Modeling temporal and spatial variation in atmospheric aerosols by geographically and temporally weighted regression with principal component analysis

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ABSTRACT: Changes in the distribution of aerosol optical depth (AOD) are closely related to climate change, air quality, environmental pollution and human health. However, null values often appear in regions of AOD data retrieved by satellite. To address this problem, we propose geographically and temporally weighted regression with principal component analysis (PCA-GTWR), which aims to make full use of the advantages of geographically and temporally weighted regression (GTWR) and principal component analysis (PCA). Taking the prediction of the AOD in Beijing as an example, the PCA-GTWR model predicted that the monthly average AOD data would have an MAE, RMSE, R^2, R_j^2 and regression coefficient of 0.0705, 0.0954, 0.8705, 0.8703, and 0.7913, respectively, in April 2015; 0.0587, 0.0757, 0.8628, 0.8627, and 0.7939, respectively, in May 2015; and 0.1059, 0.1376, 0.8185, 0.8184 and 0.7633, respectively, in June 2015. This result shows that the PCA-GTWR model can be effectively applied to AOD data prediction. The research content of this paper is of great significance to research on climate change, air quality and environmental pollution.

1. INTRODUCTION

Aerosol optical depth (AOD) is an important property of aerosols and is the main physical quantity that characterizes atmospheric turbidity (Qin, et al. 2018, Wang, et al. 2019). The distribution of AOD is closely related to climate change, air quality, environmental pollution, and human health(Kaufman, et al. 2002, Liu, et al. 2018). Therefore, accurate observations of the AOD are of great significance in aerosol research and applications. Observations of aerosols include ground observations and satellite observations. Ground observations are mainly obtained from the Global Automated Observation Network (AERONET), the European Aerosol Research Lidar Network (EARLINET), and the Micropulse Lidar Network (MPLNET)(Liu, et al. 2011). Unlike ground observations, satellite observations can enable wide-range monitoring with satisfactory spatial and temporal resolution (Kaufman, Tanré and Boucher 2002). Satellite-based sensors that can obtain AOD observations include the multiangle imaging spectroradiometer (MISR), the sea-viewing wide field-of-view sensor (SeaWiFS), ozone mapping imaging (OMI), the visible infrared imaging radiometer (VIIRS), the medium-resolution imaging spectrometer (MODIS), and the polarization and directionality of the Earth's reflectances (POLDER) instrument (Fan, et al. 2019, Yang, et al. 2017). There have been many studies on the synergistic retrieval of AOD data with multisensor observations to improve monitoring accuracy and coverage(Singh, et al. 2017, Tang, et al. 2016). Currently, studies of AOD data reconstruction are relatively rare under various situations(Davies and North 2015, Puttaswamy, et al. 2013).

As the AOD varies with time and geographical location, it has temporal and spatial instability, which leads to uncertainty in future climate predictions (Davies and North 2015). Moreover, the driving factors of the AOD are diverse, so the multicollinearity between these factors should be eliminated when studying the driving factors of aerosols (Sun, et al. 2014). To address the above problems in the AOD prediction process, we investigate principal component analysis (PCA), which represents each principal component as a linear combination of the original data, removes the driving factor multicollinearity, and uses fewer principal components to reflect more of the information of the original indicators. This multivariate statistical analysis method has been widely used in many fields. However, traditional PCA does not consider the temporal and spatial relationships in data(Qiao, et al. 2017, Ramesh Kumar 2017). Geographically weighted regression (GWR) is a local form of linear regression used to model relationships among spatial changes. The spatial weights among independent and dependent factors are used to detect nonstationarity in spatial relationships by embedding spatial information in a linear regression model (Fotheringham, et al. 1998, Huang, et al. 2010). Geographically and temporally weighted regression (GTWR) extends the GWR model to the GTWR model of panel data sets by separating the selection of the optimal temporal and spatial bandwidths. Since it was introduced, the GTWR model has become the most popular method of spatiotemporal modeling and has been applied in many fields (Chu and Bilal 2019, Dong, et al. 2019).

