Prediction of particulate matter concentrations using LSTM networks model

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Abstract
Particulate matter (PM) is a major contributor to air pollution, and exposure to its harmful effects at elevated levels poses a significant risk to human health. Therefore, it is of considerable practical importance for air quality monitoring, air pollution restoration, and human health to have an accurate prediction of PM concentration. Traditional machine learning, neural networks, and deep learning are all areas of focus. In this investigation, we have undertaken a time series analysis on PM2.5 from 2018-2022 at DTU station of Delhi. For doing the time series forecasting, we have used a model called Long Short-Term Memory networks (LSTMs). Mean squared error (MAE), root mean squared error (RMSE), Mean absolute percentage error (MAPE), and Pearson Coefficient (r) are employed to check the validity and applicability of the constructed LSTM model. MSE was obtained as 1832.06, RMSE as 42.80, MAPE as 34.07 and R² as 0.514. We have predicted PM2.5 values for next 30 days in the year 2023 based on simulated model. The values obtained were ranging from 282.6 µg/m³ to 130.9 µg/m³.

Keywords: Particulate matter; Neural networks; Prediction; LSTM; PM2.5.

1. Introduction
At present, the quality of the inhaled air is being affected due to a combination of natural factors and human activities. These factors include the rapid growth of industries, unplanned urban development, the accelerated surge in the human population, and the increase in transportation [1, 2]. Shift to industrialization in India brings growth in economic condition of the country, however, it increases the rate of air pollution. Air pollution poses a significant challenge to public health, with particulate matter (PM) emerging as a major pollutant which is harmful to the human society. The rise in air pollution has detrimental impacts on various aspects such as economic consequences, reduced visibility, and accelerated climate change. These outcomes lead to more frequent and severe weather events and cause millions of premature deaths each year.

In recent times, India has emerged as one of the highest polluted countries with high levels of PM2.5 particles. In 2020, India has 22 cities of the top 30 most polluted cities globally, according to IQ Air. Additionally, a Lancet study from the same year attributed 17.8% of all deaths in the country to ambient air pollution. PM2.5 also has various environmental impacts, like reduction in visibility and changing in the radiational balance of earth [3]. Specifically, in the National Capital Territory (NCT) of Delhi, levels of atmospheric pollutants like PM2.5, PM10 and NO2 consistently exceed both the World Health Organization (WHO) guidelines and national ambient air quality standards (NAAQS) of India [4, 5]. The alarming situation of adverse air quality in the NCT of Delhi has been sustaining since the 1990s [6].

Air pollutants consists of many gases and particulate matter which are harmful to the human health and environment. Ammonia (NH3), Nitrogen Dioxide (NO2), Carbon Monoxide (CO), Ozone (O3), Carbon Dioxide (CO2), Sulphur Dioxide (SO2) and particulate matter (PM2.5 and PM10) are common air pollutants [7]. PM consists of very tiny
particles which remain suspended in the atmosphere and causes adverse effects. Sources of these particles are many like combustion processes, such as burning of fossil fuels, biomass, wood burning as well as dust and other particles borne in air. Particles with diameter less than 10 µm in diameter are referred as PM$_{10}$, and those with diameters smaller than 2.5 µm are referred as PM$_{2.5}$ [8].

For the measurement of PM, we can use different methods like light scattering technique, chemical analysis and gravimetric methods. However, the accuracy of these methods can vary, and the equipment required can be expensive and difficult to maintain. Nowadays, techniques of machine learning are receiving more attention for predicting and monitoring air quality levels, including PM$_{2.5}$. Machine learning algorithms can analyze vast datasets and uncover complicated patterns that may be challenging for humans to decode. We can use the Recurrent Neural networks for this prediction but the major drawback is its ability to retain memory. This drawback of RNN is overcome by LSTM. Long Short-Term Memory (LSTM) is a variant of Recurrent Neural Networks (RNNs) specially used to handle sequential data characterized by long-term dependencies [9]. LSTMs prove valuable in cases having time-series data, where past observations can significantly influence future predictions. These networks are engineered to tackle the issue of vanishing gradients that are common issue in conventional RNNs, as gradients tend to diminish to an impractical scale for learning after a few time steps. LSTMs use a combination of gates and memory cells to selectively store and forget information from previous time steps, allowing them to process long sequences of data with a memory of past inputs.

