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Remote Sensing Estimation of Regional NO₂ via Space-Time Neural Networks

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Received: 26 June 2020; Accepted: 31 July 2020; Published: 5 August 2020

Abstract: Nitrogen dioxide (NO₂) is an essential air pollutant related to adverse health effects. A space-time neural network model is developed for the estimation of ground-level NO₂ in this study by integrating ground NO₂ station measurements, satellite NO₂ products, simulation data, and other auxiliary data. Specifically, a geographically and temporally weighted generalized regression neural network (GTW-GRNN) model is used with the advantage to consider the spatiotemporal variations of the relationship between NO₂ and influencing factors in a nonlinear neural network framework. The case study across the Wuhan urban agglomeration (WUA), China, indicates that the GTW-GRNN model outperforms the widely used geographically and temporally weighted regression (GTWR), with the site-based cross-validation R² value increasing by 0.08 (from 0.61 to 0.69). Besides, the comparison between the GTW-GRNN and original global GRNN models shows that considering the spatiotemporal variations in GRNN modeling can boost estimation accuracy. All these results demonstrate that the GTW-GRNN based NO₂ estimation framework will be of great use for remote sensing of ground-level NO₂ concentrations.

Keywords: ground NO₂; TROPOMI; GTW-GRNN; GRNN

1. Introduction

Nitrogen dioxide (NO₂) is an essential air pollutant and has been reported to be associated with adverse effects on human health by epidemiological studies [1–4]. Faustini et al. [5] have found that per 10 µg/m³ of NO₂ causes a 4% increase in mortality. Besides, NO₂ plays a vital role in the formation of acid rain and disorders greenhouse gas and ozone levels that can affect the global climate [6]. As a result, it is an urgent need to monitor NO₂ concentrations. Recently, remote sensing retrieval of ground NO₂ concentrations has aroused wide attention [7–13], for providing broader spatiotemporal coverages beyond ground monitoring stations, which act as the primary approach for the monitoring of NO₂ all the time.

For the remote sensing retrieval of ground NO₂, a common way is to construct the statistical relationship between satellite troposphere NO₂ data and ground NO₂ measurements, with the theoretical foundation that the close association exists in them [14,15]. Many satellite sensors can provide troposphere NO₂ products, such as the Ozone Monitoring Instrument (OMI) [16], the Global Ozone Monitoring Experiment (GOME) [17], and the TROPospheric Monitoring Instrument (TROPOMI) [18,19]. Thanks to so many satellite observations for NO₂ information, the daily (seasonal or annual) ground NO₂ concentrations can be effectively obtained via a statistical model from regional to global scales. For instance, Qin et al. [15] estimated ground NO₂ concentrations from OMI data over

east-central China using the relatively advanced geographically and temporally weighted regression (GTWR) statistical model.

In recent years, machine learning models have achieved widespread applications in remote sensing retrieval of ground NO_2 concentrations, which can be attributed to their advantages in describing the nonlinear relationship between ground NO_2 and influencing factors. These machine learning models, including random forest [9,20], neural network (NN) [21], Bayesian maximum entropy [22], extreme gradient boosting [23], and so on, have generally reported some advantages in estimation accuracy over traditional statistical models and played a critical role in remote sensing retrieval of ground NO_2 concentrations.

However, the current machine learning models for ground NO_2 estimation usually perform with an assumption that the relationship between NO_2 and influencing factors does not vary in the whole study domain and period. In other words, the machine learning models are based on a global modeling technique, and thus fail to consider the spatiotemporal variations of the relationship between NO_2 and influencing factors.

Therefore, this research aims to estimate ground NO_2 concentrations using a space-time neural network (STNN) model, which can allow for the spatiotemporal variations. The TROPOMI NO_2 product, the Goddard Earth Observing System Data Assimilation System GEOS-5 Forward Processing (GEOS 5-FP) simulated NO_2 related variable and meteorological data, and other auxiliary data are used as input for the STNN model, and the STNN model is trained with ground NO_2 station measurements. It is noteworthy that the new-generation TROPOMI sensor holds great potentials to assess NO_2 concentration [24], which helps capture detailed NO_2 distribution in this research. Through the above process, the STNN model is expected to fit the nonlinear NO_2 estimation function effectively and can be used to estimate ground NO_2 from remote sensing data.

