slopes between estimated and observed $PM_{2.5}$ closer to 1. The results in our study also showed that for FMF&AOT-PM_{2.5}, the accuracy of V3.0 was better than that of V2.1. The most significant improvement was found in the EntityDenseNet modeling results, where the R^2 increased by 0.04 and the RMSE decreased by 1.18 $\mu g/m^3$. The improvement in the accuracy of the V3.0 FMF was superior to that of the V2.1 FMF (Figure 5); this implies that when the FMF is more accurate, superior $PM_{2.5}$ estimation can be obtained. Zhao et al. [13] used MODIS FMF (mean error = 0.38) and the fused FMF, which showed a superior accuracy (mean error = 0.13), to estimate $PM_{2.5}$, and the $PM_{2.5}$ estimated from the fused FMF (mean error = 41.8 $\mu g/m^3$) was superior to that of the MODIS FMF (mean error = 45.3 $\mu g/m^3$). Our results are consistent with those of earlier studies.

3.3. Application of FMF for Conducting PM_{2.5} Estimations in China

As the EntityDenseNet model and Himawari-8 L2 V3.0 data provided the best results, we used them to retrieve PM_{2.5} in 2020 over China to verify their potential in providing superior PM_{2.5} estimations. PM_{2.5} estimations, including AOT&FMF-PM_{2.5} and AOT-PM_{2.5}, were further compared with ground-level PM_{2.5} values. The results showed that AOT&FMF-PM_{2.5} provided significantly better accuracy than AOT-PM_{2.5} on dust and haze days. Figure 8 shows the regional performances of AOT&FMF-PM_{2.5} and AOT-PM_{2.5} over China on typical dust and haze days. On 12 February 2020, according to the true color image (Figure 8c), haze covered the Beijing-Tianjin-Hebei (BTH) region, and the PM_{2.5} concentration was significantly higher (>85 µg/m³) than in other regions of China (Figure 8a,b). AOT&FMF-PM_{2.5} showed close agreement with ground-based PM_{2.5} (Figure 8d) and it thus captured the high PM_{2.5} concentration within the central BTH region. In contrast (Figure 8e), AOT-PM_{2.5} underestimated the PM_{2.5} concentration in the main urban area of Beijing, where the ground-based PM_{2.5} exceeded 205 μg/m³. In addition, AOT-PM_{2.5} overestimated PM_{2.5}, where the ground-based measurement was less than 85 μg/m³ in southeastern Tianjin. The difference between the modeling results (Figure 8f) shows that, compared with AOT&FMF-PM_{2.5}, AOT-PM_{2.5} tended to overestimate PM_{2.5} in areas with lower pollution levels (PM_{2.5} < 85 μ g/m³), particularly in the southeastern part of the BTH regions when the reading was over 20 μ g/m³, but it also underestimated PM_{2.5} in seriously polluted areas (PM_{2.5} > 125 μ g/m³) by over 10 μ g/m³.

Figure 8i shows that on 3 June 2020, the BTH region experienced a dust day, and there was a moderate concentration of $PM_{2.5}$ nationwide (<35 $\mu g/m^3$) (Figure 8g,h). Compared with ground-level $PM_{2.5}$, AOT&FMF-PM_{2.5} (Figure 8d) corresponded well with the low $PM_{2.5}$ levels (<25 $\mu g/m^3$) in the northern BTH region and the high $PM_{2.5}$ (>45 $\mu g/m^3$) in southeastern Tianjin, while AOT-PM_{2.5} (Figure 8k) clearly underestimated $PM_{2.5}$, with a $PM_{2.5}$ value of less than 45 $\mu g/m^3$. Moreover, the difference in the modeling results (Figure 8l) shows that, compared with AOT&FMF-PM_{2.5}, AOT-PM_{2.5} significantly overestimated $PM_{2.5}$ in the northern BTH region, the main urban area of Beijing, and southeastern Tianjin by over 5 $\mu g/m^3$. In general, Figure 8 reveals that, although FMF had little influence on the overall distribution of $PM_{2.5}$ estimations in China, it significantly improved the estimation of $PM_{2.5}$, and differences between AOT&FMF-PM_{2.5} and AOT-PM_{2.5} are evident on a regional scale.

According to Figure 9a,b, AOT&FMF-PM_{2.5} provided R² and RMSE values of 0.60 and 11.67 μ g/m³, respectively, on dust days, which were better than the results of AOT-PM_{2.5} $(R^2 = 0.57, RMSE = 13.05 \,\mu g/m^3)$. In addition, the overall accuracy of AOT&FMF PM_{2.5} $(R^2 = 0.62, RMSE=37.61 \mu g/m^3)$ on haze days also outperformed AOT-PM_{2.5} $(R^2 = 0.59, RMSE=37.61 \mu g/m^3)$ RMSE = 39.01 μ g/m³) (Figure 9c,d). This improvement can be attributed to the greater correlation achieved between fAOT and surface PM_{2.5}. As shown by the linear relationships in Figure 10, fAOT calculated by Himawari-8 FMF and AOT had a higher correlation with $PM_{2.5}$ (dust day: R = 0.77; haze day: R = 0.52) than Himawari-8 AOT (dust day: R = 0.61; haze day: R = 0.48) under both conditions. Moreover, in Figure 11, AERONET fAOT (dust day: R = 0.82; haze day: R = 0.56) also showed better correlation with AOT (dust day: R = 0.72; haze day: R = 0.52) in both dust and haze days from 2015–2019. According to the number of haze and dust days occurring every year from to 2015–2019 (Figure 11c), Beijing experienced frequent haze and dust days, especially in 2015 when 90 haze days were recorded. As haze days are dominated by fine mode aerosols and prohibitively high PM_{2.5}, fAOT becomes more important than AOT with respect to estimating PM_{2.5}. These results therefore prove that using fAOT to estimate PM_{2.5} is more suitable than using AOT, and this is in agreement with the results of previous studies, such as those of Di Nicolantonio et al. [69] and Yan et al. [16]. In addition, on haze days, Zhang and Li [59] found that the R² of PM_{2.5} with fAOT was higher than that with AOT (0.69), which indicates that dominant fine mode aerosols on haze days result in a close association between fAOT and AOT, which makes the estimation of PM_{2.5} more accurate when using FMF.

