TEHRAN AIR POLLUTION MODELING USING LONG-SHORT TERM MEMORY ALGORITHM: AN UNCERTAINTY ANALYSIS

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ABSTRACT:

Air pollution is a major environmental issue in urban areas, and accurate forecasting of particles 10 µm or smaller (PM_{10}) level is essential for smart public health policies and environmental management in Tehran, Iran. In this study, we evaluated the performance and uncertainty of long short-term memory (LSTM) model, along with two spatial interpolation methods including ordinary kriging (OK) and inverse distance weighting (IDW) for mapping the forecasted daily air pollution in Tehran. We used root mean square error (RMSE) and mean square error (MSE) to evaluate the prediction power of the LSTM model. In addition, prediction intervals (PIs), and Mean and standard deviation (STD) were employed to assess the uncertainty of the process. For this research, the air pollution data in 19 Tehran air pollution monitoring stations and temperature, humidity, wind speed and direction as influential factors were taken into account. The results showed that the OK had better RMSE and STD in the test (32.48 ± 9.8 µg/m³) and predicted data (56.6 ± 13.3 µg/m³) compared with those of the IDW in the test (47.7 ± 22.43 µg/m³) and predicted set (62.18 ± 26.1 µg/m³). However, in PIs, IDW ([0, 0.7] µg/m³) compared with the OK ([0, 0.5] µg/m³) had better performance. The LSTM model achieved in the predicted values an RMSE of 8.6 µg/m³ and a standard deviation of 9.8 µg/m³ and PIs between [2.7 ± 4.8, 14.9 ± 15] µg/m³.

1. INTRODUCTION

Since the beginning of the 20th century, people have faced new problems and one of the most common health and environmental problems in developing and in some of the developed countries is the air pollution. Tehran, the capital of Iran, is one of the air-polluted cities in the world. Tehran is a large and rapidly growing metropolis (Statistical Center of Iran, 2021). In 2022, Tehran had just three days of clean air and had only 63 days of clean air during the last 3 years. The average annual concentration of particulate materials in the formation of fine particles 10 µm or smaller (PM_{10}) in Tehran has frequently exceeded the national and international air quality recommended limits (Tehran Municipality, 2023; Iran Ministry of Health, 2023). High levels of air pollution have posed a serious threat to public health. World Health Organization (WHO) data show that a significant rate of the global population breathes air that exceeds WHO guideline limits and contains high levels of pollutants, with low- and middle-income countries suffering from the highest exposures (WHO, 2023).

PM_{10} which is also called particle pollution, is a mixture of solid particles and liquid droplets found in the air. The source of particulate matter can vary, some particles are emitted directly from a source, such as construction sites, unpaved roads, fields, smokestacks or fires and most form in the atmosphere as a result of complex reactions of chemicals such as sulphur dioxide and nitrogen oxides, which are pollutants emitted from power plants, industries and automobiles (EPA, 2023). Particulate matters are an especially important source of health risks, as these very small particles that can penetrate deep into the lungs, enter the bloodstream, and travel to organs causing systemic damages to tissues and cells (WHO, 2023). In addition, the effect of particulate matter (PM_{10}) on human health has been well-documented as one of the most harmful air pollutants with long-term exposure, as they can cause pneumoconiosis, respiratory disease, cardiovascular disease, gestational diabetes mellitus and cause higher numbers of lung cancer (Ferreira et al., 2022; Prinz et al., 2022; Sun et al., 2022; So et al., 2022; Hvidtfeldt et al., 2021).

One way for protecting public health is to adopt smart environmental management policies through accurate monitoring and forecasting PM level. There are different types of air pollution monitoring, one of them is 'ambient air monitoring'. Ambient air monitoring typically uses fixed-location ground-based monitoring stations as geo-sensor networks (GSN). These stations use particulate monitor sensors which can continuously monitor PM at specific time intervals (EEA, 2020; Clements et al., 2022). Forecasting models are often classified into two categories including statistical and numerical models. Numerical models consider meteorological principles and mathematical methods which are based on atmospheric physical and chemical processes to simulate the air quality in vertical and horizontal

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dimensions at a large scale (An et al., 2001). Statistical air quality prediction models are data-driven models which do not use explicitly atmospheric processes (Yan et al., 2021). Researchers have frequently employed air pollution forecasting based on monitoring acquired data as time series (Andrii, 2022).