2. Study Area and Materials

2.1. Study Area

The Wuhan urban agglomeration (WUA) region was selected as the study area, which is displayed in Figure 1. The WUA region is situated in the central part of China. It consists of the Wuhan city and eight surrounding cities, i.e., Ezhou, Huangshi, Xianning, Xiaogan, Huanggang, Tianmen, Qianjiang, and Xiantao [25]. In recent years, the WUA region is suffering from a severe air pollution problem, due to the rapid development of the economy [26,27]. Hence, it is of considerable significance to dynamically monitor ground NO_2 concentrations in the WUA region.

Figure 1. The WUA region and the distribution of ground NO_2 stations.

The NO₂ monitoring stations in the WUA region are used for analysis, as shown in Figure 1. Also, we further include the monitoring stations outside the WUA region to make full use of the ground NO₂ measurements, which are located in the range of 28.4°~32.3° N and 112.0°~116.7° E. A total of 84 NO₂ monitoring stations were collected in this research.

2.2. Materials

2.2.1. NO₂ Station Measurements

The hourly NO₂ data measured from 84 monitoring stations (see Figure 1) were obtained from <http://106.37.208.233:20035/>. In this research, the data during the period of 1 January 2019 to 31 December 2019 were used. The measurement method for ground NO₂ concentration is determined in the Chinese National Ambient Air Quality Standard (GB 3095-2012), which has high standards of calibration and quality control. In this research, the hourly NO₂ data corresponding to the overpass time of the satellite was extracted for modeling.

2.2.2. TROPOMI Tropospheric NO₂ Data

The Sentinel-5 Precursor (S5P) satellite can provide daily global products of trace gases and aerosols, which are of great use for air quality monitoring. The sensor onboard S5P satellite is the TROPOMI [18,28], which covers the spectral bands of the shortwave infrared, the near-infrared, the visible, and the ultraviolet. These spectral bands of observations make the TROPOMI sensor able to monitor ozone (O₃), NO₂, sulfur dioxide (SO₂), and aerosols, etc.

The TROPOMI tropospheric NO₂ product was retrieved based on the Dutch OMI NO₂ data approach and European “Quality Assurance for Essential Climate Variables” project (QA4ECV) processing systems [29]. The TROPOMI tropospheric NO₂ products were available at <https://disc.gsfc.nasa.gov/datasets?keywords=Sentinel-5P>. A previous study has revealed the high consistency between TROPOMI NO₂ and widely-used OMI NO₂ data over China [24]. In our study, the data field of “nitrogendioxide_tropospheric_column” was extracted, and this product was resampled to 0.05° × 0.05°.

2.2.3. GEOS 5-FP NO₂ Related Variable and Meteorological Conditions

We introduced two main types of GEOS 5-FP data [30] into the ground NO₂ estimation modeling. The first is NO₂ related variable, i.e., nitric acid surface mass concentration (denoted as NO_{sim}). The other is meteorological conditions, i.e., surface pressure, 10-m specific humidity, 2-m air temperature, 10-m eastward wind, 10-m northward wind, planetary boundary layer height, and evaporation from turbulence. The former type of data is recognized as a primary factor, and the latter is incorporated as the covariates for the ground NO₂ estimation modeling. The resolution of the above data is 0.25° × 0.3125°, and the additional information can be found at <https://fluid.nccs.nasa.gov/weather/>.

2.2.4. Other Auxiliary Data

In addition, Moderate-resolution Imaging Spectroradiometer (MODIS) normalized difference vegetation index (NDVI) data (identifier: MYD13C1) is used as the land cover-related covariate in the ground NO₂ estimation modeling. The NDVI data can be obtained at <https://ladsweb.modaps.eosdis.nasa.gov>. Also, the terrain-related variable, i.e., digital elevation model (DEM), is adopted, and its details can refer to Danielson et al. [31].

