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Spatial modeling of $PM_{2.5}$ concentrations using an optimized land use regression method in Jiangsu, China

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Abstract. Land use regression method (LUR) has been recognized as a promising way to predict surface air pollutants concentration and spatial distribution of them globally. While linited studies have been conducted in China, especially in rather large areas. We therefore promoted an optimized LUR method which refined the predictor variables and improved the regression modeling method for $PM_{2.5}$ spatial distribution in Jiangsu, China. Firstly, the integrated predictor variables which combined the total emission, distance to the monitoring station and wind direction are used to explore a more appropriate expression of variables e.g. pollution from point sources and line sources (traffic). The results showed that a model generated by integrated variables (R^2=0.52) outperformed that generated by traditional variables (R^2=0.34). Secondly, we compared the method of geographically weighted regression (GWR) which reflect the influence of geographical location on the effect of regression process with traditional multivariate linear regression (MLR) method. The model comparison results suggested that the overall prediction accuracy is significantly improved by 19% when using GWR model (R^2=0.62). Furthermore, the spatial distribution map of predicted $PM_{2.5}$ concentrations from GWR model was definitely finer than that from MLR model. It can be concluded that more appropriate expression of variables and the GWR modeling could definitely improve LUR modeling prediction accuracy. This study would not only demonstrate the applicability of the optimized LUR models in large geographical areas, but also support for fine population exposure studies in the future.

1. Introduction

In 2013, many parts of China experienced an unprecedented smog crisis. Fine particulate matter, or $PM_{2.5}$, had become a focal word in China. $PM_{2.5}$ refers to particles whose aerodynamics equivalent diameter is less than 2.5 μm in ambient air. $PM_{2.5}$ is easy to adsorb toxic substances and has long residence time and long transport distance in the atmosphere, which has a great impact on human health and atmospheric environment[1;2]. This phenomenon has aroused the government's and the whole society's concern about air pollution. To deal with and solve this environmental problem arising mainly from $PM_{2.5}$, China's State Council issued the Action Plan for Air Pollution Prevention and Control in September 2013, which pointed out the air quality goals for the next five years and some specific targets.

Numerous environmental epidemiology studies have shown that exposure to $PM_{2.5}$ pollution is kind of associated with cardiovascular and respiratory diseases and consequently increased mortality [1;3]. In addition, epidemiological studies launched in China estimated high health effects incurred by $PM_{2.5}$

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pollution[4;2]. Although some epidemiological studies concerning air pollution e.g. $PM_{2.5}$ have been kindly successfully carried out in China during these years, for finer human health effects data, more accurate exposure concentration estimates are especially needed.

Many models were used to simulate the spatial distribution of pollutant concentration, such as spatial interpolation, atmospheric diffusion simulation, remote sensing inversion and land use regression (LUR) models[5]. LUR modeling is a multivariate regression modeling method based on air quality monitoring station observation concentration and its surrounding geographical predictor variables that commonly include land use, population, traffic, meteorological and local pollution data[5]. LUR models were widely used all over the world. The earliest prediction area is Europe, and later it was extended to North America, Asia, etc. The predicted pollutants include NO_2, NO_X, particulates(PM_{10}, $PM_{2.5}$ and UFP), BC and some organic matters[6-10]. With the improvement of research methods, the deepening of research theory, the improvement of data availability and precision, and the development of GIS software, LUR models have become one of the most commonly used methods to assess air pollutants exposures in epidemiologic studies. [6;11].

After 20 years of development, the LUR models still had two main limitations. One was the deficiency of irregular selection of characteristic variables and uncertain expression of variables, which lead to insufficient explanatory power of the model[5]. Concerning the very reality of China, the $PM_{2.5}$ pollution from Point sources deserved more attention than the other areas in the world. Some previous studies have tried putting point sources predict variables into LUR models, but the precise expression of this variable have not been identified[12;13]. Learning from a former study carried out by Chen in Tianjin, integrated independent variables were used in this study to explore a more appropriate expression of variables e.g. pollution from point sources and line sources (traffic)[14]. The other was that the traditional method of multivariate linear regression (MLR) could not reflect the influence of geographical location on the effect of regression. The technique of GWR is a variant of MLR with a weight function included, which only takes the samples within a defined neighbourhood (band width or number of samples) into calculation and also may weigh the contributions of closer samples more than those farther away [15]. GWR has obvious advantages over MLR in spatial data analysis and spatial mapping because it takes into account the spatial nonstationarity of the relationship between variables[16;17]. It is necessary to probe into the method of geographically weighted regression (GWR) for the optimization effect of the model.