Recently, deep learning models have been applied to time series to forecast future air pollution levels. The results have confirmed reliable performance of air pollution forecasting in this type of data (Espinosa, 2022; Yan et al., 2021). Long Short-Term Memory (LSTM) model is one of the deep learning methods that has been regularly used. Some studies showed that this method is superior to traditional machine learning algorithms including support vector regression (SVR), gradient boosted tree regression (GBTR) and other traditional statistical models such as ARIMA (Autoregressive integrated moving average) (Yan et al., 2021; Hvidtfeldt et al., 2021; Jiang et al., 2020; Ma et al., 2019; Li, et al., 2017).

Sensors at monitoring sites sporadically cannot get concentration at random or specific times, and they do not save data because of device failure, broken sensors and other issues (Jangho et al., 2022; Laencina, 2009). Often spatially continuous data are required for environmental sciences and management. Therefore, scientists usually use spatial interpolation methods (SIM) to generate spatially continuous data retrieved from district monitoring stations (Ma et al., 2019). For this purpose, some studies have used inverse distance weighting (IDW) and ordinary kriging (OK) (Aldegunde, 2022; Bao et al., 2022; Ma et al., 2019; Zhao et al, 2018;). Air pollution spatial variability constitutes a significant source of uncertainty for environmental modeling. Assessing air pollution models has an important role in developing statistical models of climate change, agricultural and water resources management, and air dynamics (Bayat et al., 2021; Bui et al., 2018; Bui et al., 2023).

Quantifying the uncertainty associated with these predictions can assist the concerned decision-making processes and provide insights into the limitations of the employed models. Uncertainty analysis is a critical component in many fields of research, particularly those involving predictions and modeling (Gawlikowski et al., 2021; Psaros et al., 2023).

In the previous studies, the uncertainty assessment of the spatial interpolation for air pollution forecasting has been rarely reported (Ribeiro et al., 2016), seems researches not focused on impact of forecast on performance of SIM in the context of air pollution modeling and forecasting. Therefore it is vital to study the effect of forecasting on the interpolation models for better air pollution management, modeling and forecasting.

In this research, based on the type of data and previous studies we employed LSTM model for forecasting air pollution and investigated different interpolation methods performance in terms of uncertainty analyses in the spatial interpolation and how well uncertainty analyses can assist in assessing the implemented methods and forecasting models. The remaining parts of the paper is as follows. Section 2 focuses on the materials and the research methodology. Section 3 elaborates the research results. Finally, section 4 concludes the paper and suggests some directions for future research.

2. MATERIALS AND METHODS

In this section, the study area, employed data, LSTM model as the implemented deep learning model, as well as IDW and OK as SIM are discussed.

2.1 Data sources

The data used in this study consists of climatology data acquired every three hours and hourly PM_{10} air pollution concentration data obtained from January 2017 to June 2022. The climatology data was collected from 4 meteorological stations operated by Iran Meteorological Organization, located throughout the study area, and includes information on temperature, humidity, wind speed and direction as meteorological parameters (https://data.irimo.ir/). The hourly PM_{10} concentrations data was obtained from 19 ground-based monitoring stations operated by the Air Quality Control Company of Municipality of Tehran (http://air.tehran.ir/). Figure (1) illustrates the locations of the climatological and monitoring stations as well as Tehran megacity urban districts.

2.2 Study area

Tehran, the capital of Iran is divided into 22 urban districts. According to the 2021 census data, Tehran contains over 9 million urban residents (Statistical Center of Iran, 2021), and 10 million population related to daily immigrant (Amini et al., 2014). Climatologically, Tehran has a semi-arid climate, with hot summers and cold winters. Geographically, the city is situated at an altitude of 1200 meters above mean sea level, spreads from Latitude 35°35' N to 35°48' N and Longitude 51°17' E to 51°33' E. The city, surrounded by the Alborz mountain range to the north and desert areas to the south, and Jajroud road in the east.