3. Methodology

3.1. The STNN Model for NO₂ Estimation

The NN models have been applied for satellite-based NO₂ estimation, and they usually establish a global relationship between ground NO₂ and influencing factors, i.e., $NO_2 = f(NO_{2,sat}, X)$,

where $NO_{2,sat}$ means satellite observations of NO_2 and X refers to other influencing factors, such as meteorological data, NDVI, etc. However, global NN modeling fails to allow for the spatiotemporal variations of the relationship between ground NO_2 and influencing factors. To address this issue, an STNN model is adopted in this research, whose general structure is shown as follows.

$$NO_2 = f_{(x_j, y_j, t_j)}(NO_{2,sat}, NO_{sim}, Meteorology, NDVI, DEM) \quad (1)$$

where NO_{sim} means the GEOS 5-FP simulated NO_2 related variable, $Meteorology$ is the GEOS 5-FP meteorological data. The details of the input variables can be found in Section 2.2. $f_{(x_j, y_j, t_j)}$ refers to the location-time-specific NN model, which varies in space and time to cope with the spatiotemporal variations. (x_j, y_j) denotes the spatial coordinate and t_j stands for the time of grid cell j .

In this research, the generalized regression neural network (GRNN) [32,33] model is utilized for mapping the relationship between ground NO_2 and influencing factors, that is, $f_{(x_j, y_j, t_j)}$ is represented by the GRNN model. Figure 2 shows the schematic of the space-time varying GRNN model for ground NO_2 estimation, which is denoted as geographically and temporally weighted GRNN (GTW-GRNN). The GTW-GRNN model is separately constructed for each location and time, and the modeling process contains two main steps, i.e., spatiotemporal weighting and GRNN modeling, which are simply described as follows. For details, please refer to our previous study [34].

Figure 2. GTW-GRNN model for estimating ground-level NO_2 .

For the spatiotemporal weighting, the widely used Gaussian function is applied to describe the contribution of each sample to the estimation of NO_2 for grid cell j . To be specific, the weight of sample k can be depicted as Equation (2):

$$w_k = \exp\left(-\frac{ds_k^2 + \lambda dt_k^2}{h_{ST}^2}\right) \quad (2)$$

where ds_k and dt_k respectively stand for the spatial and the temporal distance of sample k to grid cell j . λ is a factor to counterweigh the spatial distance and temporal distance. h_{ST} is considered as spatiotemporal bandwidth in the spatiotemporal weighting scheme [35,36].

For the GRNN modeling, the critical issue is how to incorporate spatiotemporal weighting into the GRNN model (i.e., establishing the GTW-GRNN model). Compared with the original GRNN model, the GTW-GRNN model does not change the neural network structure, but it introduces the spatiotemporal weighting into the weights between the pattern layer and the summation layer. Thus, a joint weighting of spatiotemporal weighting and GRNN weighting is used for estimating ground NO_2 concentrations. Additional details about GTW-GRNN modeling can be found in our previous study [34].

3.2. The Procedure of STNN-Based NO_2 Estimation

Figure 3 shows the procedure of satellite-based NO_2 estimation using the GTW-GRNN model, which can be divided into three main steps: (1) data pre-processing and matching, (2) GTW-GRNN modeling and validation, and (3) spatiotemporal mapping of ground NO_2 .

Figure 3. The procedure of satellite-based NO_2 estimation via the GTW-GRNN model.

(1) Data pre-processing and matching. The variables mentioned in Section 2.2. are firstly extracted from the original datasets to form the input dataset. During this process, all the data are converted to the WGS84 geographic coordinate system and resampled to 0.05° in accordance with the spatial resolution of TROPOMI observation. Subsequently, the values of TROPOMI observation, GEOS 5-FP data, and other auxiliary data are extracted according to the locations of NO_2 monitoring stations. Meanwhile, multiple NO_2 station measurements are averaged in each 0.05° grid cell.