Jiangsu Province is a developed and polluted area , and few researchers have studied the spatial distribution of $PM_{2.5}$ exposure in this area. We therefore promoted an optimized LUR method which refined the predictor variables and improved the regression modeling method for $PM_{2.5}$ spatial distribution in Jiangsu. This study made up the gap in the study of $PM_{2.5}$ spatial distribution in Jiangsu Province, and laid a foundation for further study on population exposure.

2. Materials and methods

Annual average $PM_{2.5}$ concentrations from routine air quality monitoring stations and the selected predictor variables were combined to develop LUR models in Jiangsu Province.

2.1. $PM_{2.5}$ concentration data

There are 97 routine air quality monitoring stations being distributed among Jiangsu Province, the types of them include urban accessing stations, regional accessing stations, background stations, source impact stations and traffic stations. Two of these 97 stations were deleted in this study owing to lack of partial monitoring data during the study time. Finally the daily $PM_{2.5}$ concentration measurement of 95 stations (Figure 1) from 1 January 2015 to 31 December 2015 were selected as the study data. Each station had more than 27 daily mean concentration in a month and more than 324 daily mean concentration in a year, which conformed to the rule of data validity. For each station, all daily mean concentration measurements were averaged to calculate the annual average.

2.2. Predictor data for LUR models

Considering the selection experience of variables in previous studies and the reality of this study, there were five types of predictor variables included in the process of modeling[5]. Table 1 shows the selected predictor variables, and the priori hypotheses made for LUR model developing, including the unit, buffer sizes, transformations and the priori defined direction of effects of the variables[18].

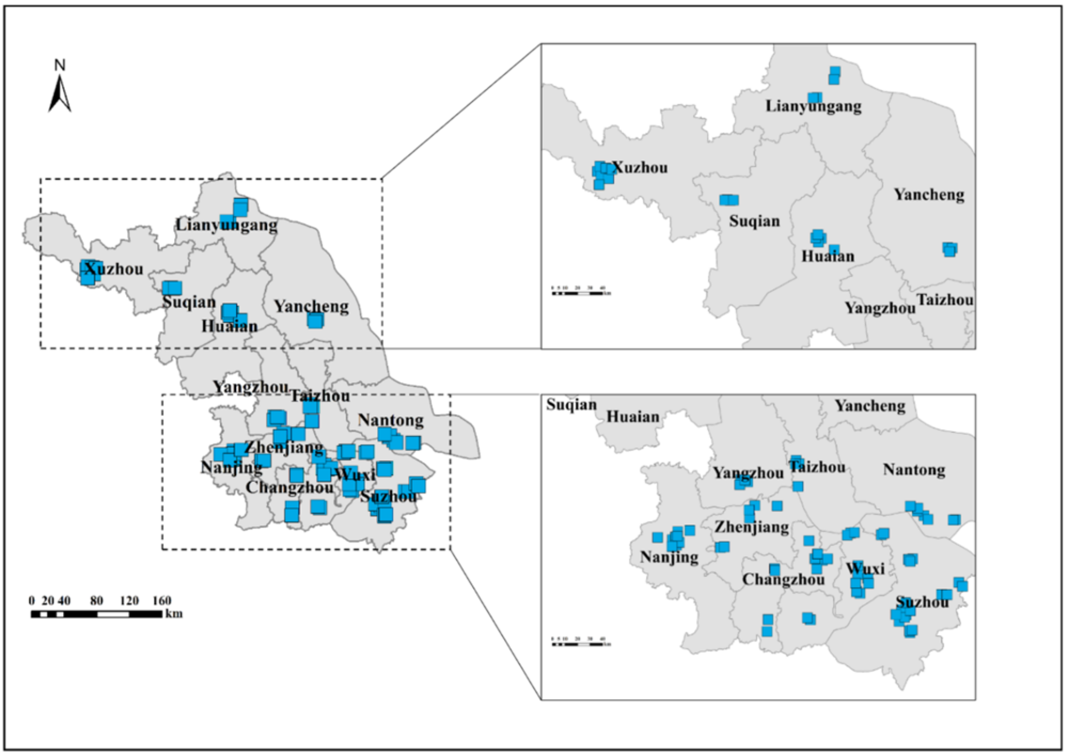

Figure 1. Air quality monitoring stations in Jiangsu Province.

