Prediction of particle level behavior in atmospheric air based on laws of physics of motion and geographic interpolation

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Abstract. Given the global problem of high levels of pollutants in the atmosphere, it is essential to use tools to measure and determine these levels. Unfortunately, it is impossible to have devices that allow direct pollutants' direct measurements in a place of interest. Due to this limitation, in this work, a computer tool was developed to predict contaminants' behavior and their concentration levels in a reliable way. In this methodology, equations of the physics of motion were implemented to predict particles' behavior in a given area and an interpolation technique based on the Kriging method. In the initial stage, a preliminary analysis of the pollution data of the city of Bogotá, Colombia, downloaded from the Air quality monitoring network of Bogotá, Colombia, was performed. In the next stage, the variables of most significant interest in the analysis were defined, and the data to be characterized is explored. Finally, the selected method's calculation algorithm is implemented in Python, taking an ArcGIS library as a programming reference. From the results, it was possible to determine the contaminants' levels for some regions of Bogota, Colombia, between values of 0.067 to a maximum weight of 0.4039 μg/m³, for January 2013.

1. Introduction
Implementing different techniques for the processes of energy conversion and transport has always contributed to the increase of pollutants in the air [1]. High contaminants are often found in areas with high vehicle traffic [2], industrial zones, and nearby regions [3]. Generated a considerable impact on people's health and the environment. About the effect on people's health, different contaminating agents can be related, such as CO₂, CH, SOₓ, NOₓ, and particle matter (PM), represent the leading causes of damage to people's health and a valuable indicator for measuring air quality [4]. Faced with this problem, measuring and determining the levels of [5], represents an area of great interest as a way to guarantee and contribute to the continuous development of environmental management programs [6]. For this reason, being able to measure directly using measuring stations is one of essential for controlling direct and indirect sources of pollutant generation [7]. However, because of the limitation of having this equipment in all regions and the desired quantity, it allows the implementation of mathematical and statistical techniques to gain more and more importance as a practical and useful tool to determine the behavior of the pollutants in regions where it becomes indispensable to have some type of measurement of these agents [8]. Research on the development of tools and techniques to determine the level of contamination in a region includes Tegavarapu et al. [9] show in their study that geospatial interpolation methods can be applied as a faire as an accurate technique for predicting atmospheric variables. Beauchamp et al. [10] presented a geostatistical analysis based on the kriging method as a way of
determining pollution levels along roads. Morley and Gulliver [11], used the land use regression (LUR) technique to estimate exposure to air pollution for epidemiological studies. Shen et al. [12], present in their research various methods of interpolation, their characteristics and specific conditions for the numerous case studies. Highlighting within statistical methods, the kriging, which complies with the typology required for the research carried out in this study.

This research’s main contribution is based on the implementation of a methodology that uses the laws of the physics of motion and geographic interpolation to predict the behavior of particulate material in a given region. Based on this methodology, a mathematical model is established to analyze particle matter PM$_{10}$ in areas with no direct measurement systems. This model allows integrating Web tools and the geographic information system (GIS), to use time series models.

2. Methodology
This section shows each of the stages (Figure 1) used to analyze and predict the behavior of PM10 in the atmospheric air.

![Figure 1. Stages implemented for the analysis and prediction of PM10 in atmospheric air.](image)

In the first stage (Figure 1), the preliminary analysis seeks to understand and comprehend the characteristics that allow us to study the defined analysis phenomenon or requirements. In this stage, another interest is to organize, prepare the data, and establish the necessary criteria to guarantee the reliability report review to be carried out. Then we move on to the variable definition stage, where the variable most significant test interest or those that most significant most considerable influence on the study is identified. Next, the information is explored to identify and filter any data that present unusual behavior within the data set and that finally affect negatively, by generating deviations or errors in predicting the action of the PM$_{10}$. Once these stages of the work are completed, the interpolation method that best suits the requirements of the process and characteristics of the data sample to be analyzed is selected.

The method selected and used in this study is the Kriging, which is widely recognized for its geostatistical estimation potential that provides the most likely value of a non-experimental point attribute, with a high degree of accuracy [13]. Knowing the mathematical basis and technical aspect of the selected methodology, we precedent the calculation algorithm in Python of the method Kriging. From the implementation of algorithms from the ArcGIS library in Python. Once the Kriging method was applied, the simulations and processing of the data on the concentration of pollutants present in the atmospheric air were carried out. With the results obtained with the simulations in Python, the comparison of the real data collected from the Bogotá air quality monitoring network (RMCAB) and the data collected with the mathematical model developed in this work is carried out. To guarantee the highest precision of the prediction model developed.
It is essential to mention that the data used for this research was obtained from RMCAB, which provides information on the concentration of pollutants of anthropogenic and natural origin that regulate the atmosphere of the city of Bogotá, Colombia.