(2) GTW-GRNN modeling and validation. For each location and time, a GTW-GRNN model is established and trained with local samples (see Section 3.1). Then a cross-validation (CV) technique [37] is adopted to evaluate model performance and to be specific, the site-based CV [38] is utilized for the model validation in this research. For the site-based CV, all the grid cells with NO_2 monitoring stations are partitioned into ten folds randomly and averagely, where one fold is used as the validation set, and nine folds are adopted for model fitting. This process will be repeated ten times until each fold has been used for model validation. At the same time, the following statistical indicators are calculated for accuracy evaluation: root-mean-square error (RMSE, unit: $\mu\text{g}/\text{m}^3$) and coefficient of determination (R^2 , unitless).

(3) Spatiotemporal mapping of ground NO₂. After the validation process, the GTW-GRNN model can be utilized for the mapping of ground NO₂ concentrations. For each grid cell in the spatiotemporal dimension, the data samples are inputted into the GTW-GRNN model, and the output NO₂ value can be obtained. Thus, the spatiotemporal distribution of NO₂ concentrations can be mapped through the above processes.

4. Results and Analysis

To fully assess the performance of the GTW-GRNN model, it was compared to the global GRNN model and the GTWR model, both of them have been widely used in remote sensing estimation modeling of air quality [39–41]. The selection for these two models is subject to the following reasons: (1) the global GRNN does not consider the spatial and temporal variations of the relationship between NO₂ and influencing factors, the comparison between the global GRNN and GTW-GRNN models can thus reveal the function of considering the spatiotemporal variations in GRNN. (2) the GTWR and GTW-GRNN models share similar modeling strategies, whereas the former is based on a linear assumption, and the latter uses the nonlinear NN modeling technique.

4.1. Overall Performance of the Models

Figure 4 shows the site-based CV performance of the GTWR, global GRNN, and GTW-GRNN models. As can be observed from Figure 4, the GTWR model shows a relatively poor performance, with RMSE and R² values being 9.25 µg/m³ and 0.61, respectively. Then a slightly better performance is achieved by the global GRNN model, whose CV RMSE and R² values are 9.14 µg/m³ and 0.62, respectively. The GTWR model can allow for the spatiotemporal variations of the association between ground NO₂ and influencing factors, whereas it is based on a linear assumption. On the contrary, the global GRNN model can fit the nonlinear relationship, whereas it fails to consider the spatiotemporal variations. Comparing the GTWR and global GRNN models, the global GRNN model shows a slight advantage in such a relatively small WUA region. Thanks to the ability to simultaneously cope with nonlinear fitting and spatiotemporal variations, the GTW-GRNN model performs the best for ground NO₂ estimation, with CV RMSE and R² values of 8.29 µg/m³ and 0.69, respectively. In addition, the GTW-GRNN model shows the lightest degree of underestimation/overestimation among the three models, which has a CV slope value of 0.75. The underestimation/overestimation is a common phenomenon in remote sensing of air quality modeling [42], and the possible reasons could be that the station measurements cannot represent the grid cell. The lack of high values for model training is also likely to result in that phenomenon. In summary, all the results demonstrate that the GTW-GRNN model is advantageous for the remote sensing retrieval of ground NO₂ concentrations.

Figure 4. Site-based CV performance of the (a) GTWR, (b) global GRNN, and (c) GTW-GRNN models (N = 21,065). The dashed line refers to $y=x$ reference, and the coordinate axis means NO₂ concentration with the unit of µg/m³.