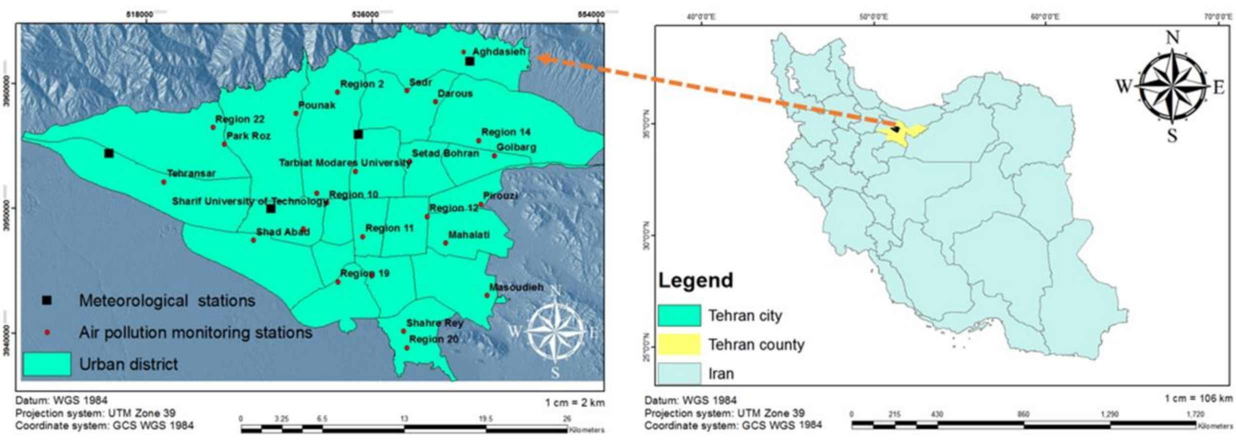

Figure 1. Study area and location of the climatological and air pollution monitoring stations and Tehran districts

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2.3 Long-Short Term Memory Model

LSTM model has shown promising results in predicting air quality levels based on historical data (Ma et al., 2019; Jiang et al., 2020). By utilizing historical air quality data and meteorological variables such as temperature, humidity, and wind speed, LSTM models can learn patterns and trends in the data and make reliable predictions for future time steps (Yan et al., 2021; Hvidtfeldt et al., 2021; Jiang et al., 2020;). LSTM model is a type of recurrent neural network (RNN) introduced by Hochreiter and Schmidhuber (1997) which has been successfully employed in modeling and forecasting time series data. LSTM models were specifically designed to overcome the limitations of traditional RNNs, such as the vanishing gradient problem, which occurs when the gradients used to update the network weights during training become too small, causing the network to stop the learning process. LSTM models were specifically designed to overcome this problem by introducing a memory cell that can selectively forget or remember information over time (Hochreiter et al, 1997; Nagabushanam et al, 2020). Activation function is a mathematical function applied to the weighted sum of the inputs to a neuron to determine its output in neural networks, which helps to determine whether the neuron should be activated or not (Han and Moraga, 1995; Vijayaprabakaran and Sathiyamurthy, 2022).
Figure (2) presents a LSTM network, every time step LSTM cells get time series data and can selectively forget or remember information over time. LSTM uses hidden and current states in the forecasting process. These cells are composed of three gates including input gate, forget gate, and output gate that control the flow of information into and out of the memory cell. The input gate determines the information to let into the cell, the forget gate decides the information to forget, and the output gate determines the information to output from the cell. The gates use sigmoid activation functions to control the flow of information, and a hyperbolic tangent activation function (tanh) to transform the cell state (Hochreiter et al, 1997; Sak et al, 2014; Nagabushanam et al, 2020).
The sigmoid activation function formulated as Eq. (1) (Fathi and Maleki Shoja, 2018) and hyperbolic tangent formulated as Eq. (2) (Fathi and Maleki Shoja, 2018):

$$\mathrm{f(z)} = \sigma(z) = \frac{1}{1+e^{-z}} \qquad (1)$$

$$\tanh(z) = \frac{2}{1+e^{-2z}} - 1 = 2\sigma(2z) \qquad (2)$$

where z, is the value of input.

2.4 Spatial Interpolation Methods

Spatial interpolation is a method used to estimate unknown values at a particular location based on the values observed at known locations. There are two broad categories of spatial interpolation methods including deterministic and stochastic methods, while deterministic interpolation methods assume a deterministic relationship between the known and unknown points, stochastic methods take into account the statistical distribution and spatial correlation of the data being interpolated (Tan and Xu, 2014; Zhao et al, 2018;). In this study, we have employed two popular interpolation methods to produce PM_{10} maps based on the forecasted data retrieved from the LSTM model using the acquired data at each Tehran Municipality air pollution monitoring stations. We employed Inverse Distance Weighting (IDW) and Ordinary Kriging (OK) methods based on the results achieved in some previous research (Tan and Xu, 2014; Roberts et al., 2004; Ma et al, 2019; Oliver and Webster, 2014; Ding et al., 2018).