2.2.1. Land use data. The Remote Sensing Monitoring data of Land use in China in 2015 were available from the Resource and Environmental Science data Center of the Chinese Academy of Sciences as a 30m grid database. The land use types of the national are divided into 6 primary (Urban and rural, Industrial and mining, residential land; Water area; Grass; Forest land; Cultivated land; and Unutilized land) types. Based on the national database, part of Jiangsu Province was extracted from the whole country. The area of each type of land-use was calculated in buffers of 100, 300, 500, 1000, 2000, 3000m.

2.2.2. Population density data. The population density data were available from the Ministry of Civil Affairs of the People's Republic of China. Administrative divisions are compiled according to the information of the national administrative divisions at or above the county level approved by the State Council, ending on December 31, 2015. The population of administrative districts at or above the county level in 2015 came from the National Bureau of Statistics of the people's Republic of China. Population density data (in 10,000people/km2) of each air quality monitoring station used population density data of the district or county where it set as a proxy.

2.2.3. Meteorological data. The meteorological data of 23 Meteorological observation stations distributed over the Jiangsu Province were available from National Meteorological Information Center. 365 daily observation data of air pressure, wind speed, relative humidity and precipitation of each station were averaged to calculate the annual average. Meteorological data of observation station nearest to air quality monitoring station were used as the proxy of meteorological data of this air quality monitoring station.

2.2.4. Point source pollution data. Point source pollution data were available from Jiangsu Province key Monitoring Enterprise Self-monitoring Information Publishing platform. Only the State key Supervision and Control Enterprise of exhaust Gas in Jiangsu Province in 2015 were considered as the waste gas pollution sources. After investigation and confirmation, 6 of total 194 State-controlled enterprises shut down in 2015, and 13 enterprises were lack of monitoring data, finally the annual emission of NO2, SO2 and soot of 175 enterprises were used as the proxy of PM2.5. Learning from a former study carried out by Chen in Tianjin, integrated independent variables are used in this study to explore a more appropriate expression of variables of emission from point sources and line sources (traffic)[14]. To synthetically account for the distance of the monitoring station and wind direction relative to the point source, the PSIndex was calculated (Figure 2) .The point source variables were calculated in buffers of 3, 5, 7, 10, 13 and 15km.

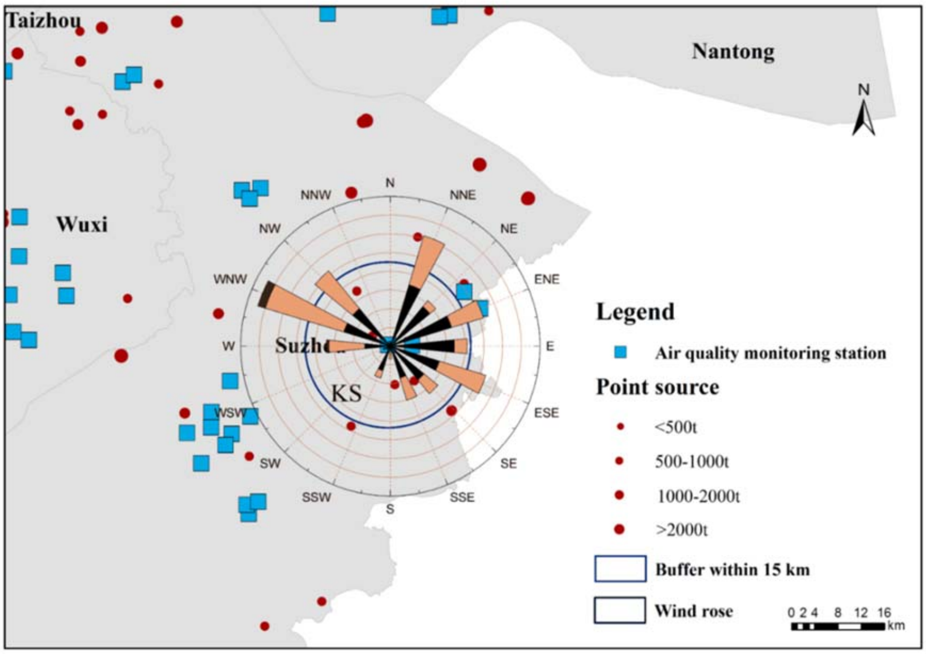

Figure 2. Point sources within 15 km buffer and the wind speed and frequency rose at the Kunshan Experimental Primary School monitoring station in 2015.