Remote Sens. 2021, 13, 2779 13 of 20

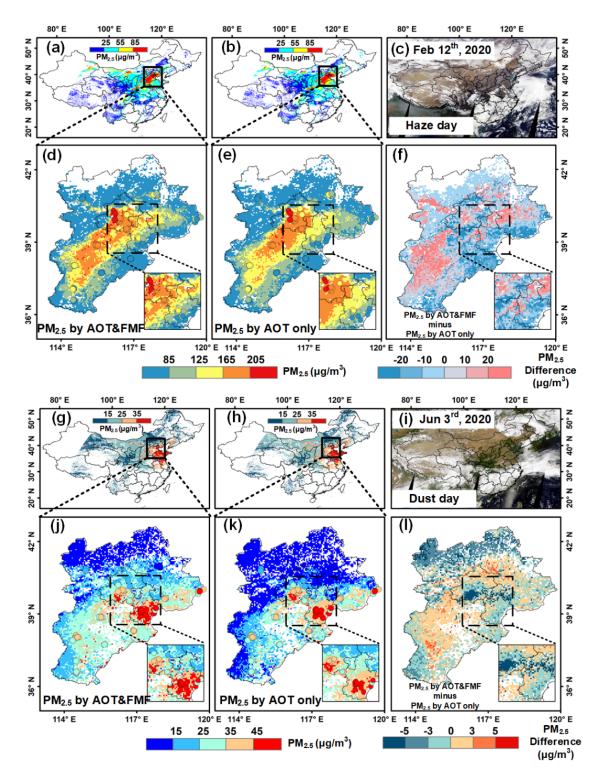


Figure 8. PM_{2.5} estimation on 12 February 2020 (haze day) and on 3 June 2020 (dust day). (**a,g**) AOT&FMF-PM_{2.5} in China; (**b,h**) AOT-PM_{2.5} in China; (**c,i**) true color image on haze/dust day where the black line is the boundary of China; (**d,j**) AOT&FMF-PM_{2.5} in Beijing-Tianjin-Hebei (BTH) region; (**e,k**) AOT-PM_{2.5} in BTH region; (**f,l**) differences in PM_{2.5} between AOT&FMF-PM_{2.5} and AOT-PM_{2.5} in BTH regions.

Remote Sens. 2021, 13, 2779 14 of 20

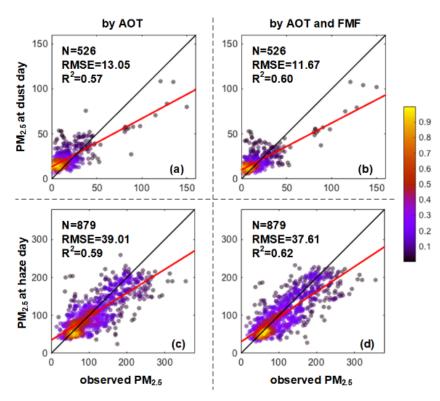


Figure 9. Density plot of EntityDenseNet retrieved $PM_{2.5}$ with ground-based $PM_{2.5}$ on dust (**a,b**) and haze (**c,d**) days in 2020 based on different Himwari-8 V3.0 input data (AOT only/AOT&FMF data). The black and red lines are 1:1 and fitting lines, respectively.

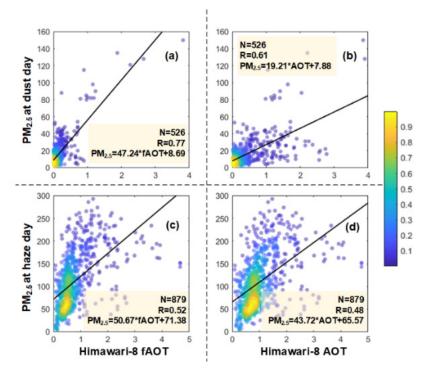


Figure 10. (a) linear correlation between Himawari-8 fAOT and $PM_{2.5}$ on dust day (3 June 2020); (b) linear correlation between Himawari-8 AOT and $PM_{2.5}$ on dust day (3 June 2020); (c) linear correlation between Himawari-8 fAOT and $PM_{2.5}$ on haze day (12 February 2020); (d) linear correlation between Himawari-8 AOT and $PM_{2.5}$ on haze day (12 February 2020).

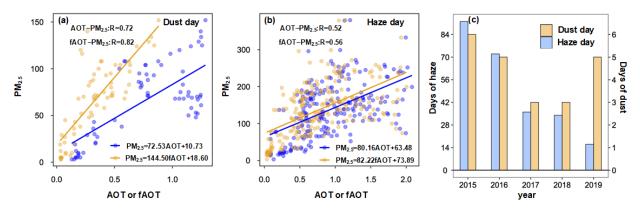


Figure 11. (a) Linear correlation between AERONET AOT (blue) and fAOT (orange) and PM_{2.5} on dust days during 2015–2019; (b) linear correlation between AERONET AOT (blue) and fAOT (orange) and PM_{2.5} on haze days during 2015–2019; (c) the number of haze and dust days occurring every year during 2015–2019.