Inverse Distance Weighting: Inverse Distance Weighting (IDW) is a deterministic interpolation method. IDW estimates the value at a target location by assigning weights to the known data points based on their distance from the target location, assuming that the value at a target location is inversely proportional to its distance from the known data points (Ma et al, 2019; Roberts et al., 2004). Using IDW for spatial interpolation is supported by Tobler's first law of geography which indicates that "everything is related to everything else, but near things are more related than distant things" (Tobler, 1970). In IDW, $Z_{(x_0)}$ is the estimated value at a target location (x_0). $Z_{(x_i)}$ is the known value at surrounding data points (x_i). IDW can be calculated using Eq. (3) (Roberts et al., 2004), where λ_i is the weight assigned to the i_{th} target location, which is quantified using Eq. (4) (Roberts et al., 2004):

$$Z_{(x_0)} = \sum_{i=1}^{n} \lambda_i Z_{(x_i)}\,, \qquad (3)$$

$$\lambda_i = \left|d_{(x_i,x_0)}\right|^p \sum_{i=1}^{n} \left|d_{(x_i,x_0)}\right|^p\,, \qquad (4)$$

where, $d_{(x_i,x_0)}$ is Euclidian distance between the target location and the data point. The parameter p determines the degree of influence of the surrounding data points on the estimated value at the target location (Roberts et al., 2004; Ma et al, 2019).

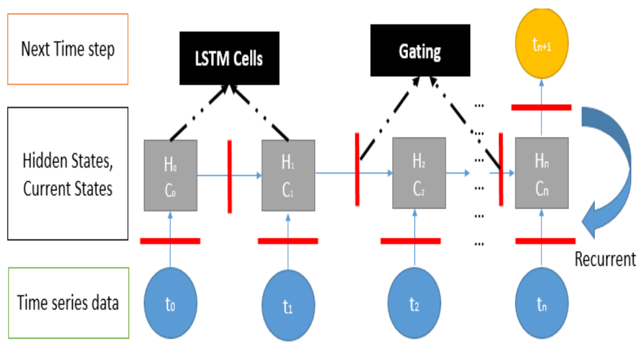

Figure 2. LSTM network adapted from Hamad et al. (2021)

2.4.1 Ordinary Kriging: Ordinary Kriging (OK) is a stochastic method used for spatial interpolation, which assumes that the underlying spatial structure of the data can be modeled by a spatial autocorrelation function (Ding et al., 2018).
This geostatistical method uses a linear combination of the weighted values. The weights are determined by the spatial autocorrelation function and the covariance between the target location and the surrounding data points. This basic geostatistics assumption (Oliver and Webster, 2014) is formulated as Eq. (5):

$$Z_{(x)} = \mu_{(x)} + \varepsilon_{(x)} \qquad (5)$$

where, $Z_{(x)}$ is the woody cover variable (density, species), decomposed into a random autocorrelated variations form, ε(x), at location x and a deterministic trend, μ(x) (mean of the process).

3. RESULTS

Our study confirmed that integrating spatial interpolation and LSTM forecasting model can be a useful method to produce a

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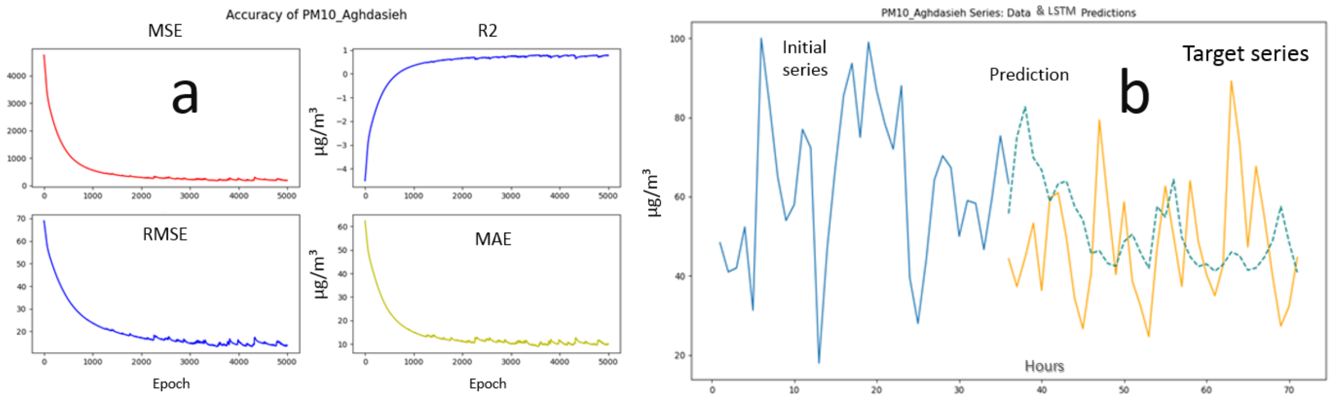