2.2.5. Road traffic data. Road traffic data of Jiangsu Province in 2015 were available from National Geomatics Center of China. Only 5 main classe s of roads were considered as the study data, which were Express way, Trunk road, Main road, Minor road and Ordinary street. Similar to the idea of PSIndex calculation, the LSIndex was calculated[14]. The road traffic variables were calculated in buffers of 50, 100, 150, 200, 300, 400 and 500m.

2.3. Model development

2.3.1. Multiple linear regression modeling. Variables in the Distance to the nearest point source.

Emission of point source and Integrated point source variable were considered as mutually exclusive point source variables and combined with other variables respectively to construct models for $PM_{2.5}$, the same rule to three variables of Road Traffic[17]. According to the previous research experience, there are two kinds of model building algorithms, one is backward algorithm, the other is forward algorithm[5;19]. The former modeling method is used here in this study.

Table 1. Predictor variables uesd to build models.

Variable classification	Predictor variable	Variable name	Unit	Buffer size (radius of buffer)	Transformation	Direction of effect
Land Use	Industrial and mining land	INDUSTRY	m^2	100, 300, 500, 1000, 2000, 3000m	NA	+
	Residential land	RESIDENCE				+
	Water area	WATER				-
	Grass land	GRASS				-
	Forest land	FOREST				-
	Cultivated land	CULTIVATION				NA
Population Density	Population density of administrative districts or county	POP	10,000 people/m^2	using population density data of the district or county where monitoring station set as a proxy	NA	+
Meteorological Element	Precipitation	PRCP	mm	using meteorological data of observation station nearest to monitoring station as a proxy	NA	-
	Air pressure	PRS	hPa			NA
	Relative humidity	RHU	1%			-
	Wind speed	WP	m/s			-
Point Source	Distance to the nearest point source	DIS TO PS	km		Inverse distance	+
	Emission of point source	EMISSION	t	3, 5, 7, 10, 13, 15km	NA	+
	Integrated point source variable	PSINDEX	-			+
Road Traffic	Distance to the nearest road	DIS TO ROAD	m		Inverse distance	+
	Road length of major roads (5 classes)	ROADLENGTH	m	50, 100, 150, 200, 300, 400, 500m	NA	+
	Integrated line source variable	LSINDEX	-			+

NA is not applicable
Variable name: Combining variable name with buffer size

2.3.2. Geographically weighted regression modeling. Geographically weighted regression model (GWR) is based on multivariate linear regression model and adds the influence of geographical location to regression parameters[20]. Multivariate linear regression model is essentially a global regression model, while GWR is a local regression model, which could generate the specific regression parameters at each monitoring station[16]. The Geographically Weighted Regression tool in ArcGIS 10.2 software was used to build the model. GWR is a linear model with the same preconditions as MLR, the same variables remained in the final MLR model were used in the GWR modeling. In the process of modeling, due to the uneven distribution of monitoring stations in Jiangsu Province, the adaptive Gaussian kernel function was used to specify the nearest neighbor number and the Akaike Information Criterion (AICc) was adapted to identify the scope of the nucleus.

2.4. Model validation
Cross validation (CV) methods are often used to verify the final model in case of model overfitting. Considering the relatively few monitoring stations[21], Leave-one-out cross validation (LOOCV) method was applied here. In addition, mean prediction error (MPE), mean relative prediction error (MRPE, defined as the MPE divided by the mean observed $PM_{2.5}$ concentration) and root mean square error (RMSE) were employed to evaluate the model prediction accuracy[16].

3. Results and discussion
LUR Modeling have been operated in several areas over the world during the last 20 years. As the development of geographic information technology and availability of sources of data, LUR modeling were gradually used in large scale regions[11]. The researchers applied such models in some areas in China in the last 10 years[14;13]. However, prior to this, there have been no relevant researches carried out in Jiangsu Province. This study was the first time that LUR model was used in the whole area of Jiangsu Province. This study tried to improve the expression of variables (point source, road traffic) by calculating integrated variables. Besides, considering the spatial heterogeneity and nonstationarity of geographical prediction factors, traditional global regression statistical method (MLR) may be not the best way to model. To explore a better way to establish a LUR model, this study compared MLR and GWR modeling methods especially.

