Meteorological and Environmental Research 2017, 8(3): 1 -4, 9 Editor: Yang Yingying Proofreader: Yang Yingying

A Review of Methods of Studying the Spatial Distribution of Atmospheric Pollutants

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Abstract Characteristics of studies on the spatial distribution of atmospheric pollutants are shown as follows: the main object of the studies in China is a single city instead of a region and the country; studying the spatial distribution of fine particulate matter becomes a hot spot presently; research methods have developed from traditional techniques into modernized techniques. Current methods of studying the spatial distribution of atmospheric pollutants mainly include spatial interpolation model, remote sensing method, land use regression model and BP neural network approach, *etc.* Each method has both advantages and disadvantages, and combining various methods to study the spatial distribution of atmospheric pollutants becomes a new problem that needs to be solved urgently.

Key words Atmospheric pollutants; Spatial distribution; Research methods

DOI 10.19547/j.issn2152 -3940.2017.03.001

With the rapid development of urbanization in China, environmental problems caused by urban expansion have become important factors restricting healthy, orderly and coordinated development of cities, especially the deterioration of atmospheric environmental quality. Scientifically, accurately and quantitatively describing the situation of atmospheric environmental quality in a city to provide scientific reference for the implementation of effective and scientific urban environmental management and future urban development planning has become key problems of current assessment of atmospheric environmental quality and related studies. Scientifically and accurately describing the spatial distribution of air pollutant concentration in a city is one of bases and cores of atmospheric environmental quality assessment, planning and management, as well as a difficulty in research of atmospheric environmental quality in a city presently[1]. The way to monitor atmospheric environment at a fixed point is often adopted internationally to obtain the pollution situation of a city, and the observation results of a monitoring point can reflect pollutant concentration around the monitoring point instead of the pollution situation of the whole city and its spatial difference. Therefore, how to obtain the continuous spatial surface of pollution in a city based on the monitoring data of pollutant concentration at discrete monitoring points is also a key problem that needs to be solved urgently[2].

Received: February 3, 2017 Accepted: May 15, 2017

Supported by the Major Research and Development Plan of Shandong Province, China (2015GSF117032); Scientific Research Foundation of Binzhou University (BZXY1501); Major Subject of Binzhou University (2015ZDL03).

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1 Characteristics of studies on the spatial distribution of atmospheric pollutants

1.1 The main object of studies is a single city instead of a region and the country in China The main object of studies on the spatial distribution of atmospheric pollutants in China is a single city instead of a region and the country. The spatial distribution of atmospheric pollutants in Beijing, Tianjing, Wuhan, Chongqing, Urumqi, Lanzhou, Hangzhou and Jinan have been studied[3-21]. In addition, the spatial distribution of atmospheric pollutants in Beijing City, Tianjin City, and Hebei Province, five cities (Mianyang, Deyang, Chengdu, Meishan, and Leshan cities) in Chengdu Plain, Jiaodong Peninsula, the Pearl River Delta region, many key cities in China[22-31].

1.2 Studying the spatial distribution of fine particulate matter becomes a hot spot presently $PM_{2.5}$ refers to particulate matter that is smaller than or equal to 2.5 μm in diameter in the atmosphere, and it is called fine particulate matter. $PM_{2.5}$ size is small and rich in toxic and harmful substances, so it can cause respiratory diseases and lung cancer[32-33], so it has become one of the most important object of prevention and control of environmental pollution in various countries in the world. Among atmospheric pollutants, the spatial distribution of sulfur dioxide, nitrogen oxides, total suspended particulates, and PM_{10} was mainly studied at the early period. After China has monitored and issued data of $PM_{2.5}$ concentration in main urban monitoring points since 2013, research of spatial distribution of $PM_{2.5}$ has become a hot spot.