4. Discussion

Satellite data have been used with various models to estimate ground-level $PM_{2.5}$ by building a relationship between $PM_{2.5}$ and AOT (Figure 1). However, as shown in Figure 10, the correlations between $PM_{2.5}$ and AOT are mediocre because they lack identical size information, and this difference in aerosol size information affects the correlations between $PM_{2.5}$ and AOT. For example, when coarse mode aerosols are dominant, the relationships between $PM_{2.5}$ and AOT are weakened compared to when fine mode aerosols dominate [28]. Yang et al. [70] reported that, although all the cities in the BTH region are located in urban agglomerations, the aerosols in the region mainly consist of fine particles, such as sulfates and nitrates. This means that the correlations between $PM_{2.5}$ and AOT are higher than in cities within the Pearl River Delta (PRD) region, where aerosols comprise coarse particles, such as sea salt. In the BTH region, the proportions of fine particles vary among seasons, with higher numbers of fine mode aerosols during winter and higher numbers of coarse mode aerosols during spring; therefore, the relationship between $PM_{2.5}$ and AOT is better in winter [71]. As $PM_{2.5}$ is mainly composed of fine particles, separating the fine mode information from the total AOT helps to build a better and closer relationship with $PM_{2.5}$.

In this study, we found that fAOT separated by FMF from total AOT had both significant linear and non-linear correlations with $PM_{2.5}$ (Figure 4). This phenomenon has also been reported in a previous study, which showed that fAOT (R = 0.74) had a better correlation with $PM_{2.5}$ than AOT (R = 0.49) [16]. In addition, the study of Wei et al. [24] also found that the distribution of fAOT was closer to $PM_{2.5}$ than AOT over China, which indicated the superiority of the relationship between fAOT and $PM_{2.5}$.

FMF has already been introduced in statistical models for estimating PM2.5; for example, the study of She et al. [72] employed a linear mixed effect model that also combines FMF to estimate PM_{2.5} in the Yangtze River Delta, China. However, FMF has rarely been applied in machine learning models. In this study, we used the deep learning model, EntityDenseNet, and four traditional machine learning methods to apply FMF in estimating PM_{2.5} over China. The results showed that, compared with using only AOT, estimations of PM_{2.5} with FMF provided higher R² and lower RMSE values for all the models (Figure 7). This indicates that the use of aerosol size information can assist in providing estimations of $PM_{2.5}$ that are more accurate than those previously obtained. Zhang and Li [59] also reported that using fAOT provides better PM_{2.5} estimates than AOT during haze days, with a reduction in the RMSE from 61 to 53 μ g/m³. Spatially, on haze days (Figure 8), AOT- $PM_{2.5}$ showed an obvious overestimation in the southeastern BTH region (>20 μ g/m³) and an underestimation in the southern BTH region (>10 μ g/m³). On dust days, AOT-PM_{2.5} provided a large overestimation in the main urban area of Beijing (of over $5 \mu g/m^3$). The superior accuracy of AOT&FMF-PM_{2.5} is partly due to the better correlation between PM_{2.5} and fAOT than AOT and PM_{2.5} (Figures 10 and 11). Therefore, using FMF in models can

achieve different distributions of $PM_{2.5}$ estimations compared to using only AOT. Owing to the high spatial and temporal resolutions of satellites such as Himawari-8, improvements in $PM_{2.5}$ estimation will generate data providing more accurate fine spatial distributions and variations of $PM_{2.5}$. This can enhance our understanding of the changes and transportation of fine mode pollutants.

In addition, Figure 7 shows that the FMF&AOT-PM_{2.5} by Himawari-8 V3.0 outperforms FMF&AOT-PM_{2.5} by Himawari-8 V2.1, which indicates that a more accurate FMF product is required to provide superior estimations of PM_{2.5}. Although Figure 5 provides evidence of the improvements in V3.0 FMF compared to V2.1, it still provides a low accuracy (R = 0.33) and large RMSE of 0.26, which hinders the application of FMF on PM_{2.5} estimations. Some studies have proposed using modified satellite-based FMF retrievals to improve the accuracy of FMF. For example, Yan et al. [38] applied an improved LUT-SDA for FMF retrieval, which resulted in an RMSE of 0.168, and Chen et al. [73] used deep learning to improve the accuracy of FMF, and achieved an RMSE of 0.157. However, FMF products with a high spatial resolution on a global scale are currently rare. Although Yan et al. [74] generated a 10-year FMF product on a global scale, it has a spatial resolution of 1° × 1°, which cannot fulfill the needs of estimating PM_{2.5} at a high spatial resolution. Therefore, the generation of a highly accurate FMF product with a high spatial resolution is urgently required.

5. Conclusions

This study investigated the linear and non-linear relationships between fAOT and PM_{2.5} over five AERONET stations in China (Beijing, Baotou, Taihu, Xianghe, and Xuzhou) using AERONET fAOT and ground-level PM_{2.5} data. The linear relationships were significant over the stations (with an overall R of 0.45), and the non-linear relationships between fAOT and PM_{2.5} were significant for all stations in China. Data obtained from Himawari-8 aerosol product data and meteorological data obtained in the year 2020 were then used to estimate PM_{2.5} employing a deep learning method (EntityDenseNet) and four traditional machine learning methods (Extratree, RF, XGBoost, and LightGBM). The PM_{2.5} estimations were found to be more accurate when adding FMF as input data (FMF&AOT-PM_{2.5}) than when using only AOT (AOT-PM_{2.5}). Compared with the FMF&AOT-PM_{2.5} by V2.1 FMF, the FMF&AOT-PM_{2.5} by V3.0 FMF showed further improvement. These results indicate that when FMF is more accurate, superior PM_{2.5} estimations can be obtained. When both FMF&AOT-PM_{2.5} and AOT-PM_{2.5} from 2020 over China were applied, the agreement between FMF&AOT-PM_{2.5} and ground-level PM_{2.5} was obviously closer than that of AOT-PM_{2.5} on both dust and haze days. These results are related in part to the better correlation between $PM_{2.5}$ and fAOT (dust days: R = 0.82; haze days: R = 0.56) than with AOT (dust days: R = 0.72; haze days: R = 0.52).