4.2. Model Performance for Each Season

The seasonal performance of the models is shown in Table 1. Firstly, the GTW-GRNN model has obtained the best performance among the three models, with R^2 s being 0.55, 0.34, 0.61, and 0.64 for spring (March to May), summer (June to August), autumn (September to November), and winter (December, January, and February), respectively. Meanwhile, the seasonal R^2 values for the global GRNN (GTWR) model are 0.50 (0.40), 0.25 (0.18), 0.56 (0.58), and 0.54 (0.56), respectively. Also, from the view of RMSE and slope, the GTW-GRNN model shows some advantages over the other two models for ground NO_2 estimation for all the four seasons. Specifically, the RMSE values decrease from $10.06 \mu\text{g}/\text{m}^3$ to $8.57 \mu\text{g}/\text{m}^3$ (spring), from $7.12 \mu\text{g}/\text{m}^3$ to $6.28 \mu\text{g}/\text{m}^3$ (summer), from $7.99 \mu\text{g}/\text{m}^3$ to $7.73 \mu\text{g}/\text{m}^3$ (autumn), and from $11.39 \mu\text{g}/\text{m}^3$ to $10.27 \mu\text{g}/\text{m}^3$ (winter), respectively, when comparing the GTW-GRNN model to the GTWR model.

Secondly, large seasonal variations can be found in Table 1, where summer shows the most miserable performance, and autumn and winter report significant increase for model fitting goodness. Taking the GTW-GRNN model as an example, the RMSE, R^2 , and slope values are $6.28 \mu\text{g}/\text{m}^3$, 0.34, and 0.48, respectively, for summer, whereas the corresponding metric values are $10.27 \mu\text{g}/\text{m}^3$, 0.64, and 0.70, apiece, for winter. A higher slope value generally means a lighter degree of underestimation/overestimation, so the models tend to better estimate NO_2 high/low values in winter than in summer. Besides, it should be noted that winter has a higher RMSE value than other seasons. RMSE value is an absolute metric and the high level of NO_2 concentrations in winter results in the high RMSE value. The reason for seasonal variations could be related to seasonal differences of NO_2 values, formation conditions, etc.

Table 1. Site-based cross-validation (CV) performance of the models for each season.

Season	Sample (N)	GTWR			Global GRNN			GTW-GRNN		
		R^2	RMSE	Slope	R^2	RMSE	Slope	R^2	RMSE	Slope
Spring	5485	0.40	10.06	0.52	0.50	9.25	0.63	0.55	8.57	0.65
Summer	5335	0.18	7.12	0.31	0.25	6.86	0.42	0.34	6.28	0.48
Autumn	5354	0.58	7.99	0.61	0.56	8.33	0.66	0.61	7.73	0.68
Winter	4891	0.56	11.39	0.59	0.54	11.69	0.61	0.64	10.27	0.70

4.3. Model Performance for Each Grid Cell

We also evaluate the model performance for each grid cell, which is shown in Figure 5. Overall, the mean R^2 (RMSE) for the GTWR, global GRNN, and GTW-GRNN models are 0.64 ($9.08 \mu\text{g}/\text{m}^3$), 0.66 ($8.82 \mu\text{g}/\text{m}^3$), and 0.72 ($7.95 \mu\text{g}/\text{m}^3$), respectively. Meanwhile, 45, 44, and 53 out of 63 grid cells respectively achieve high R^2 values of greater than 0.6 for the GTWR, global GRNN, and GTW-GRNN models. These results indicate that the GTW-GRNN model performs the best, whereas the GTWR is the poorest for the overall performance. Spatially, higher values of R^2 are found for GTW-GRNN compared to the GTWR and global GRNN models in Wuhan, Ezhou, and Xianning cities. Accordingly, lower RMSE values for the GTW-GRNN model can be observed in Ezhou city.

On the other hand, the site-based CV is considered as an effective solution to reflect spatial prediction accuracy [38]. As shown in Figure 5c, most of the grid cells can obtain a high R^2 value (as mentioned before, 84% grid cells with $R^2 > 0.6$), indicating that the GTW-GRNN predictions show high consistency to ground station measurements. The above results reveal GTW-GRNN modeling is an appropriate approach for satellite-based spatial mapping of ground NO_2 concentrations.

Figure 5. Site-based CV performance for each grid cell. (a–c) are R^2 distributions for the GTWR, global GRNN, and GTW-GRNN models, respectively. (d–f) are RMSE distributions for the GTWR, global GRNN, and GTW-GRNN models, respectively.