Figure 3. (a) Accuracy of air pollution at Aghdasieh station, (b) predicted test values.

map based on air pollution ground-based monitoring stations. IDW and OK were used on the interpolated data to predict air pollution concentration at unknown points. By completing the learning time series for each station and adding meteorological parameters as feature, LSTM model has been implemented by Python programming using Keras library as an interface for the TensorFlow library. We found that the LSTM model with two hidden layers of 256 units with batch size of 1000 and 5000 epochs achieved the best performance. Statistical indices including Mean Absolute Error (MAE), Mean Square Error (MSE), Root Mean Square Error (RMSE) (Chai and Draxler, 2014) and R-Squared (R^2) (Weisberg, 2005) were calculated to evaluate the model in training of the monitoring stations according to Eqs. (6, 7, 8 and 9).

$$MAE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i) \quad (6)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad (7)$$

$$RMSE = \sqrt{MSE} \quad (8)$$

$$R^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \quad (9)$$

where, $\bar{y}_i$ is the mean of the observed data, n = number of observations, y_i = actual value, and $\hat{y}_i$= predicted value.

Date	MSE (µg/m³)	RMSE (µg/m³)
2022-05-21	602.044	5.765
2022-05-22	321.693	4.143
2022-05-23	336.846	4.382
2022-05-24	12722.429	27.207
2022-05-25	6998.291	20.916
2022-05-26	197.283	3.199
2022-05-27	66.529	1.604
2022-05-28	56.711	1.529
Mean	2662.72	8.60
STD	4701.69	9.80

Table 1. MSE and RMSE of the predicted PM_{10}

Figure (3.a) illustrates Aghdasieh air pollution station among the stations employed as an example of training LSTM model on the station where R^2 has increased over time with increasing epochs in which MSE, RMSE, and MAE have decreased with the learning model. Figure (3.b) shows the predicted and main train data. In addition, we evaluated the uncertainty of the LSTM model using prediction intervals (PIs), Mean and Standard Deviation (STD). Prediction interval (PIs) (Eq. 10) is a place where is expected as a future value to fall (Tian et al., 2020). Mean (Eq. 11) is the average of a set of values (Manikandan, 2011) and Standard Deviation (STD) (Eq 12) is dispersion of a set of values (Batanero et al, 1994).

$$PI = \hat{y}_i \pm t\left(\frac{a}{2}, n-2\right) * \sqrt{MSE\left(1 + \frac{1}{n} + \frac{(y_i - \bar{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}\right)} \quad (10)$$

$$Mean = \frac{\sum_{i=1}^{n} y_i}{n} \quad (11)$$

$$\text{Standard Deviation } (STD) = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}{n-1}} \quad (12)$$

where, t(a/2, n-2) is the critical value of the t-distribution for a given significance level (α), degrees of freedom for the error assessment.

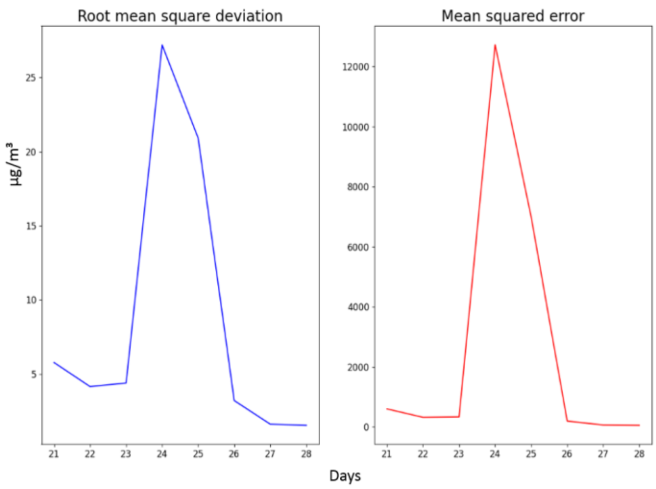

Figure 4. MSE and RMSE of the air pollution prediction using LSTM during May 21-28, 2022