This study demonstrates that incorporating FMF can effectively improve the ability of machine learning models to accurately estimate $PM_{2.5}$ from satellite data. However, a more accurate, higher spatial and temporal resolution of the FMF product is required to further improve $PM_{2.5}$ estimation.

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10 .3390/rs13142779/s1. Figure S1: Map of Himawari-8/AHI imaging zone with the base map showing the DEM in meters. Blue and orange dots represent Level 1.5 (L1.5) and Level 2.0 (L2.0) AERONET stations that were used in validation, respectively; Figure S2: The study area (China) for PM2.5 estimation and the ground-level stations of (a) 1701 PM2.5 stations (pink scatters), (b) 95 radiosonde stations (black scatters) and the DEM over China, (c) 405 meteorology stations (magenta scatters) and (d) climate zones over China classified by Koppen-Geiger climate classifications; Figure S3. Differences between validation results (R and RMSE) for Himwari-8 V3.0 and V2.1 (V3.0 minus V2.1) data over AERONET sites: (a,b) for AE; (c,d) for AE after quality control (AE QA); and (e,f) for FMF; Figure S4. Validation results (R and RMSE) for Himwari-8 V3.0 and V2.1 AE over AEROENT sites: (a,e) for V2.1 AE; (b,f) for V3.0 AE; (c,g) for V2.1 AE QA; (d,h) for V3.0 AE QA; Figure S5. Validation results (R and RMSE) for Himwari-8 V3.0 and V2.1 FMF over AEROENT sites: (a,c) for V2.1 FMF;

(b,d) for V3.0 FMF; Figure S6. Density scatter plots of modeling results of ground-based $PM_{2.5}$ retrieved by four machine learning models (Extratree, Random Forest, LightGBM and XGBoost) based on four different FMF products (Himawari-8 V2.1 and V3.0 FMF, MODIS and VIIRS FMF) with the same lengths for training and test datasets. The black and red lines represent 1:1 and fitting lines, respectively. Because the amount of training data is small (N = 1321), which is unsuitable for applying deep learning models, EntityDenseNet was not used for $PM_{2.5}$ estimations here. Table S1. Previous studies of machine learning retrieved $PM_{2.5}$ since 2014. Table S2. AERONET stations and their data level used in this study. Table S3. The parameters for the four machine learning models used in this study. Table S4. The class types and their abbreviations of global climate zone. Table S5. The evaluation of MODIS, VIIRS and Himawari-8 V2.1 and V3.0 FMF against the AERONET stations mainland China.

Author Contributions: Conceptualization, X.Y. and Z.Z.; methodology, X.Y.; software, X.Y.; validation, Z.Z.; formal analysis, Z.Z.; investigation, Y.G.; data curation, D.L.; writing—original draft preparation, Z.Z.; writing—review and editing, W.S.; visualization, Z.Z.; supervision, X.Y.; funding acquisition, X.Y. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded by the National Natural Science Foundation of China (42030606, 41801329 and 91837204), the National Key Research and Development Plan of China (2017YFC1501702), the Open Fund of State Key Laboratory of Remote Sensing Science (OFSLRSS201915) and the Fundamental Research Funds for the Central Universities.

Data Availability Statement: The Himawari-8 was collected from the Himawari Monitor and the P-Tree system (ftp.ptree.jaxa.jp, accessed on 4 June 2021). The AERONET data are available at https://aeronet.gsfc.nasa.gov/ (accessed on 4 June 2021). The radionsonde data are from NOAA's Integrated Global Radiosonde Archive data (https://www.ncdc.noaa.gov/data-access/weatherballoon/integrated-global-radiosonde-archive, accessed on 4 June 2021). The in-situ meteorological data are from NOAA's National Centers for Environmental Information (https://www.ncei.noaa.gov/products/integrated-surface-database, accessed on 4 June 2021). The in-situ PM2.5 data are available at the China National Environmental Monitoring Center (http://www.cnemc.cn) (accessed on 4 June 2021).

Acknowledgments: The authors gratefully acknowledge the Japan Meteorological Agency (JMA) for providing Himawari-8 data, Goddard Space Flight Center for providing the AERONET ground-based measurements, NOAA's National Centers for Environmental Information (NCEI) for providing the Global Historical Climatology Network data and the Integrated Global Radiosonde Archive data, and the China National Environmental Monitoring Center for providing the ground-based PM_{2.5} data.

Conflicts of Interest: The authors declare no conflict of interest.