3.1. Predictor variable selection
Bivariate correlation analysis was used to explore the correlation between predictive variables and $PM_{2.5}$ concentration. Strong correlation variables were selected from many influencing factors for model building. In this study, the correlation strength was set as the only index to determine the contribution of characteristic variables to the spatial variation of concentration[22]. In order to reduce the collinearity of same type variables with different buffer radius in the subsequent multivariate linear regression, only the variables of the same type with the highest correlation with $PM_{2.5}$ concentration were retained, and other similar variables were removed. After a series of screening processes, 7 valid predictor variables were left behind (Table 2).

Among the 7 valid predictor variables, PSINDEX_15km ranked the highest correlation of 0.697, which was conformed to the reality that major sources of $PM_{2.5}$ in Jiangsu are industrial emissions, coal combustion et al. The second highest correlated variable was EMISSION_13km, and the correlation between it and annual $PM_{2.5}$ concentration was 0.585, which is lower than that of integrated variable (PSINEX_15km). The degree of correlation between the other predictor variables and the concentration was consistent with previous studies[23;19]. For example, population agglomeration increased $PM_{2.5}$ concentration, water reduced pollution to a certain extent, and meteorological factors such as relative humidity and wind speed were negatively correlated with $PM_{2.5}$ concentration. Variables in the Emission of point source and Integrated point source variable were considered as mutually exclusive point source variables and combined with other variables respectively to construct models for $PM_{2.5}$. The adjusted R^2 of the two models were 0.34 and 0.52 respectively, and the PSINDEX model was 0.18 higher than the EMISSION model. The relatively higher R^2 suggested that point source integrated variables would partly improve the explanatory power of the model. Final regression equation remained 3 predictor variables, POP, WATER_500 and PSINDEX_15km. Higher population density and higher PSINDEX induced higher $PM_{2.5}$ concentration, while more water area would reduce $PM_{2.5}$ concentration contrarily.

Table 2. A summary of valid predictor variables.

Effective predictor variables	Mean	Std. Deviation	Pearson correlation	P value
POP	0.26	0.37	0.204	0.047
RHU	74.98	2.62	-0.313	0.002
WP	2.15	0.35	-0.211	0.040
INDUSTRY_100	1.88	7.47	0.205	0.046
WATER_500	27.68	116.41	-0.202	0.050
PSINDEX_15km	23.52	32.82	0.697	0.000
EMISSION_13km	1635.43	1925.88	0.585	0.000

3.2. Model fitting, validation and comparison

After stepwise multivariate linear regression, three predictor variables entered the final regression equation in this study (Table 3). The final 3 predictor variables were POP, WATER_500 and PSINDEX_15km for MLR and GWR models. It can be seen from the table that the adjusted R^2 was 0.52 and 0.62 for MLR and GWR model respectively, and the latter is about 19 % higher than the former. In general, when the difference between the two models' AICc values is greater than 3, the model with lower AICc value will be considered as a better model[16;22]. The AICc value of GWR was 7.6 lower than that of MLR, which definitely meant that GWR model performed better. Residuals should be randomly distributed in space and not clustered. The Moran's I was adopted to evaluate the spatial autocorrelation of residuals, and the smaller absolute value of Moran's I is, the lower the spatial autocorrelation of residual is. GWR model outperformed MLR model by a smaller Moran's I (0.069).

Table 3. The final regression results and evaluating indicators of MLR and GWR model.

Model	Predictor variables	Adjusted R^2	AICc	Moran's I
MLR	POP, WATER_500, PSINDEX_15km	0.52	515.5	0.178
GWR		0.62	507.9	0.069

Figure 3 shows the model fitting and LOOCV results of the MLR and GWR models. For the MLR and GWR models, the model fittings adjusted R^2 values were 0.52 and 0.62 respectively, and the latter is about 19 % higher than the former. Besides, the MPE of GWR model was 0.5 lower than that of MLR model, and similarly was the MRPE. The RMSE of both models were relatively lower compared to previous studies, and GWR model performed better than MLR model by a lower RMSE (2.85). For LOOCV results, the LOOCV R^2 of MLR was 0.38 which was much lower than model fitting R^2 (0.52). However, the LOOCV R^2 of GWR was only 0.02 lower than that of model fitting. The LOOCV results of MPE, MRPE and RMSE all indicated that GWR model outperformed MLR model.