The PIs were calculated using the quantile regression method with a 95% confidence level, the inclusion of PIs, STD and Mean is important for understanding the uncertainty associated with the model predictions and can be useful for the concerned decision-making in practical applications. According to Tables (1, 2) and Figure (6), we developed a LSTM prediction air pollution deep learning model with a RMSE of 8.6 ± 9.7 µg/m³ and PIs between [2.7 ± 4.8, 14.9 ± 15] µg/m³ with 95% confidence level. Then, we performed spatial interpolation methods on the predicted and source data. For this purpose, we split data to train (70%) and test (30%) then calculated RMSE based on the two categorized data.

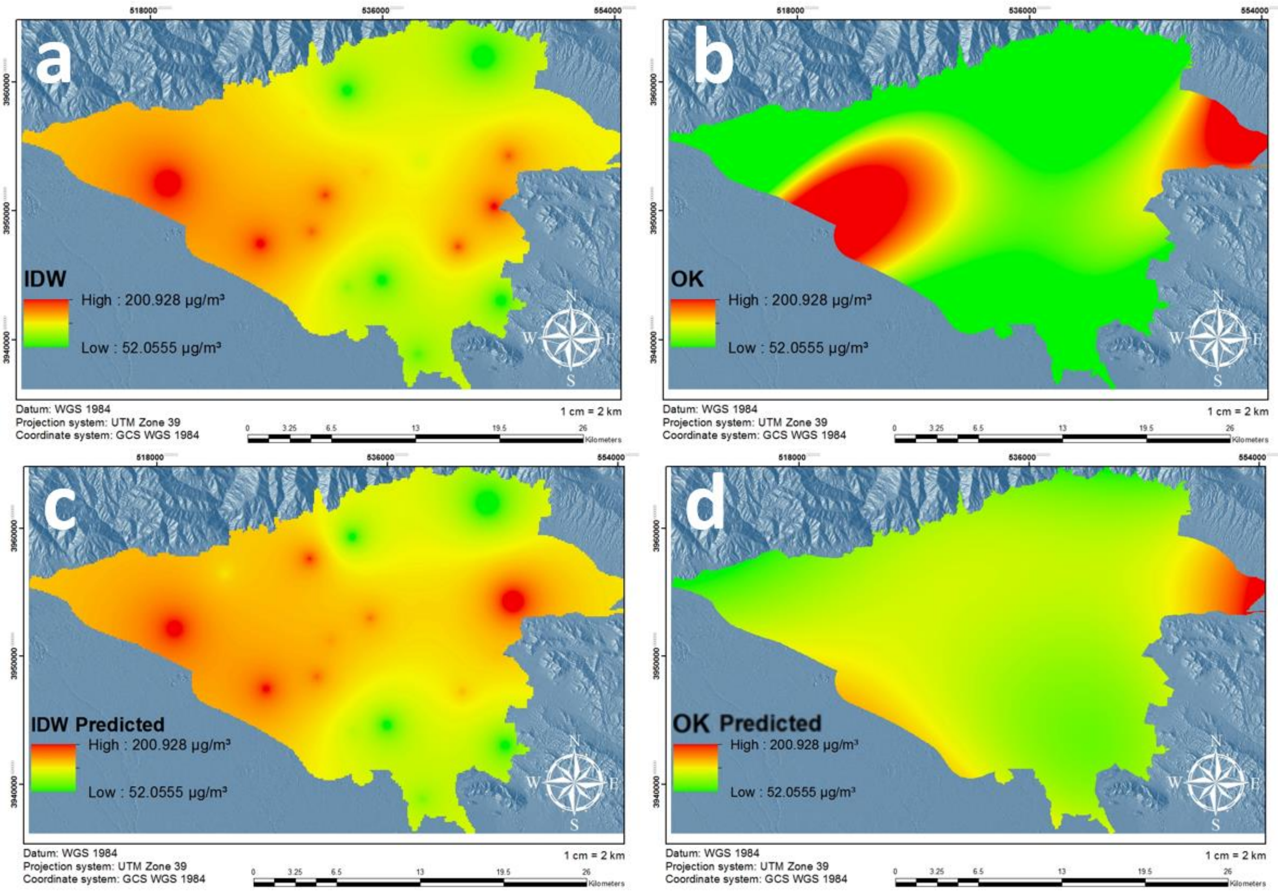

Figure 5. Air pollution map of mean of the 8 days on the test set using IDW (a), OK (b) and on the test set using IDW (c), OK (d)