References

- 1. Bell, M.L.; Ebisu, K.; Peng, R.D. Community-level spatial heterogeneity of chemical constituent levels of fine particulates and implications for epidemiological research. *J. Expo. Sci. Environ. Epidemiol.* **2011**, *21*, 372–384. [CrossRef]
- 2. Xu, P.; Chen, Y.; Ye, X. Haze, air pollution, and health in China. Lancet 2013, 382, 2067. [CrossRef]
- 3. Van Donkelaar, A.; Martin, R.; Brauer, M.; Hsu, N.C.; Kahn, R.A.; Levy, R.C.; Lyapustin, A.; Sayer, A.; Winker, D.M. Global Estimates of Fine Particulate Matter using a Combined Geophysical-Statistical Method with Information from Satellites, Models, and Monitors. *Environ. Sci. Technol.* **2016**, *50*, 3762–3772. [CrossRef]
- 4. Schaap, M.; Apituley, A.; Timmermans, R.M.A.; Koelemeijer, R.B.A.; De Leeuw, G. Exploring the relation between aerosol optical depth and PM_{2.5} at Cabauw, the Netherlands. *Atmos. Chem. Phys. Discuss.* **2009**, *9*, 909–925. [CrossRef]
- 5. Gupta, P.; Christopher, S.A.; Wang, J.; Gehrig, R.; Lee, Y.; Kumar, N. Satellite remote sensing of particulate matter and air quality assessment over global cities. *Atmos. Environ.* **2006**, *40*, 5880–5892. [CrossRef]
- 6. Guo, Y.; Feng, N.; Christopher, S.A.; Kang, P.; Zhan, F.B.; Hong, S. Satellite remote sensing of fine particulate matter (PM_{2.5}) air quality over Beijing using MODIS. *Int. J. Remote Sens.* **2014**, *35*. [CrossRef]
- 7. Van Donkelaar, A.; Martin, R.V.; Brauer, M.; Kahn, R.; Levy, R.; Verduzco, C.; Villeneuve, P.J. Global Estimates of Ambient Fine Particulate Matter Concentrations from Satellite-Based Aerosol Optical Depth: Development and Application. *Environ. Health Perspect.* 2010, 118, 847–855. [CrossRef]
- 8. Zhang, Y.; Li, Z.; Bai, K.; Wei, Y.; Xie, Y.; Zhang, Y.; Ou, Y.; Cohen, J.; Zhang, Y.; Peng, Z.; et al. Satellite remote sensing of atmospheric particulate matter mass concentration: Advances, challenges, and perspectives. *Fundam. Res.* **2021**, *1*, 240–258. [CrossRef]

9. Remer, L.A.; Kaufman, Y.J.; Tanré, D.; Mattoo, S.; Chu, D.A.; Martins, J.V.; Li, R.R.; Ichoku, C.; Levy, R.C.; Kleidman, R.G.; et al. The MODIS Aerosol Algorithm, Products, and Validation. *J. Atmos. Sci.* 2005, 62, 947–973. [CrossRef]