The GWR method effectively solves spatial problems in regression analysis. The PCA method effectively reduces the redundancy and multicollinearity problems of auxiliary variables. Guo, et al. [7]) used geographically weighted regression with principal component analysis (PCA-GWR) to estimate soil organic carbon density (SOCD). The results show that PCA can play an important role in reducing the redundancy and multicollinearity of auxiliary variables and that GWR had the highest prediction accuracy among the four models proposed. In this paper, a geographically and temporally weighted regression method with principal component analysis (PCA-GTWR) is proposed. This method represents principal components as linear combinations of the original data; this strategy can effectively eliminate multicollinearity, reflect more of the original index information with fewer principal components, reduce the information loss in the original data, and improve the dimensionality reduction effect and accuracy of the model estimation of the AOD. At the same time, the model incorporates the spatiotemporal characteristics of the data into the regression model, which effectively solves the problem of the spatiotemporal nonstationarity of the regression model and demonstrates the superiority of the PCA-GTWR method for estimating AOD. The PCA-GTWR model is used to predict high-precision AOD values, providing a reliable basis for research on climate change, air quality, environmental pollution, and human health.

2. STUDY AREA AND DATA

The research area of this article is Beijing (115.7°E-117.4°E, 39.4°N-41.6°N). As the capital of China, Beijing's rapid economic development has aggravated air pollution, and the concentration of $PM_{2.5}$-based particulate matter has increased sharply. Temporal and spatial changes in AOD are closely related to $PM_{2.5}$, climate change, and environmental pollution. Therefore, it is of great significance to carry out complete and accurate AOD predictions in this region.

The MODIS 3 km Level 2 AOD products (MYD04_3K and MOD04_3K) of both the Terra and Aqua platforms from April 1, 2015, to June 30, 2015, were obtained from the NASA website (https://ladsweb.nascom.nasa.gov/data). Meteorological data (including wind speed, temperature, humidity, and air pressure) were obtained from the China meteorological data network (http://data.cma.cn/site/index.html). In this study, the hourly observation data same as the temporal coverage of MODIS data were downloaded. The geographical distribution of the data from meteorological ground monitoring stations in the study area is shown in Figure 1. The geographic data (including the digital elevation model (DEM), slope and aspect) are from the geospatial data cloud website (http://www.gscloud.cn/). The resolution of the elevation, slope and aspect data used in this paper is 90 m.

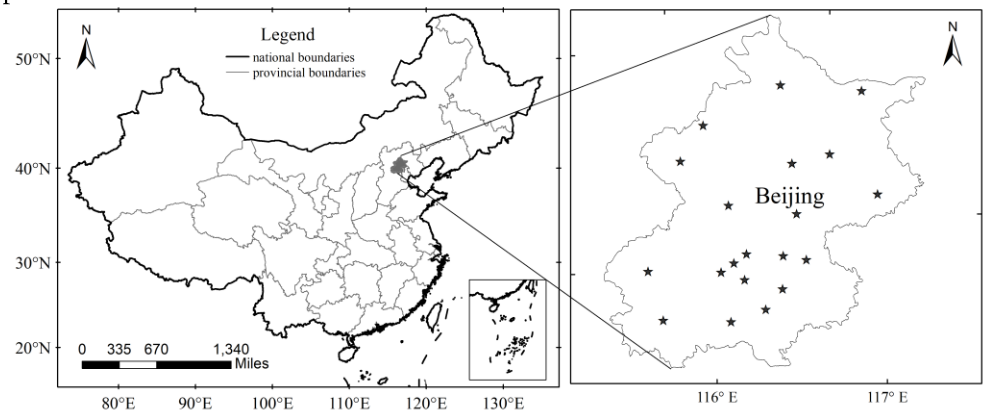

Figure 1 Distribution of meteorological data monitoring stations in Beijing

3. METHODOLOGY

3.1 Technical Route

To unify the spatial and temporal resolution, the AOD, meteorological and geographic data were preprocessed and projected to the same spatial resolution and coordinates. The average-value method was used to obtain the monthly average of each index in the AOD data and meteorological data. Regarding the spatial resolution, the AOD and geographical data are surface data, and the meteorological data are site data, which requires further processing. The meteorological data were interpolated to 3 km * 3 km grid data with the kriging method. The AOD, meteorological and geographic data of the center point of the 3 km * 3 km grid were extracted.