1.3 Research methods have developed from traditional techniques into modernized techniques Traditional methods of studying the spatial distribution of atmospheric pollutants include combining surface observation data and isoline drawing technology and establishing models of atmospheric motion in small and middle cities[34]. The two traditional methods have certain defects. The former has disadvantages of high cost and too long study period in terms of setting and observation of monitoring points in the early period and result output in the late period. The latter often make achievements lose representative significance.

Geographic information technology is a new peripheral discipline integrating geography, geometry and computer science, as well as a computer system that collect, store and manage, analyze and process, show and output spatial information and attribute information. It can combine a variety of information about natural processes and human societal activities with spatial position, distribution and relationship by digitization[35], so it is very suitable for research of problems in the field of environmental science[36]. In recent years, the development of GIS technology has provided new technological means for simulating the spatial distribution of atmospheric pollutants.

2 Methods of studying the spatial distribution of atmospheric pollutants

2.1 Spatial interpolation model Air pollution is prominent in China presently. With the transformation of pollution sources from a single pollution source to several pollution sources, air pollution has shown regional and complex features, and data of discrete atmospheric environmental monitoring points can not reflect the continuous change of regional air quality. Using spatial interpolation to realize visualization of spatial distribution of air quality is an important method to analyze characteristics and regional distribution trends of air pollution. In China, spatial interpolation algorithm has been widely applied in fields of geology, medicine, building, environment and meteorology, but its application in the spatial distribution of atmospheric pollutants was started relatively late.

Commonly used spatial interpolation methods mainly include inverse distance weighted interpolation (IDW), completely regularized spline (CRS), ordinary Kriging (OK), indicator Krining (IK), and radial basis function (RBF). The method IDW is a deterministic local interpolation method[37], and the distance between an interpolation point and an actual observed sample point is used as weight; the contribution of weight is in inverse proportion to the distance. The method CRS, a spline function interpolation method using mathematical functions as theoretical foundation, uses the functions to approximate to surfaces, produces a curve with a second-order continuous derived function based on data of the known sample points, and estimate the attribute value of an unknown point according to the curve. The method OK means that unbiased optimal estimation of regionalized variables is conducted in a limited region Based on variation function theory and structural analysis, and it is one of main contents of geostatistics. It is complex, and many model parameters are adjustable; it is needed to set up parameters according to properties of regionalized variables. The method IK is the most commonly used non-parametric geostatistics method, in which indicator functions are studied instead of regionalized variables[38-39]. This method does not depend on stationarity of space phenomena, does not demand that regionalized variables follow certain distribution, and dose not need to reject abnormal values. To realize the algorithm of RBF, based on Green's function interpolation, the linear combination of Green's functions around various sampling points is used to constitute an interpolating surface, and the weight of each point is regulated to make the surface pass through each sampling point; the quantity of Green's theorems can be smaller than that of data points, so interpolating curves will not be matched with inaccurate data points, and they can be solved by using least square method; the quantity of model parameters is adjusted to make the fitted standard deviation equal to the standard deviation of original data.