5. Discussion

5.1. Mapping Results of Ground NO_2 Concentrations

Based on the GTW-GRNN model, the spatial distributions of ground NO_2 concentrations are mapped. As shown in Figure 6, four days (1 January 2019, 9 May 2019, 21 August 2019, and 8 October 2019) of mapping results are presented as an example. Overall, the distributions of the remote sensing retrievals of NO_2 show an excellent agreement to station measurements for the given four days. Among the four days, 1 January 2019 reports relatively high levels of NO_2 concentrations, and 9 May 2019 and 21 August 2019 are cleaner. Spatially, Wuhan is a severe NO_2 pollution center, which has the most urbanized degree in the WUA region.

Figure 6. Mapping results of ground NO_2 concentrations. The top row is remote sensing retrievals of NO_2 concentrations, and the bottom row is station measurements.

To quantitatively evaluate the consistency between remote sensing retrievals and station measurements, we calculate the RMSE and R^2 values, as shown in Table 2. For the whole year, a good agreement is found, with the RMSE and R^2 values being $4.55 \mu\text{g}/\text{m}^3$ and 0.91, respectively, indicating that the GTW-GRNN model achieves a good fit for the relationship between ground NO_2 and influencing factors. For the above mentioned four days, the R^2 s are 0.76, 0.75, 0.84, and 0.81, respectively, which confirms the high consistency between remote sensing retrievals and station measurements.

Table 2. R^2 and RMSE between remote sensing mapping results and station measurements.

Time	Whole Year	20190101	20190509	20190821	20191008
R^2	0.91	0.76	0.75	0.84	0.81
RMSE	4.55	4.57	4.73	3.08	3.11

5.2. The Novelty of Incorporating Spatiotemporal Weighting into GRNN

A GTW-GRNN model was applied to estimate ground NO_2 concentrations in this research, of which the novelty lies in two main aspects when comparing to the original GRNN model. The first is the GTW-GRNN model uses a local modeling strategy and thus can address the spatiotemporal variations. The other is that a spatiotemporal weighting scheme is introduced to capture the relation of data samples for NO_2 estimation. We now compare the GTW-GRNN model with the global GRNN model and the local GRNN model without spatiotemporal weighting, that is, the spatiotemporal weights are all set as 1 in the GTW-GRNN modeling process.

As Table 3 shows, the global GRNN performs the poorest, with CV RMSE and R^2 values being $9.25 \mu\text{g}/\text{m}^3$ and 0.61, respectively, for the reason that the global GRNN model cannot address the spatiotemporal variations and estimate ground NO_2 concentrations using constant model coefficients. Based on a local modeling strategy, the local GRNN model can consider the spatiotemporal variations, and the ground NO_2 is estimated using spatially and temporally varying model coefficients. Thus, the local GRNN model obtains a more advantageous performance, the CV RMSE, R^2 , and slope values are $8.61 \mu\text{g}/\text{m}^3$, 0.66, and 0.71, respectively. By further incorporating spatiotemporal weighting, the GTW-GRNN model achieves the best performance. These results demonstrate that combining spatiotemporal weighting derived from geographical laws and neural networks can boost the estimation accuracy.

Table 3. Site-based CV performance of the global GRNN, local GRNN, and GTW-GRNN models.

Model	Site-Based CV Performance		
	R^2	RMSE	Slope
Global GRNN	0.61	9.25	0.68
Local GRNN	0.66	8.61	0.71
GTW-GRNN	0.69	8.29	0.75