The PCA-GTWR method fully combines the advantages of PCA and GTWR. The technical process of PCA-GTWR is shown in Figure 2, and the corresponding steps are as follows: 1) Use the Pearson correlation coefficient to test the correlation of each factor, and remove the factors that have a small correlation with the dependent variable. 2) Perform PCA on the remaining impact factors to obtain n new comprehensive evaluation indicators. 3) From the n new comprehensive evaluation indicators, select the first m evaluation indicators with a cumulative contribution exceeding 85% as the input variables of the GTWR model, and estimate the values of the dependent variables. 4) Using the test results, calculate the mean absolute error (MAE), root-mean-square error (RMSE), R-squared coefficient (R^2) and corrected R-squared coefficient (R_j^2) as the four evaluation indexes to evaluate the effectiveness of this method.

3.2 Principal Component Analysis

PCA is a classical statistical method for analyzing the covariance structure of multiple variables (Viana, et al. 2006) that maps high-dimensional data to low-dimensional data (Zhao, et al. 2018). PCA uses orthogonal transformation to transform the covariance matrix of the original random vector into a diagonal matrix so that it points to the most open orthogonal directions of the distribution of P at the sample point, carries out dimensionality reduction on the system of multidimensional variables and replaces the original variables with a few principal components. PCA principles can be found in the literature (Qiao, et al. 2017, Ramesh Kumar 2017).