- 10. Veihelmann, B.; Levelt, P.P.; Stammes, P.; Veefkind, J.P. Simulation study of the aerosol information content in OMI spectral reflectance measurements. *Atmos. Chem. Phys. Discuss.* **2007**, *7*, 3115–3127. [CrossRef]
- 11. Jackson, J.M.; Liu, H.; Laszlo, I.; Kondragunta, S.; Remer, L.A.; Huang, J.; Huang, H.-C. Suomi-NPP VIIRS aerosol algorithms and data products. *J. Geophys. Res. Atmos.* **2013**, *118*, 12673–12689. [CrossRef]
- 12. Bessho, K.; Date, K.; Hayashi, M.; Ikeda, A.; Imai, T.; Inoue, H.; Kumagai, Y.; Miyakawa, T.; Murata, H.; Ohno, T.; et al. An Introduction to Himawari-8/9—Japan's New-Generation Geostationary Meteorological Satellites. *J. Meteorol. Soc. Jpn.* **2006**, *94*, 151–183. [CrossRef]
- 13. Zhao, A.; Li, Z.; Zhang, Y.; Li, D. Merging MODIS and Ground-Based Fine Mode Fraction of Aerosols Based on the Geostatistical Data Fusion Method. *Atmosphere* **2017**, *8*, 117. [CrossRef]
- 14. Zhang, Y.; Li, Z. Remote sensing of atmospheric fine particulate matter (PM_{2.5}) mass concentration near the ground from satellite observation. *Remote Sens. Environ.* **2015**, *160*, 252–262. [CrossRef]
- 15. Liang, C.; Zang, Z.; Li, Z.; Yan, X. An Improved Global Land Anthropogenic Aerosol Product Based on Satellite Retrievals From 2008 to 2016. *IEEE Geosci. Remote Sens. Lett.* **2021**, *18*, 944–948. [CrossRef]
- 16. Yan, X.; Shi, W.; Li, Z.; Li, Z.; Luo, N.; Zhao, W.; Wang, H.; Yu, X. Satellite-based PM_{2.5} estimation using fine-mode aerosol optical thickness over China. *Atmos. Environ.* **2017**, *170*, 290–302. [CrossRef]
- 17. Geng, G.; Meng, X.; He, K.; Liu, Y. Random forest models for PM_{2.5} speciation concentrations using MISR fractional AODs. *Environ. Res. Lett.* **2020**, *15*, 034056. [CrossRef]
- 18. Huang, K.; Xiao, Q.; Meng, X.; Geng, G.; Wang, Y.; Lyapustin, A.; Gu, D.; Liu, Y. Predicting monthly high-resolution PM_{2.5} concentrations with random forest model in the North China Plain. *Environ. Pollut.* **2018**, 242, 675–683. [CrossRef]
- Li, L. A Robust Deep Learning Approach for Spatiotemporal Estimation of Satellite AOD and PM_{2.5}. Remote Sens. 2020, 12.
 [CrossRef]
- 20. Wang, Q.; Ding, X.; Tong, X.; Atkinson, P. Spatio-temporal spectral unmixing of time-series images. *Remote Sens. Environ.* **2021**, 259, 112407. [CrossRef]
- Levy, R.C.; A Remer, L.; Kleidman, R.; Mattoo, S.K.; Ichoku, C.; Kahn, R.; Eck, T.F. Global evaluation of the Collection 5 MODIS dark-target aerosol products over land. *Atmos. Chem. Phys. Discuss.* 2010, 10, 10399–10420. [CrossRef]
- 22. Yang, X.; Zhao, C.; Luo, N.; Zhao, W.; Shi, W.; Yan, X. Evaluation and Comparison of Himawari-8 L2 V1.0, V2.1 and MODIS C6.1 aerosol products over Asia and the oceania regions. *Atmos. Environ.* **2020**, 220, 117068. [CrossRef]
- 23. Choi, M.; Kim, J.; Lee, J.; Kim, M.; Park, Y.J.; Jeong, U.; Kim, W.; Hong, H.; Holben, B.; Eck, T.F.; et al. GOCI Yonsei Aerosol Retrieval (YAER) algorithm and validation during the DRAGON-NE Asia 2012 campaign. *Atmos. Meas. Tech.* 2016, *9*, 1377–1398. [CrossRef]
- 24. Wei, Y.; Li, Z.; Zhang, Y.; Chen, C.; Dubovik, O.; Xu, H.; Li, K.; Chen, J.; Wang, H.; Ge, B.; et al. Validation of POLDER GRASP aerosol optical retrieval over China using SONET observations. *J. Quant. Spectrosc. Radiat. Transf.* 2020, 246, 106931. [CrossRef]
- 25. Zhang, Y.; Li, Z.; Liu, Z.; Wang, Y.; Qie, L.; Xie, Y.; Hou, W.; Leng, L. Retrieval of aerosol fine-mode fraction over China from satellite multiangle polarized observations: Validation and comparison. *Atmos. Meas. Tech.* **2021**, *14*, 1655–1672. [CrossRef]
- 26. Wang, Q.; Tang, Y.; Tong, X.; Atkinson, P. Virtual image pair-based spatio-temporal fushion. *Remote Sens. Environ.* **2020**, 249, 112009. [CrossRef]
- 27. Okuyama, A.; Andou, A.; Date, K.; Hoasaka, K.; Mori, N.; Murata, H.; Tabata, T.; Takahashi, M.; Yoshino, R.; Bessho, K. Preliminary validation of Himawari-8/AHI navigation and calibration. *Earth Obs. Syst. XX* **2015**, *9607*, *96072*. [CrossRef]
- 28. Xu, Q.; Chen, X.; Yang, S.; Tang, L.; Dong, J. Spatiotemporal relationship between Himawari-8 hourly columnar aerosol optical depth (AOD) and ground-level PM_{2.5} mass concentration in mainland China. *Sci. Total Environ.* **2021**, 765, 144241. [CrossRef]
- 29. Fukuda, S.; Nakajima, T.; Takenaka, H.; Higurashi, A.; Kikuchi, N.; Nakajima, T.Y.; Ishida, H. New approaches to removing cloud shadows and evaluating the 380 nm surface reflectance for improved aerosol optical thickness retrievals from the GOSAT/TANSO-Cloud and Aerosol Imager. *J. Geophys. Res. Atmos.* 2013, 118, 13520–13531. [CrossRef]
- 30. Yoshida, M.; Kikuchi, M.; Nagao, T.M.; Murakami, H.; Nomaki, T.; Higurashi, A. Common Retrieval of Aerosol Properties for Imaging Satellite Sensors. *J. Meteorol. Soc. Jpn.* **2018**, *96B*, 193–209. [CrossRef]
- 31. Gao, L.; Chen, L.; Li, C.; Li, J.; Che, H.; Zhang, Y. Evaluation and possible uncertainty source analysis of JAXA Himawari-8 aerosol optical depth product over China. *Atmos. Res.* **2021**, 248, 105248. [CrossRef]
- 32. Eck, T.F.; Holben, B.N.; Reid, J.S.; Dubovik, O.; Smirnov, A.; O'Neill, N.T.; Slutsker, I.; Kinne, S. Wavelength dependence of the optical depth of biomass burning, urban, and desert dust aerosols. *J. Geophys. Res. Atmos.* **1999**, *104*, 31333–31349. [CrossRef]
- 33. Giles, D.M.; Sinyuk, A.; Sorokin, M.G.; Schafer, J.S.; Smirnov, A.; Slutsker, I.; Eck, T.F.; Holben, B.N.; Lewis, J.R.; Campbell, J.R.; et al. Advancements in the Aerosol Robotic Network (AERONET) Version 3 database–automated near-real-time quality control algorithm with improved cloud screening for Sun photometer aerosol optical depth (AOD) measurements. *Atmos. Meas. Tech.* **2019**, *12*, 169–209. [CrossRef]
- 34. O'Neill, N.T.; Eck, T.F.; Smirnov, A.; Holben, B.N.; Thulasiraman, S. Spectral discrimination of coarse and fine mode optical depth. *J. Geophys. Res. Space Phys.* **2003**, *108*, 4559–4573. [CrossRef]

35. Levy, R.C.; Remer, L.A.; Mattoo, S.; Vermote, E.F.; Kaufman, Y.J. Second-generation operational algorithm: Retrieval of aerosol properties over land from inversion of Moderate Resolution Imaging Spectroradiometer spectral reflectance. *J. Geophys. Res. Space Phys.* **2007**, *112*. [CrossRef]