3. **Kriging method mathematical bases**

During the implementation of the kriging method, it is possible to assume that the regionalized variable is stationary (at least the central hypothesis is fulfilled). However, in many cases, the variable does not satisfy these conditions and is characterized by a trend. For example, in hydrology, the piezometric levels (an instrument used to measure compressibility coefficients of solids, liquids, and gases) of an aquifer may show an overall slope in the direction of flow [14]. To treat this type of variable, it is common to decompose the variable \( Z(s) \) as the sum of the trend, treated as a deterministic function, plus a stationary stochastic component of zero average. In this way, it can be assumed, as show the Equation (1) [14].

\[
Z(s) = m(s) + \varepsilon(s),
\]

with \( E(\varepsilon(s)) = 0 \) and \( V(\varepsilon(s)) = \sigma^2 \), and therefore, Equation (2).

\[
E(Z(s)) = m(s).
\]

The trend can be expressed by Equation (3).

\[
m(x) = \sum_{i=1}^{p} a_i f_i(s),
\]

where the functions \( f(s) \) are known, and \( p \) is the number of terms used to adjust \( m(s) \) and \( Z(s) \) the variable of interest measured at site \( s \). The Universal Kriging predictor can be expressed with Equation (4) [14].

\[
m(x) = \sum_{i=1}^{n} \lambda_i Z(s_i),
\]

where \( \lambda_i \) represents the coefficients for each observed value of the variable \( S_i \). To the Kriging method presented above, the correction factor is applied, as a way of considering the movement of the particles and their trajectories, expressed with Equation (5) [14].

\[
m(x)'_{PS(t+1)} = m(x) * (X_{jdst} + C_{jdst}).
\]

The term \( C_{jdst} \) is known as the correction factor based on the historical trend, which is expressed with Equation (6) [15].

\[
C_{jdst} = \sum_{i=1}^{\Omega} \frac{u_i (X_{jdst} - X_{jdst(0)})}{\sum_{i=1}^{\Omega} u_i},
\]

where the term \( X_{jdst} \) is associated with the displacement of the particles, described by Equation (7) [15].

\[
X_{jdst} = (X_{i+1} + Y_{i+1}).
\]

The Equation (8) is associated with the displacement of the particles in the longitude, associated with the displacement of the particles, considering the classical equations of motion [15].
\[ X_{i+1} = X_i + v \Delta t. \]  

(8)

The Equation (9) is associated with the displacement of the particles in the latitude, considering the classical equations of motion [15].

\[ Y_{i+1} = Y_i + v \Delta t, \]  

(9)

where \( X_i \) and \( Y_i \) are the position of the particle in a step time, \( v \) is the velocity of the particle, \( \Delta t \) is the period of time analyzed, \( J \) is each of the antennas in the inventory, \( D \) is the days of the week, \( T \) is the reading hours of the day and \( \alpha \) is the adjustment factor that must be between zero and one.

4. Results and discussions

Figure 2 shows the behavior of the distribution of particulate matter for Bogotá, Colombia, obtained for three simulation conditions of the Kriging method. In Figure 2, the particulate material's behavior for different simulation conditions of the Kriging method is shown, in blue the Kriging method considers the trajectory of the particle and the correction factor. In red, the Kriging method assumes only the revolution and the yellow color, corresponds to the results of the standard Kriging method. For the analysis shown in Figure 2, the data obtained from 13 fixed meteorological stations and one mobile station in the city of Bogotá, Colombia were used. Data, which represent the calculation base of the geographic interpolation model implemented in this work.

In Figure 2, the reference base from which to establish the error values shown, represent the real values of PM10 concentration, measured by meteorological stations. For the periods shown in the simulation, the Kriging method, considering the trajectory of the particles and the correction factor, presents the best predictions of the level of particulate material, of the selected region in Bogotá Colombia. This behavior can be corroborated by identifying that of the three conditions of the simulated method. For the evaluated time range, this method has more significant contact with the base of this graph's surface, representing the data obtained from the meteorological stations. Followed by the Kriging method that considers the trajectory.

![Figure 2. Prediction of particulate matter behaviors for Bogotá, Colombia.](image)

Figure 3 shows the behavior of contamination levels in Bogotá, Colombia. The data shown in Figure 3 corresponds to the graphic distribution of the action and distribution obtained with the calculation methodology implemented in Python, where the contamination levels obtained for the city of Bogotá, for January 2013, are shown. From the results obtained and shown in Figure 2, it is possible to determine that for the areas studied the contamination values; it is possible to observe that the concentration levels were between values of 6.7328 up to a maximum amount of 40.397 \( \mu g/m^3 \). At this stage, the prediction of February 2, 2013, was made based on data from January 28, 24, 21, and 7, 2013, to calculate the
correction factor. Thus, most of the analyzed areas are above the intermediate objective III defined by the world health organization (WHO) for PM$_{10}$ (30 μg/m$^3$) [16].

Finally, Figure 4 illustrates the distribution and behavior of the pollution level in the city of Bogotá, Colombia, applying the interpolation technique by the kriging method, implemented in Python. To identify the value of contamination in each area analyzed and shown in Figure 4, the colored bar defined in Figure 3 is used. Each value is determined based on the historical values obtained from the RMCAB database, and the interpolation calculations derived from the analysis carried out in this investigation. For these of the level of particulate material, shown in Figure 4, it is possible to observe that for the analyzed zone, almost in all of this the highest levels of particulate material reported were obtained, 40.397 μg/m$^3$, and only in small region values of 6.7328 μg/m$^3$ are obtained.

5. Conclusions
According to those described during the development of this research and based on the background, having tools that integrate web and GIS components are of great importance since they support decision making, considering the relative levels of pollution that directly affect health and the environment. For this reason, the main conclusion of this work is the implementation of a useful methodology, which can be used as a tool to predict the behavior of PM$_{10}$, based on historical data from contaminant measurement stations. Additionally, this methodology can be applied to predict the behavior of other types of pollutants present in the air. From the analysis carried out in this research, it was possible to identify in detail the regions of the areas under investigation, which exceeded the limits established by the WHO. Therefore, in this case, it is necessary to take preventive measures to control the level of pollutants for these sectors of Bogotá, Colombia and thus avoid more critical conditions. That can generate further deterioration of people's health and quality of life.
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