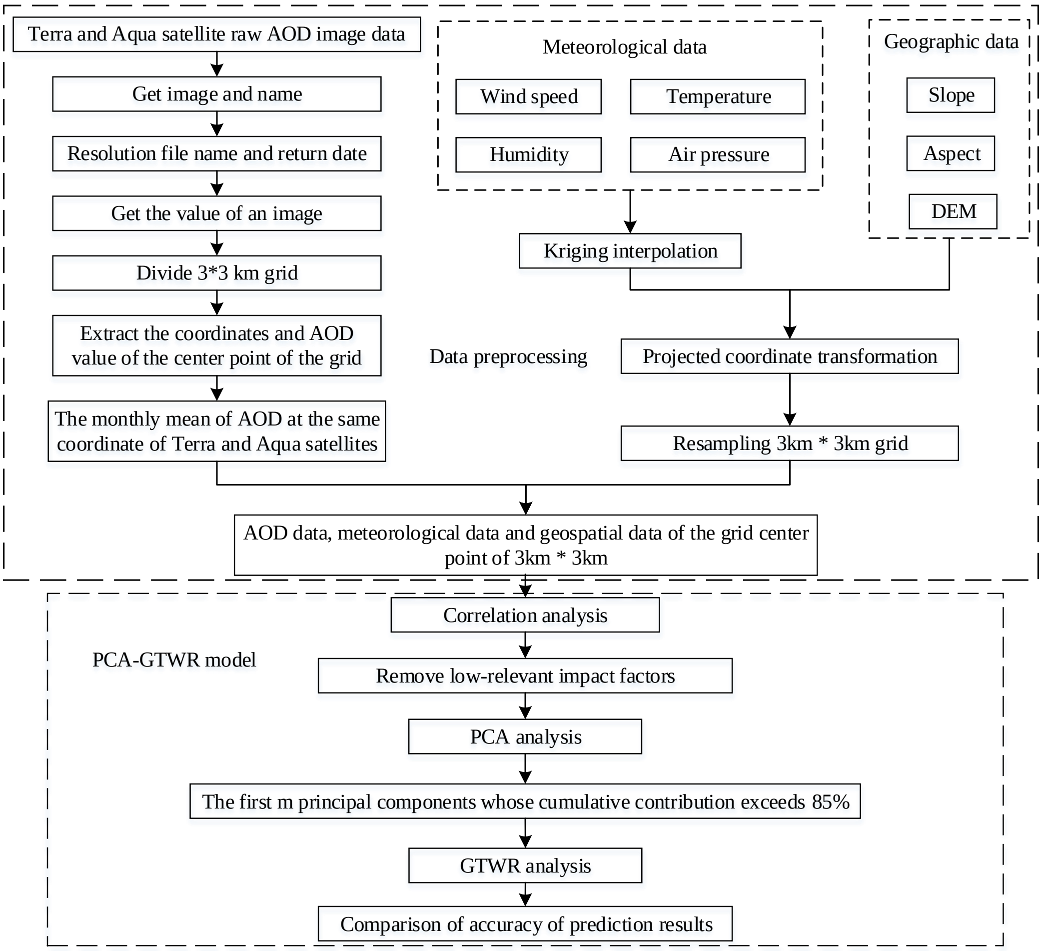

Figure 2 PCA-GTWR technology flowchart

3.3 Geographically Weighted Regression

The GWR model is an extension of the ordinary least-squares regression (OLS) model to solve the problem of the local estimation of parameters (Brunsdon, et al. 1996). The GWR principle is as follows (Nilsson 2014):

$$y_i = \beta_0(u_i, v_i) + \sum_{k=1}^{d} \beta_k(u_i, v_i) x_{ik} + \varepsilon_i . \quad (1)$$

In formula (1), $(y_i, x_{i1}, x_{i2}, \cdots x_{id})$ are the n data sets at the point (u_i, v_i) for the dependent variable y and the independent variables $(x_1, x_2, \cdots x_d)$, and $\beta_k(u_i, v_i)(k = 1, 2, \cdots, d)$ is the unknown parameter at the observation point (u_i, v_i) of i. $\varepsilon_i (i = 1, 2, 3 \ldots, n)$ is an independent and identically distributed error term, usually assumed to follow an $N(0, \delta^2)$ distribution. In matrix notation, the estimated expression of this parameter is as follows:

$$\hat{\beta}(u_i, v_i) = (X^T W(u_i, v_i) X)^{-1} X^T W(u_i, v_i) Y . \quad (2)$$

From equation (2), the local estimate of the regression function $\hat{\beta}(u_i, v_i)$ is obtained at all observation positions; X is the independent variable matrix, Y is the dependent variable vector, and $W(u_i, v_i)$ is the spatial weight matrix. The regression parameters in GWR are related to the geographical locations of the sample data, and the spatial weights can be represented by a distance function, which is referred to as a kernel function. Commonly used kernel functions include the Gauss function and the Bisquare function. In this paper, the Gauss function is used to generate the spatial weight matrix. The formula is as follows:

$$\omega_{\mathrm{i}}\left(u_j, v_j\right) = \mathrm{K}_h(d_{ij}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{d_{ij}}{h}\right)^2\right). \tag{3}$$

In equation (3), h is the bandwidth and d_{ij} is the distance between the points (u_i, v_i) and (u_j, v_j). Bandwidth is an important factor in calculating the spatial weight matrix. This paper uses cross-validation (specifically, cross-validation residual sum of squares (CVRSS)) to determine the optimal bandwidth of the GWR. Assuming that the predicted value of y_i in the GWR is represented by $\hat{y}(h)$ as a function of h, the formula for the sum of squared errors can be written as follows:

$$CVRSS(\mathrm{h}) = \sum_i (y_i - \hat{y} \neq 1(h))^2. \tag{4}$$

3.4 Geographically and Temporally Weighted Regression

GTWR assumes that the regression coefficient is an arbitrary function of the geographic location and observation time and simultaneously detects nonstationarity in time and space. The principle of GTWR is as follows (Huang, Wu and Barry 2010):

$$y_i = \beta_0\left(u_i, v_i, t_i\right) + \sum_{k=1}^{d} \beta_k\left(u_i, v_i, t_i\right) x_{ik} + \varepsilon_i. \tag{5}$$

In formula (5), $\left(y_i, x_{i1}, x_{i2}, \cdots x_{id}\right)$ are the n sets of observations of the dependent variable y and the independent variables $\left(x_1, x_2, \cdots x_d\right)$ at the observation point (u_i, v_i, t_i). $\beta_k(u_i, v_i, t_i)(k{=}1, 2, 3\ldots, d)$ is the unknown parameter at the i th observation point (u_i, v_i, t_i), and $\varepsilon_i(i{=}1, 2, 3\ldots, n)$ is an independent and identically distributed error term, usually assumed to follow an $N(0, \delta^2)$ distribution.