5.3. Impact of Aerosol on Satellite-Based NO_2 Modeling

Aerosol optical depth (AOD) has been reported to be closely correlated to NO_2 , and ul-Haq et al. [43] have revealed that the correlation coefficient between NO_2 and AOD is as high as 0.49 over South Asia during 2005–2015. Hence, the AOD data is likely to be useful for the remote sensing retrieval of ground NO_2 . In this research, the AOD product is not adopted for the following reasons. First, in the remote sensing of air quality field, AOD product has been widely considered as a proxy to estimate ground particulate matter [7,44], and the remote sensing retrieval of ground NO_2 usually uses satellite observed NO_2 data [8,9,15]. Hence, the selection of satellite data of this work is in line with previous studies. Second, the widely used AOD products (e.g., MODIS AOD) are often missing, whose missing proportion is greater than that of TROPOMI NO_2 data. If the AOD product is incorporated, it may introduce more data absence in the ground NO_2 estimates. In summary, this work pays more attention

to address the spatiotemporal variations in the NO₂ neural network estimation framework, so we did not further investigate the influencing factors of NO₂. However, considering the high correlation between AOD and NO₂, it remains an interesting direction to introduce AOD data in remote sensing retrieval of ground NO₂.

5.4. Limitations

There are still some limitations to the remote sensing retrieval of ground NO₂ concentrations in this study. Firstly, the missing TROPOMI data results in the incomplete information of remote sensing NO₂ retrievals, which may bring limitations for further applications. The data filling for TROPOMI data is not conducted in this research, for the reason that the fundamental purpose of this research is to develop the GTW-GRNN based remote sensing NO₂ retrieval framework, the data filling may introduce additional errors. Secondly, the study region focuses on WUA, which is a relatively small area. New challenges and problems will come out for estimating ground NO₂ over a broader geographical region. Hence, it remains our further studies to estimate larger scales of NO₂ data using the GTW-GRNN based NO₂ estimation framework proposed in this research.

6. Conclusions and Future Work

In this study, a GTW-GRNN model was applied to estimate ground NO₂ concentrations by integrating ground NO₂ station measurements, TROPOMI NO₂ products, GEOS 5-FP data, and other auxiliary data. The contribution of this study lies in two main aspects: (1) the proposed remote sensing retrieval framework of ground NO₂ based on the GTW-GRNN model can simultaneously address the nonlinearity and spatiotemporal variations. (2) the ground NO₂ estimation framework introduces multi-source data, including TROPOMI observations, GEOS 5-FP simulations, land cover-related variable, and terrain-related variable. Thanks to the advanced model and sufficient data, this study achieves a satisfactory result for remote sensing retrieval of ground NO₂, with CV RMSE and R² values being 8.29 µg/m³ and 0.69, respectively. The comparison between the GTW-GRNN and global GRNN models indicates that considering spatiotemporal variations in GRNN helps improve estimation accuracy for NO₂ concentrations. Also, the comparison between the GTW-GRNN and GTWR models shows that the neural network nonlinear modeling holds advantages over linear modeling. On this basis, the mapping results of the GTW-GRNN model agree perfectly with station measurements. In conclusion, this study will be an essential supplement to the field of remote sensing of ground NO₂ concentrations.

In future studies, we will focus on two aspects. First, we will develop geographically and temporally weighted deep learning models for remote sensing of ground NO₂ concentrations, because deep learning is expected to have high potentials for environmental remote sensing [45,46]. Second, we would like to produce remote sensing NO₂ products using GTW-GRNN modeling over broader geographical regions in China, to provide fundamental data for monitoring the increasing NO₂ levels [47–49].

Author Contributions: Data preparation and curation, Y.W. and T.L.; Conceptualization, T.L. and Q.Y.; methodology, T.L.; validation, T.L. and Y.W.; supervision, Q.Y.; writing—original draft preparation, T.L.; writing—review and editing, T.L., Y.W., and Q.Y. All authors have read and agreed to the published version of the manuscript.

Funding: This study was supported by the Strategic Priority Research Program of the Chinese Academy of Sciences (No. XDA19090104), the National Natural Science Foundation of China (No. 41922008), and the Fundamental Research Funds for the Central Universities of Wuhan University (No. 2042019kf0213).

Acknowledgments: The authors would like to thank the data provider listed in Section 2.2 for freely releasing the fundamental data for use.

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

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