- 36. Levy, R.C.; Munchak, L.A.; Mattoo, S.K.; Patadia, F.; Remer, L.A.; Holz, R.E. Towards a long-term global aerosol optical depth record: Applying a consistent aerosol retrieval algorithm to MODIS and VIIRS-observed reflectance. *Atmos. Meas. Tech.* **2015**, *8*, 4083–4110. [CrossRef]
- 37. Kleidman, R.G.; O'Neill, N.T.; Remer, L.A.; Kaufman, Y.J.; Eck, T.F.; Tanré, D.; Dubovik, O.; Holben, B.N. Comparison of Moderate Resolution Imaging Spectroradiometer (MODIS) and Aerosol Robotic Network (AERONET) remote-sensing retrievals of aerosol fine mode fraction over ocean. *J. Geophys. Res. Space Phys.* 2005, 110. [CrossRef]
- 38. Yan, X.; Li, Z.; Shi, W.; Luo, N.; Wu, T.; Zhao, W. An improved algorithm for retrieving the fine-mode fraction of aerosol optical thickness, part 1: Algorithm development. *Remote Sens. Environ.* **2017**, *192*, 87–97. [CrossRef]
- 39. Chen, C.; Dubovik, O.; Fuertes, D.; Litvinov, P.; Lapyonok, T.; Lopatin, A.; Ducos, F.; Derimian, Y.; Herman, M.; Tanré, D.; et al. Validation of GRASP algorithm product from POLDER/PARASOL data and assessment of multi-angular polarimetry potential for aerosol monitoring. *Earth Syst. Sci. Data* 2020, 12, 3573–3620. [CrossRef]
- 40. Yan, X.; Zang, Z.; Jiang, Y.; Shi, W.; Guo, Y.; Li, D.; Zhao, C.; Husi, L. A Spatial-Temporal Interpretable Deep Learning Model for improving interpretability and predictive accuracy of satellite-based PM_{2.5}. *Environ. Pollut.* **2021**, 273, 116459. [CrossRef]
- 41. Holzworth, G.C. Estimates of Mean Maximum Mixing Depths in the Contiguous United States. *J. Mon. Weather Rev.* **1964**, 92, 235. [CrossRef]
- 42. Seibert, P.; Beyrich, F.; Gryning, S.-E.; Joffre, S.; Rasmussen, A.; Tercier, P. Chapter 20 Review and intercomparison of operational methods for the determination of the mixing height. *Atmos. Environ.* **2000**, *34*, 1001–1027. [CrossRef]
- 43. Geurts, P.; Ernst, D.; Wehenkel, L. Extremely randomized trees. Mach. Learn. 2006, 63, 3-42. [CrossRef]
- 44. Chu, Z.; Yu, J.; Hamdulla, A. Throughput prediction based on ExtraTree for stream processing tasks. *Comput. Sci. Inf. Syst.* **2021**, 18, 1–22. [CrossRef]
- 45. Carruba, V.; Aljbaae, S.; Domingos, R.C.; Lucchini, A.; Furlaneto, P. Machine learning classification of new asteroid families members. *Mon. Not. R. Astron. Soc.* **2020**, *496*, 540–549. [CrossRef]
- 46. Ho, T.K. Random decision forests. In Proceedings of the 3rd International Conference on Document Analysis and Recognition, Montreal, QC, Canada, 14–16 August 1995; Volume 1, p. 278.
- 47. Chen, T.; Guestrin, C. XGBoost: A Scalable Tree Boosting System. In Proceedings of the 22nd ACM Sigkdd International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, 13–17 August 2016; pp. 785–794.
- 48. Pan, B. Application of XGBoost algorithm in hourly PM_{2.5} concentration prediction. *IOP Conf. Ser. Earth Environ. Sci.* **2018**, 113, 012127. [CrossRef]
- 49. Zhong, J.; Zhang, X.; Gui, K.; Wang, Y.; Che, H.; Shen, X.; Zhang, L.; Zhang, Y.; Sun, J.; Zhang, W. Robust prediction of hourly PM2.5 from meteorological data using LightGBM. *Natl. Sci. Rev.* **2021**. [CrossRef]
- 50. Yan, X.; Zang, Z.; Luo, N.; Jiang, Y.; Li, Z. New interpretable deep learning model to monitor real-time PM_{2.5} concentrations from satellite data. *Environ. Int.* **2020**, 144, 106060. [CrossRef] [PubMed]
- 51. Guo, C.; Berkhahn, F. Entity Embeddings of Categorical Variables. arXiv 2016, arXiv:1604.06737.
- 52. Yan, X.; Liang, C.; Jiang, Y.; Luo, N.; Zang, Z.; Li, Z. A Deep Learning Approach to Improve the Retrieval of Temperature and Humidity Profiles from a Ground-Based Microwave Radiometer. *IEEE Trans. Geosci. Remote Sens.* **2020**, *58*, 8427–8437. [CrossRef]
- 53. Nair, V.; Hinton, G.E. Rectified linear units improve restricted boltzmann machines. In Proceedings of the 27th International Conference on Machine Learning, Haifa, Israel, 21 June 2010; pp. 807–814.
- 54. Ioffe, S.; Szegedy, C. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In Proceedings of the 32nd International Conference on International Conference on Machine Learning, Lille, France, 6–11 July 2015; Volume 37, pp. 448–456.
- 55. Srivastava, N.; Hinton, G.; Krizhevsky, A.; Sutskever, I.; Salakhutdinov, R. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. *J. Mach. Learn. Res.* **2014**, *15*, 1929–1958.
- 56. Beck, H.E.; Zimmermann, N.E.; McVicar, T.; Vergopolan, N.; Berg, A.; Wood, E.F. Present and future Köppen-Geiger climate classification maps at 1-km resolution. *Sci. Data* **2018**, *5*, 180214. [CrossRef] [PubMed]
- 57. Wang, B.; Yuan, Q.; Yang, Q.; Zhu, L.; Li, T.; Zhang, L. Estimate hourly PM_{2.5} concentrations from Himawari-8 TOA reflectance directly using Geo-intelligent long short-term memory network. *Environ. Pollut.* **2020**, 271, 116327. [CrossRef] [PubMed]
- 58. Glorot, X.; Bengio, Y. Understanding the difficulty of training deep feedforward neural networks. *J. Mach. Learn. Res. Proc. Track* **2010**, *9*, 249–256.
- 59. Zhang, Y.; Li, Z. Estimation of PM_{2.5} from fine-mode aerosol optical depth. *J. Remote Sens.* **2013**, *17*, 929–943.
- 60. Tian, S.; Pan, Y.; Liu, Z.; Wen, T.; Wang, Y. Size-resolved aerosol chemical analysis of extreme haze pollution events during early 2013 in urban Beijing, China. *J. Hazard. Mater.* **2014**, 279, 452–460. [CrossRef]
- 61. Lang, H.; Qin, K.; Yuan, L.; Xiao, X.; Hu, M.; Rao, L.; Wang, L. Particles size distributions and aerosol optical properties during haze-fog episodes in the winter of Xuzhou. *China Environ. Sci.* **2016**, *36*, 2260–2269.
- 62. Jiang, Q.; Wang, F.; Sun, Y.-L. Analysis of Chemical Composition, Source and Evolution of Submicron Particles in Xianghe, Hebei Province. *China Environ. Sci.* **2018**, *39*, 3022–3032.