With the least-squares method, the estimated regression parameter $\hat{\beta}(u_i, v_i, t_i)$ and the regression value $\hat{y}_i$ at (u_i, v_i, t_i) can be found as:

$$\beta\left(u_0, v_0, t_0\right) = \left[X^T W\left(u_0, v_0, t_0\right) X\right]^{-1} X^T W\left(u_0, v_0, t_0\right) Y, \tag{6}$$

$$y_i\left(u_0, v_0, t_0\right) = x_0{}^T \beta\left(u_0, v_0, t_0\right) = x_0{}^T \left[X^T W\left(u_0, v_0, t_0\right) X\right]^{-1} X^T W\left(u_0, v_0, t_0\right) Y. \tag{7}$$

In equation (7), $X^T = [x_1, x_2, \cdots x_d]$, $x_0^T = [1, x_{01}, x_{02}, \cdots x_{0d}]$ is the value of the independent variable at (u_0, v_0, t_0), and $W\left(u_i, v_i, t_i\right) = diag(\omega_{i1}, \omega_{i2}, \cdots, \omega_{im})$ is the weight matrix. The spatiotemporal distance d^{ST} is defined as a linear combination of the spatial distance d^S and the time distance d^T, and its formula is as follows:

$$d^{ST} = \lambda d^{S} + \mu d^{T} . \tag{8}$$

In equation (8), λ and μ are scale factors used to balance the different effects of space and time. Therefore, if the scale factor is adjusted appropriately, d^{ST} can be used to measure the spatiotemporal distance. The spatiotemporal distance between point (u_0, v_0, t_0) and point (u_i, v_i, t_i) is defined as follows:

$$d_{0i} = \sqrt{\lambda\left[\left(u_0 - u_i\right)^2 + \left(v_0 - v_i\right)^2\right] + \mu\left(t_0 - t_i\right)^2} . \tag{9}$$

The spatiotemporal weight matrix generated by the Gaussian function is as follows:

$$\begin{aligned} w_{ij}^{ST} &= \exp\left\{-\left(\frac{\lambda[(u_i - u_j)^2 + (v_i - v_j)^2] + \mu(t_i - t_j)^2}{h_{ST}^2}\right)\right\} \\ &= \exp\left\{-\frac{(d_{ij}^S)^2}{h_S^2}\right\} \times \exp\left\{-\frac{(d_{ij}^T)^2}{h_T^2}\right\} = \omega_{ij}^S \times \omega_{ij}^T \end{aligned} . \tag{10}$$

In equation (10), h_{ST} , h_S and h_T are the spatiotemporal bandwidth, spatial bandwidth, and time bandwidth, respectively. $h_S = \sqrt{h_{ST}/\lambda}$, and $h_T = \sqrt{h_{ST}/\lambda}$. The bandwidth of the kernel function has a significant impact on the GTWR. Therefore, the key to accurate regression is choosing the right bandwidth (Dong, Zhang, Long, Zhang and Sun 2019). This paper uses cross-validation (CVRSS) to determine the optimal bandwidth of the GTWR. The calculation method is shown in equation (4).

4. RESULTS AND DISCUSSION

4.1 Correlation Test

The Pearson correlation coefficient of each factor is calculated to test the correlations among variables and determine whether there is multiple collinearity among the independent variables. The Pearson correlation coefficient of the AOD for the indexes of the elevation, slope, wind speed, air temperature, humidity and pressure was calculated to be greater than 0.4, and the Pearson correlation coefficient of the AOD for the indexes of slope and aspect direction was less than 0.1. These two factors were removed. Among the remaining six impact factors, there were many Pearson correlation coefficients above 0.6. It was concluded that there were multiple collinearities among the explanatory variables.

It must be determined whether the dependent variable has spatial correlations before GWTR model analysis is applied. This paper uses Moran's I value to pretest the spatial correlations among the AOD variables. Moran's I values of the monthly averages of the AOD in April, May, and June 2015 were calculated to be 0.833, 0.724, and 0.625, respectively, which revealed that the AOD in this study area has a strong agglomeration pattern.

4.2 PCA Analysis

The PCA method was used to calculate the principal component (PC), characteristic root, contribution degree and cumulative contribution degree of each index in the data set in April, May and June of 2015. The results are shown in Table 1. According to Table 1, the contribution degree of the first principal component (PC1) in each month is approximately 60%, the cumulative contribution degree of the first two principal component (PC2) is greater than 75%, and the cumulative contribution degree of the first three principal component (PC3) is greater than 85%. Therefore, this paper selects the first three PCs as the input variables of the model to fully reflect most of the information in the original data.