3.3. Prediction maps of $PM_{2.5}$ concentrations

The lowest concentration of Figure 4(a) and Figure 4(b) was 49.0μg/m^3 and 45.8μg/m^3 respectively. Figure 4(a) had a highest concentration of 76.7μg/m^3, while that of Figure 4(b) was 75.0μg/m^3. The total mean $PM_{2.5}$ concentrations of the two maps were 55.1μg/m^3 and 55.0μg/m^3 respectively. The upper and lower limit values of the two maps were similar, and the mean values were almost equal, which indicated that the global prediction accuracy of the two models was similar.

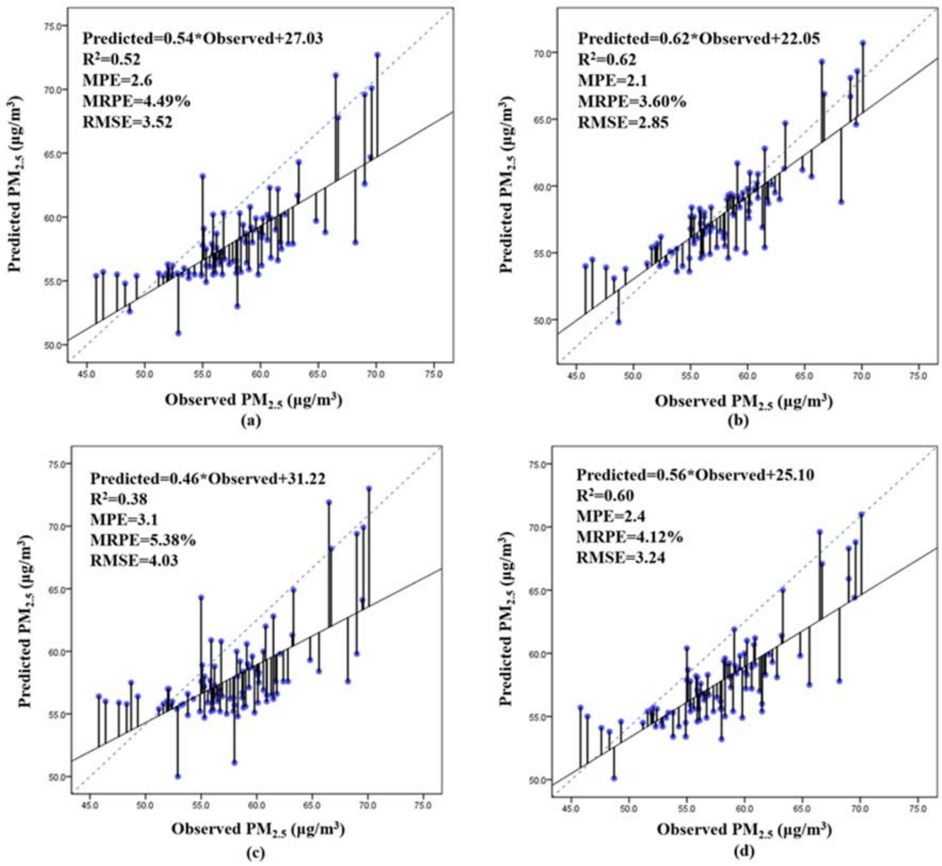

Figure 3. (a) MLR model fitting results; (b) GWR model fitting results; (c) MLR model LOOCV results; (d) GWR model LOOCV results.