At present, these methods have been widely used to study the spatial distribution of atmospheric pollutants in China. For instance, Meng Jian *et al.*[3] used indicator Krining to study the spacial variability characteristics of SO_2 concentration. Zhao Wenhui *et al.*[7] adopted indicator Krining to simulate and analyze the spatial and temporal variation of $PM_{0.3}$, $PM_{3.0}$ and $PM_{5.0}$ in Beijing City in the heating period from 2007 to 2009 based on geostatistics. Based on the optimization algorithm of inverse distance weighted interpolation, the visualization of air quality is realized[40]. By using the geostatistical analysis tool of GIS and ordinary Kriging, Zhao Wenhui also simulated the spatial distribution of $PM_{0.3}$, $PM_{0.5}$, $PM_{1.0}$, $PM_{3.0}$ and $PM_{5.0}$ and analyzed the spatial distribution characteristics of inhalable particles in the atmosphere within the Fifth Ring Road in Beijing City[5]. Zhao Chenxi *et al.*[13] used ordinary Kriging to analyze the temporal and spatial distribution of $PM_{2.5}$ and PM_{10} mass concentration in winter and spring in Beijing. By using ordinary Kriging, Li Zhan *et al.*[16] studied the spatial distribution of average mass concentration of SO_2、NO_2、PM_{10} and $PM_{2.5}$ in Beijing City in the November of 2012. Liu Yanyue *et al.*[41] used inverse distance weighted interpolation to optimize the interpolation model of ordinary Kriging and proposed an interpolation model based on inverse distance weighted interpolation to study the spatial distribution of $PM_{2.5}$ concentration in the atmosphere. By using the spherical model, circular model, exponential model, and Gaussian model of inverse distance weighted interpolation, spline function method and ordinary Kriging, Liu Yongwei *et al.*[24] conducted the spatial interpolation of API in 120 cities of China and crosscheck of the interpolation results, and the results show that the circular model of ordinary Kriging had good interpolation effect. Based on the monitoring data of atmospheric pollutants at 667 environmental monitoring stations in 118 key cities of China from November to December in 2013, Pan Jinghu *et al.*[27] adopted the spherical model, circular model, exponential model, and Gaussian model of inverse distance weighted interpolation, radial basis function, spline function method and ordinary Kriging to carry out spatial interpolation of NO_2, PM_{10}, $PM_{2.5}$ and SO_2 concentration to determine the best interpolation method. By using inverse distance weighted interpolation, spline function method and ordinary Kriging, Ding Hui *et al.*[42] conducted spatial interpolation of atmospheric pollutants ($PM_{2.5}$, SO_2, O_3, NO_2 and CO) in the Pearl River Delta region and adopted cross validation method to analyze the error of interpolation results. Liu Jie *et al.* [12,15] used radial basis function and MATLAB to study the spatial distribution of $PM_{2.5}$ and PM_{10} mass concentration at 35 monitoring stations in Beijing City in the spring of 2013.

2.2 Remote sensing method In traditional studies of atmospheric pollutant concentration, the measured concentration of a pollutant was often obtained from scattered sampling points (like an environmental monitoring site) and was used to represent the average level of the pollutant in a region. Current urban air monitoring sites are built according to administrative division, and most of them are distributed in administrative centers instead of the geographic center of each administrative region, so point-source data are less representative.

Using satellite remote sensing images to conduct inversion of spatial distribution of atmospheric pollutant concentration is a good complement to surface observation, thereby making up the disadvantages of monitoring atmospheric pollutant concentration caused by the quality position of observation points. For example, by using regression analysis and with the aid of spatial modeling function of ERDAS, Wang Xiaoxia[17] and Wei Wei *et al.* [43] carried out inversion of spatial distribution characteristics of NO_2 concentration in the atmosphere in Lanzhou City.

2.3 Land use regression model Based on multiple linear regression method, Briggs *et al.* [44] simulated the spatial distribution of NO_2 concentration in Amsterdam and other cities of Europe, and called the method Regression Mapping. This method has been widely used to simulate the concentration of pollutants such as $PM_{2.5}$ and NO_2 by researchers in Europe and America and is called Land Use Regression (LUR) model[45-46]. LUR model is established based on the correlation between the spatial distribution of atmospheric pollutants and geospatial elements like land use, and ground survey data and data of geospatial elements at monitoring points are used to build regression equations and then derive the regression relation to other regions that are not monitored, thereby simulating the spatial distribution of pollutants[47]. The spatial distribution of atmospheric pollutant concentration correlates with pollution sources, terrain, land cover, land use and other geospatial elements.