Table 1 Principal component analysis results

Time	PC	Eigenvalue	Contribution/%	Cumulative contribution/%
	PC1	3.585	59.750	59.750
April	PC2	0.959	15.977	75.727
	PC3	0.565	9.419	85.146
	PC1	3.635	60.583	60.583
May	PC2	1.156	19.266	79.850
	PC3	0.708	11.805	91.655
	PC1	3.604	60.059	60.059
June	PC2	1.505	25.091	85.151
	PC3	0.475	7.909	93.059

4.3 Comparative Results

The original monthly average AODs in April, May, and June 2015 are shown in Figure 3. Figure 4 shows the monthly average AODs in April, May, and June 2015 calculated with the PCA-GWR method by using the first three principal components in the principal component analysis results as the explanatory variables and the AOD as the dependent variable. Figure 5 shows the monthly average AODs in April, May, and June 2015 calculated with the PCA-GTWR method by using the first three principal components in the principal component analysis results as the explanatory variables and the AOD as the dependent variable. To evaluate the PCA-GWR and PCA-GTWR models, four evaluation indexes—the MAE, the RMSE, R^2, and R_j^2—are calculated, as shown in Table 2.

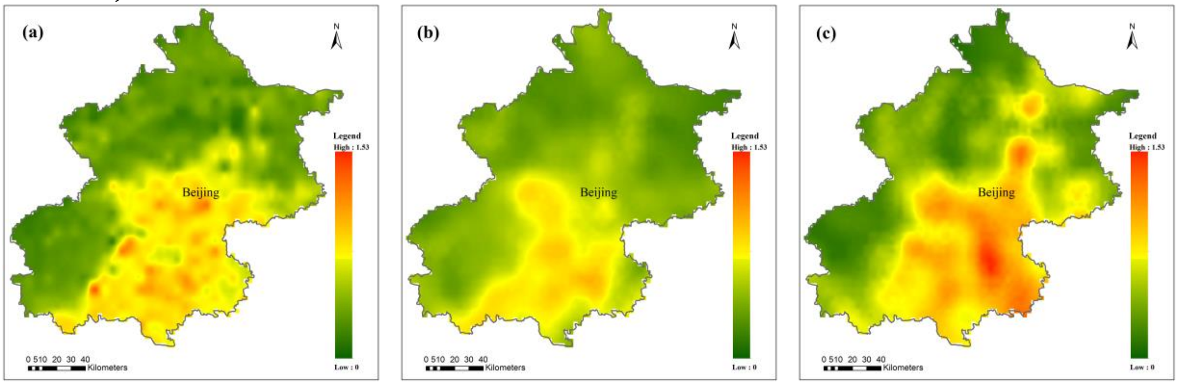

Figure 3 Original monthly average AOD in 2015: (a) April, (b) May, (c) June

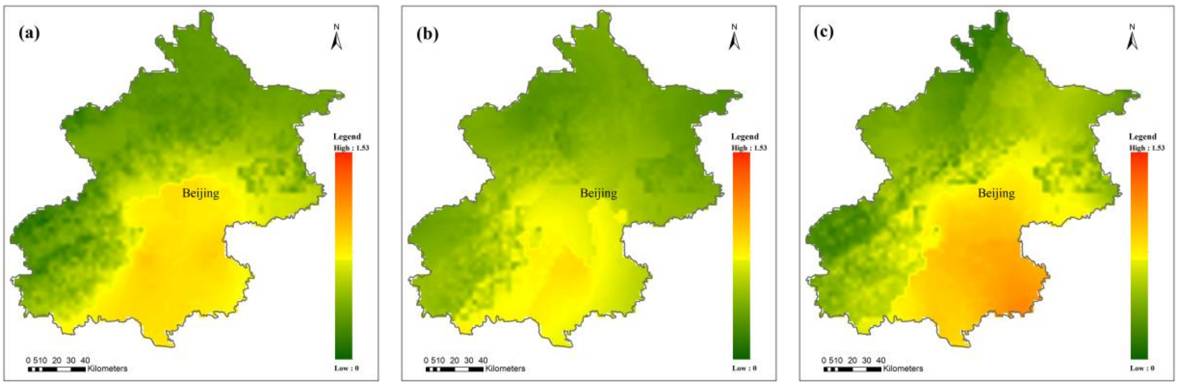

Figure 4 PCA-GWR prediction of monthly average AOD in 2015: (a) April, (b) May, (c) June