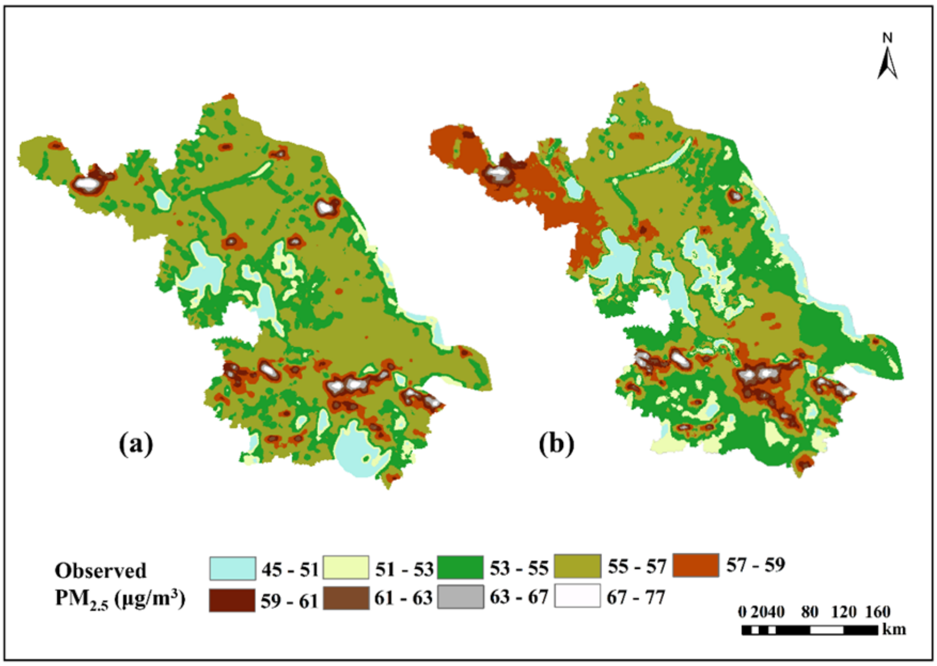

Figure 4. Prediction maps of $PM_{2.5}$ concentrations for the MLR and GWR models. (a) Prediction map for the MLR model, (b) Prediction map for the GWR model.

However, the spatial distribution map of predicted $PM_{2.5}$ concentrations from GWR model was definitely finer than that from MLR model, especially some certain areas. For northern part in Jiangsu, the map from MLR model showed a steady trend of concentration distribution, while the results from GWR model highlighted a high concentration area mainly around Xuzhou. The explanation for this phenomenon might be that there were more pollution sources in this area, resulting in a more significant pollution agglomeration effect. Compared with the global regression, the local regression highlighted this kind of agglomeration effect[2;17]. For southern part, especially for the area of Taihu Lake, tha map from GWR model showed higher concentration than that from MLR model. Similarly, although the Taihu Lake water body would reduce the pollution to a certain extent, it is worth noting that the area around the Taihu Lake water body has dense pollution sources, and which meant a pollution agglomeration effect. The local regression of the GWR model highlighted such an agglomeration effect, resulting in such a high concentration phenomenon[16].

In general, the northern parts had lower $PM_{2.5}$ concentrations except the area of Xuzhou where a lot of industries were located. In more detail, concentration was higher in the urban area or populated area than suburb area or sparsely populated area, which was corresponding to the fact that population density had a positive effect on concentration[5;22]. Most of the low-concentration areas occured in areas rich in water area, such as Taihu Lake, Gaoyou Lake and Hongze Lake. However some areas with low population density still suffered from high $PM_{2.5}$ concentration, mostly due to the industries located around these areas discharging a large amount of atmospheric pollutants. Compared to other predictor variables, point source variables (industry) had higher influence owing to the quantity and not very effective regulation[24].

4. Conclusions

In this study, we calculated integrated point source variables and integrated road traffic variables by combining emission from industries, length of main roads, wind frequency and distance to the industries or the roads. According to the results of integrated variable model and regular emission model, a model generated by integrated variable (R^2=0.52) outperformed that generated by emission(R^2=0.34). Furthermore, we compared a GWR modeling approach with traditional MLR model by evaluating the prediction accuracy of $PM_{2.5}$ concentration in Jiangsu Province. The adjusted R^2 of GWR and MLR models were 0.62 and 0.52 respectively, and the former was about 19% higher than the latter. In addition to the R^2, all other evaluation indicators (MPE,MRPE and RMSE) showed that the GWR model was superior to the MLR model. The prediction map of annual $PM_{2.5}$ concentration in Jiangsu Province in 2015 showed that the territory of the entire Jiangsu Province below the ambient air quality secondary standard. Although air quality in Jiangsu Province has improved under some pollution prevention and control measures, there is still a long way to go to reach ambient air quality primary standard. All the results suggested that more appropriate expression of variables and the GWR modeling could definitely improve LUR modeling prediction accuracy.

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