Date	Upper band (µg/m³)	Lower band (µg/m³)
2022-05-21	10.53	0.843
2022-05-22	9.267	0
2022-05-23	9.484	0
2022-05-24	45.223	9.191
2022-05-25	30.266	11.566
2022-05-26	6.705	0
2022-05-27	3.49	0
2022-05-28	3.349	0
Mean	14.80	2.70
STD	14.96	4.80

Table 2. PIs of the predicted PM_{10} over the 8 days.

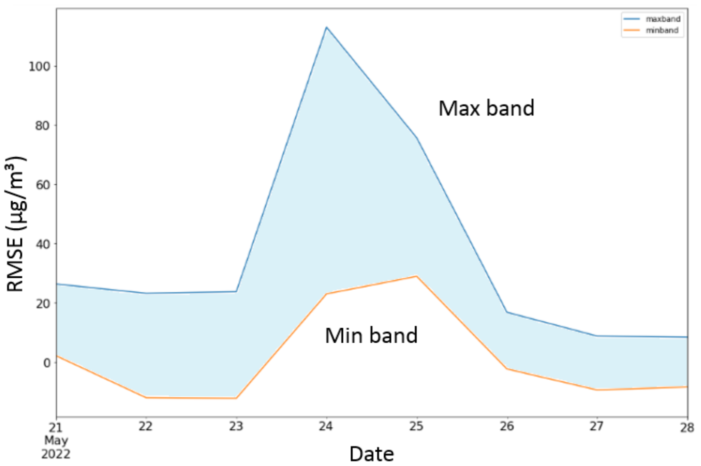

Figure 6. 95% confidence level shows with light blue color over the 8 days between upper and lower bands of the PIs.

According to Table (3), we used OK interpolation method with a RMSE of 32.48 ± 9.8 µg/m³ on test data, RMSE of 56.6 ± 13.3 µg/m³ on the predicted data and according to Table (4), PIs of this method is [0, 0.5] µg/m³.

Date	Test Data (µg/m³)	Predicted Data (µg/m³)
2022-05-21	25.276	48.931
2022-05-22	30.336	45.824
2022-05-23	22.668	41.988
2022-05-24	31.383	67.55
2022-05-25	20.562	80.261
2022-05-26	45.511	63.181
2022-05-27	45.361	59.094
2022-05-28	38.666	46.042
Mean	32.471	56.609
STD	9.783	13.251

Table 3. RMSEs of OK interpolation methods of the predicted PM_{10}.

Based on the results shown in Table (5) we used IDW interpolation method with a RMSE of 47.7 ± 22.43 µg/m³ on the test data, RMSE of 62.18 ± 26.1 µg/m³ on the predicted data and according to Table (4), PIs of this method is [0, 0.7] µg/m³.
We visualized a continuous representation of the air pollution data using ArcMap 10.4.1, as illustrated in Figure (5).

SIM	Lower Band (µg/m³)	Upper Band (µg/m³)
OK	0	0.475
IDW	0	0.662

Table 4. PIs of IDW and OK based on RMSE of the interpolated test and predicted data

Date time	Test Data (µg/m³)	Predicted Data (µg/m³)
2022-05-21	86.472	103.657
2022-05-22	62.139	82.402
2022-05-23	65.73	82.689
2022-05-24	40.104	36.436
2022-05-25	31.74	49.367
2022-05-26	47.992	59.244
2022-05-27	24.067	57.935
2022-05-28	22.93	25.659
Mean	47.647	62.174
STD	22.429	26.015

Table 5. RMSEs of IDW interpolation methods of the predicted PM_{10} over the 8 days.

According to Figure (7) in initial days OK have better accuracy on the test and predicted data, however, later on OK provides better performance on the prediction in both test and predicted data.