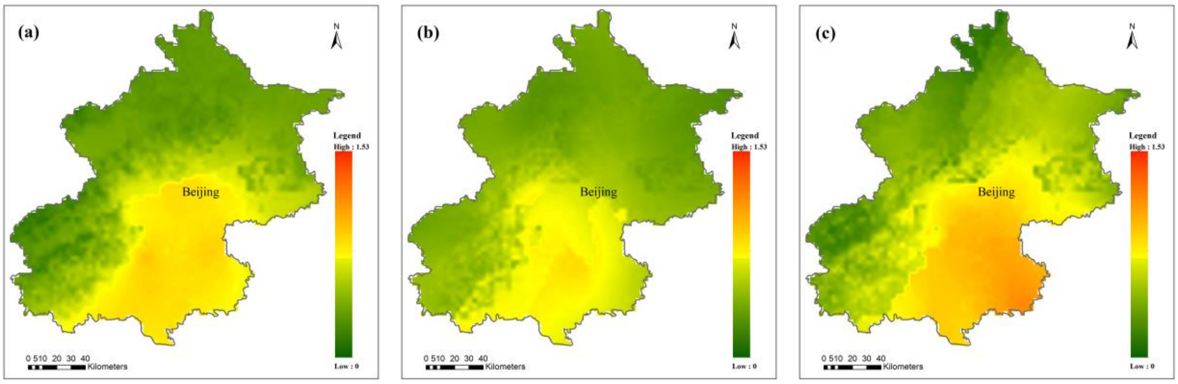

Figure 5 PCA-GTWR prediction of monthly average AOD in 2015: (a) April, (b) May, (c) June

Table 2 Comparison of the PCA-GWR and PCA-GTWR methods

Time	Model	MAE	RMSE	R^2	R_j^2
April	PCA-GWR	0.0761	0.1017	0.8530	0.8514
	PCA-GTWR	0.0705	0.0954	0.8705	0.8703
	Increase in PCA-GTWR prediction compared with that of PCA-GWR	7.36%	6.19%	2.05%	2.22%
May	PCA-GWR	0.0629	0.0806	0.8445	0.8424
	PCA-GTWR	0.0587	0.0757	0.8628	0.8627
	Increase in PCA-GTWR prediction compared with that of PCA-GWR	6.68%	6.08%	2.17%	2.41%
June	PCA-GWR	0.1087	0.1411	0.8090	0.8064
	PCA-GTWR	0.1059	0.1376	0.8185	0.8184
	Increase in PCA-GTWR prediction compared with that of PCA-GWR	2.58%	2.48%	1.17%	1.49%

Figures 4 and 5 show that the overall distribution trend of the monthly average AOD in April, May, and June 2015 using PCA-GWR and PCA-GTWR is consistent, with only a small number of regions having relatively obvious differences. From April to June, the distribution trend of the AOD in the southeast of the study area went from high to low and then from low to high. The distribution trend of the AOD in other areas did not change much from April to May, while the distribution trend from May to June was obvious. Table 2 shows that the values of the MAE, the RMSE, R^2, and R_j^2 obtained by using PCA-GTWR to estimate the monthly average AOD in April, May, and June 2015 are better than those obtained by PCA-GWR. This shows that the PCA-GTWR method provides more accurate estimates of the AOD than the PCA-GWR method. The PCA-GTWR method proposed in this paper uses PCA to analyze the explanatory variables and expresses the principal components as linear combinations of the original data. It can effectively eliminate multicollinearity and reflect more of the original index information with fewer PCs. It can reduce the loss of raw data information and improve the dimensionality reduction effect and the accuracy of the model's estimated AOD concentration. Additionally, the method incorporates the spatiotemporal characteristics of the data into the regression model, effectively solves the spatiotemporal nonstationarity problem of the regression model, and demonstrates its superiority in estimating the AOD.