For instance, Chen Li *et al.* [6,48-49] used LUR model to simulate the spatial distribution of PM_{10} and NO_2 concentration in Jinan and Tianjin cities. Based on LUR model, Jiao Limin *et al.* simulated the spatial distribution of $PM_{2.5}$ concentration in Wuhan City. By using ArcGIS platform and LUR model, Wu Jiansheng *et al.* [20] simulated the spatial distribution of $PM_{2.5}$ concentration in Chongqing City based on data of land use, road network, DEM and population. Han Ruiying *et al.* [21,29] used LUR model to simulate the spatial distribution of $PM_{2.5}$ concentration in Hangzhou City and Zhejiang Province. Xu Gang *et al.* [30] adopted LUR model to simulate the spatial distribution of $PM_{2.5}$ concentration in Beijing, Tianjin and Hebei Province.

2.4 BP neural network approach BP artificial neural network means that interpolation is conducted in high dimensional space. It is composed of three layers of neurons, including input layer, hidden layer and output layer. Each layer is composed of large quantities of disconnected simple neurons. Neurons in the input layer transmit the input data to the hidden layer, and then the data are activated, magnified and transmitted to the output layer. Finally, the data are exported by the output layer. Moreover, data information can not be transmitted between neurons in the same layer. However, when actual error exceeds anticipation error, error values spread along the network reversely to revise link weight and threshold between neurons and train the network repeatedly until meeting anticipation error, thereby determining the mapping relation between input and output. The transfer function between input and hidden is S-type transformation function, and the transfer function between hidden and output is pure linear transformation function.

In recent years, neural network algorithm and its improved algorithm have developed gradually and have been used to predict the concentration and changing trend of atmospheric pollutants in a city[50]. By using multi-layer neural network and linear regression method, Perez *et al.* [51] predicted the hourly average concentration of $PM_{2.5}$ in a city, and the results show that neural network method is superior to linear regression method. Grivas *et al.* [52] used genetic algorithm and neural network approach to predict the hourly average concentration of PM_{10}, and the results reveal that neural network method is superior to multiple linear regression method. By using ordinary Kriging interpolation and BP artificial neural network, Wang Min *et al.* [10] predicted the daily average mass concentration of $PM_{2.5}$.

3 Conclusions and discussion

The above methods to study the spatial distribution of atmospheric pollutants have advantages and disadvantages. Spatial interpolation means approximation function is established to estimate pollutant concentration at other monitoring stations based on the data of atmospheric pollutant concentration at monitoring stations. The method has advantages of simple principle, convenient operation, and wide application range, but data of many observation points are needed. In regions with lack of observation data of atmospheric pollutants, the method has no prediction function, and changes in the extreme concentration of a pollutant can be magnified easily.

Remote sensing method covers a wide area, but images in any interested time can not be obtained under the limit of imaging time phase[53]. Moreover, spatial resolution is low presently, and it is difficult to meet the demands for discerning the spatial distribution of atmospheric pollutant concentration in a city.

Establishment of land use regression model means based on the observation data of atmospheric pollutant concentration and geographic elements at air quality monitoring sites, atmospheric pollutant concentration at any spatial point in the study area is predicted by using the least square method. The method has advantages of considering complete factors and wide use range, high estimation accuracy and spatial resolution. However, this method still has disadvantages of uncertain driving factors, not normative choice of variables, poor capacity of temporal and spatial migration of the model.

BP neural network is one of neural network models that have been applied most widely at present. The network can study and store the mapping relation between input and output of a model, and does not need to reveal the mathematical equations that can be used to describe the mapping relation. Its learning rule means that steepest descent method and back-propagation are combined to regulate the weight and threshold of network until its error is the minimum. In comparison with ordinary Kriging, BP neural network has certain advantages in terms of predicting atmospheric pollutant concentration and can overcome the problem of reducing prediction accuracy of atmospheric pollutant concentration in low-value regions by prediction accuracy of extremely maximum value, so its prediction effect is superior to that of ordinary Kriging.

It is clearly seen that each method has advantages and disadvantages, and combining various methods to study the spatial distribution of atmospheric pollutants becomes a new problem that needs to be solved urgently.

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