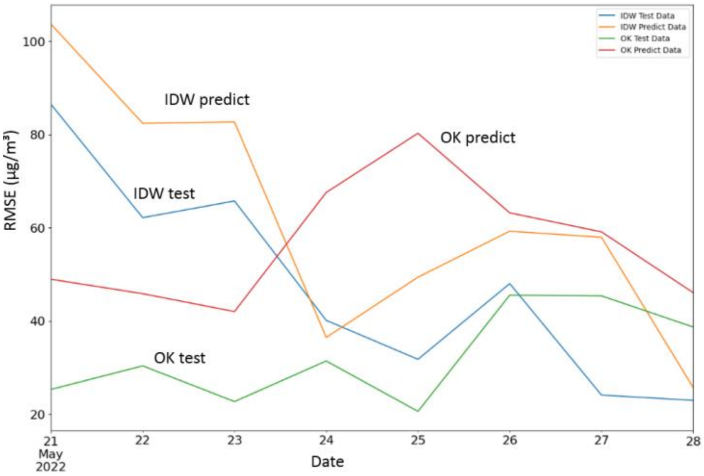

Figure 7. RMSEs of OK and IDW interpolation of the test and Predicted PM_{10} (µg/m³)

4. CONCLUTIONS AND FUTURE DIRECTIONS

WHO (2023) and some other studies (Ferreira et al., 2022; Prinz et al., 2022; Sun et al., 2022; So et al., 2022; Hvidtfeldt et al., 2021) have emphasized that air pollution is a critical issue globally. Tehran Municipality and Iran Statistical Center data confirm that Tehran megacity and its inhabitants are suffering from the highest exposures to air pollution. On the other hand, PM_{10} is among the air pollutants that can lead to serious health issues. For these reasons, it is important to predict the level of air pollution to take precautionary measures and informed management policies for public health. Therefore, knowing the error and reliability of the air pollution prediction model should be considered in the Municipal environmental management policies. In this study, air pollution maps were produced by implementing a deep learning model, LSTM, based on the interpolated data using IDW and OK. In addition, the uncertainty of the methods was assessed using PIs, STD, RMSE and Mean.
LSTM model has been also implemented for predicting the level of air pollution and producing air pollution maps using the SIM in previous studies (Bao et al., 2021; Ma et al., 2019; Yan et al. 2019), however, assessing the uncertainty of the model have not yet been extensively reported in the previous research. In this research, we have considered the uncertainty assessment of the air pollution predictions. According to the achieved results in this study, the LSTM model has had better learned over time (Figure 3). With the increased learning time, R-squared has been closer to 1 and MAE, MSE, as well as RMSE have been closer to 0. The predicted values had an RMSE of 8.6 and a standard deviation of 9.8 µg/m³ and PIs between [2.7 ± 4.8, 14.9 ± 15] µg/m³, indicating some degree of uncertainty in the model predictions.
OK have better RMSE and STD in the test (32.48 ± 9.8 µg/m³) and predicted data (56.6 ± 13.3) than those of IDW in the test (47.7 ± 22.43) and predict set (62.18 ± 26.1), however, in PIs IDW ([0, 0.7]) compared to those of the OK ([0, 0.5]) has better performance.
The reason behind the uncertainty of LSTM model can be limited training data which is essential for forecasting air pollution and model complexity can effect on generalization capability (Hochreiter et al, 1997; Sak et al, 2014; Nagabushanam et al, 2020). Spatial variation and model assumptions which based on spatial covariance structure, the weights assigned to neighbouring data points and spatial stationarity can affect OK uncertainty model (Oliver and Webster, 2014; Ding et al., 2018). And data density and distribution and parameter selection can be some source of the uncertainty of the IDW model (Tobler, 1970; Roberts et al., 2004).
Both of the employed interpolation methods presented a higher PM_{10} concentration in southwest and northeast of Tehran megacity in the air pollution map.
The major strength of this research was using LSTM as a deep learning model for air pollution predicting and spatial interpolation using IDW and OK for modelling and uncertainty assessment. There were some limitations in this study such as the lack of comparison of the results with other deep learning models like gated recurrent units (GRUs). On the other hand for uncertainty assessing, we can use of other methods for example Monte Carlo simulation (Basil and Jamieson, 1999), and Bayesian inference (Oakley and O'Hagan, 2002) for get other assessing test values. Also we can implementation of other interpolation methods such as inverse multiquadric (IMQ) and radial basis Function (RBF) (Ding et al., 2018; Jiang et al., 2020), which using these method can give us better view for answer the questions like what model could be better for forecasting air pollution time series, which model can have better performance in SIM and which one assess method is better for have good view of uncertainty of models, these questions will be considered in our future research.

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