The PCA-GWR method predicts the monthly average AODs in April, May, and June 2015 and the monthly average monitored AODs for linear regression. The PCA-GTWR method predicts the monthly average AODs in April, May and June 2015 and the monthly average AODs for linear regression analysis. The resulting graph, fitting equation and Pearson value obtained by regression analysis are shown in Figures 6 and 7. The regression coefficients and Pearson's r data values obtained by the PCA-GTWR method are greater than those obtained by the PCA-GTWR method, so the PCA-GTWR method has the best linear fit between the predicted AOD and the monitored AOD.

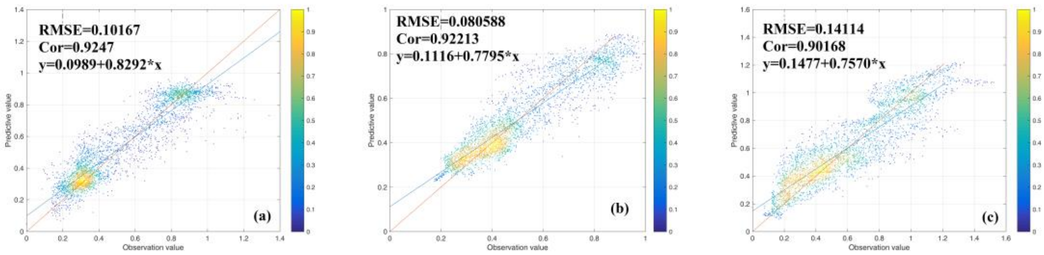

Figure 6 Regression analysis of the PCA-GWR prediction of AOD compared with the monitored AOD: (a) April, (b) May, (c) June

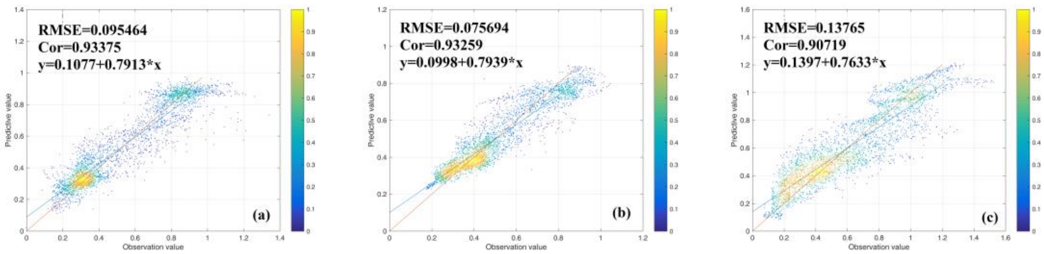

Figure 7 Regression analysis of the PCA-GTWR prediction of AOD compared with the monitored AOD: (a) April, (b) May, (c) June

5. CONCLUSIONS

With the aim of predicting the AOD in Beijing, this paper proposes geographically and temporally weighted regression with principal component analysis (PCA-GTWR), which makes full use of the advantages of both geographically and temporally weighted regression and principal component analysis. PCA was used to conduct dimensionality reduction on 6 explanatory variables of the meteorological data and geographical data to obtain several principal components. Each PC was expressed as a linear combination of the original data, and fewer PCs were used to reflect more of the information from the original index than would have been possible with previous methods. The first three PCs obtained were input as dependent variables to the GTWR model to predict the AOD. The spatial and temporal characteristics of the AOD were considered in the regression model, which effectively solved the problem of the spatial and temporal nonstationarity of the regression model and improved the accuracy of the model's predicted AOD. The results show that the PCA-GTWR method is better than the PCA-GWR method in estimating the monthly average AOD.

The PCA-GTWR model proposed in this paper has high accuracy in predicting the value of the AOD. This method represents the PCs as linear combinations of the original data and enhances the dimensionality reduction effect while effectively addressing the spatiotemporal nonstationarity of the AOD. PCA-GTWR can predict the value of the AOD, and it can also be applied in research fields involving data that are nonstationary in space and time (such as house prices in different regions, $PM_{2.5}$, soil moisture, and climate change), thereby improving the accuracy of data prediction in different fields and reducing the workload of the prediction process.

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