63. Butler, T.; Lawrence, M.; Gurjar, B.R.; van Aardenne, J.; Schultz, M.; Lelieveld, J. The representation of emissions from megacities in global emission inventories. *Atmos. Environ.* **2008**, 42, 703–719. [CrossRef]

- 64. De Meij, A.; Pozzer, A.; Lelieveld, J. Global and regional trends in aerosol optical depth based on remote sensing products and pollutant emission estimates between 2000 and 2009. *Atmos. Chem. Phys. Discuss.* **2010**, *10*, 30731–30776.
- 65. Kaskaoutis, D.G.; Kharol, S.K.; Sinha, P.R.; Singh, R.P.; Badarinath, K.V.S.; Mehdi, W.; Sharma, M. Contrasting aerosol trends over South Asia during the last decade based on MODIS observations. *Atmos. Meas. Tech. Discuss.* **2011**, *4*, 5275–5323.
- 66. Reisen, F.; Meyer, C.P.; Keywood, M. Impact of biomass burning sources on seasonal aerosol air quality. *Atmos. Environ.* **2013**, 67, 437–447. [CrossRef]
- 67. Sawyer, V.; Levy, R.C.; Mattoo, S.; Cureton, G.; Shi, Y.; Remer, L.A. Continuing the MODIS Dark Target Aerosol Time Series with VIIRS. *Remote Sens.* **2020**, *12*, 308. [CrossRef]
- 68. Choi, Y.-S.; Park, R.J.; Ho, C.-H. Estimates of ground-level aerosol mass concentrations using a chemical transport model with Moderate Resolution Imaging Spectroradiometer (MODIS) aerosol observations over East Asia. *J. Geophys. Res. Atmos.* **2009**, 114. [CrossRef]
- 69. Di Nicolantonio, W.; Cacciari, A.; Bolzacchini, E. MODIS Aerosol Optical Properties Over North Italy for Estimating Surface-level PM_{2.5}. In Proceedings of the Envisat Symposium, Montreux, Switzerland, 23–27 April 2007; pp. 3–27.
- 70. Yang, Q.; Yuan, Q.; Yue, L.; Li, T.; Shen, H.; Zhang, L. The relationships between PM2.5 and aerosol optical depth (AOD) in mainland China: About and behind the spatio-temporal variations. *Environ. Pollut.* **2019**, 248, 526–535. [CrossRef] [PubMed]
- 71. Zheng, C.; Zhao, C.; Zhu, Y.; Wang, Y.; Shi, X.; Wu, X.; Chen, T.; Wu, F.; Qiu, Y. Analysis of influential factors for the relationship between PM_{2.5} and AOD in Beijing. *Atmos. Chem. Phys. Discuss.* **2017**, *17*, 13473–13489. [CrossRef]
- 72. She, Q.; Choi, M.; Belle, J.H.; Xiao, Q.; Bi, J.; Huang, K.; Meng, X.; Geng, G.; Kim, J.; He, K.; et al. Satellite-based estimation of hourly PM_{2.5} levels during heavy winter pollution episodes in the Yangtze River Delta, China. *Chemosphere* **2020**, 239, 124678. [CrossRef]
- 73. Chen, X.; de Leeuw, G.; Arola, A.; Liu, S.; Liu, Y.; Li, Z.; Zhang, K. Joint retrieval of the aerosol fine mode fraction and optical depth using MODIS spectral reflectance over northern and eastern China: Artificial neural network method. *Remote Sens. Environ.* **2020**, 249, 112006. [CrossRef]
- 74. Yan, X.; Zang, Z.; Liang, C.; Luo, N.; Ren, R.; Cribb, M.; Li, Z. New global aerosol fine-mode fraction data over land derived from MODIS satellite retrievals. *Environ. Pollut.* **2021**, *276*, 116707. [CrossRef]