Applications of LSTM are many like, prediction of time series data, applicable in recognition of speech, management of airport passengers, in the field of robot control [10], and for translating sign communication [11], etc. The success of this network in predicting PM$_{2.5}$ levels can be attributed to its ability to process sequential data and identify complex patterns. Meteorological factors such as temperature, humidity, and wind speed also affect PM$_{2.5}$ levels significantly, and LSTM can capture the long-term dependencies between these factors and PM$_{2.5}$ levels. Thus, in this paper we are using LSTM for forecasting the PM$_{2.5}$ values with the help of data obtained from Central Pollution Control Board (CPCB) for the monitoring station in DTU (Delhi). The present study aims to (1) study temporal variation of particulate matter at urban station over Delhi region; (2) predict the particulate matter for the year 2022 based on LSTM model; (3) test and validate predicted model using MSE, RMSE, MAPE, and Pearson Coefficient.

2. Material and Methods

2.1. Site Description

Figure 1 Map displaying geographical location of the study area
Delhi is a diverse metropolis located in the northern region of India. As per the census report of 2011, Delhi is home to approximately 16.75 million people. Geographically, Delhi is situated within the geographic coordinates of approximately 28°24′17″ and 28°53′00″ North latitude and 76°50′24″ and 77°20′37″ East longitude, with an elevation of 216 meters above sea level, as depicted in Fig. 1. Situated mainly on the right bank of the Yamuna River, Delhi covers an area of 1,483 square kilometers and it shares its borders with three neighboring states; (1) To the east, it has borders attached with UP, (2) To the south, it shares border with the state of Haryana and (3) To the west, Delhi shares its border with the state of Rajasthan. This geographical proximity to neighboring states contributes to the city’s diverse culture and influences. Delhi is located on the eastern periphery of the Gangetic plains. The area is bordered by the alluvial plains of Indo-Gangetic region in the north and east, west side is bordered by Thar desert, and on its south, it has Aravali hill range. The National Capital Territory (NCT) covers a total area of 1,484 square kilometers.

The city experiences an average of 15 pollution episodes annually and also exceeds the NAAQS limits for PM$_{2.5}$ for more than 200 days each year [12]. It enjoys a varied climate with four different seasons. The winters from April to June are usually hot and humid, with temperatures often exceeding 40°C (104°F). The rainy season arrives in July and lasts until September, with light to heavy rainfall. Autumn: October to November, temperatures range from 20°C to 30°C. Winter which lasts from December to February is very cold and foggy, with temperatures as low as 5°C and occasional cold waves. One of the important characteristics of climate of Delhi is its extreme temperature variations. The ambient temperature can rise to as high as 47 degrees Celsius, while during winter, it can fall to as low as -0.6 degrees Celsius.

2.2. Data collection

In this work, the dataset of monitoring station of CPCB at DTU, New Delhi, is acquired from online platform of data monitoring provide by CPCB, which is accessible at http://cpcb.nic.in/ for a duration spanning from January 2018-December 2022 (i.e., five years). The Central Pollution Control Board (CPCB) is carrying out a nationwide program called the National Air Quality Monitoring Programme (NAMP) in India. This program involves setting up 804 monitoring stations which are to be established in 344 cities and towns across 28 states and 6 UTs of India. The goal of NAMP is to monitor the levels of four specific air pollutants (SO$_2$, NO$_2$, RSPM/PM$_{10}$, PM$_{2.5}$). Pollutants are continuously monitored over a 24-hour period, with PM sampled once in 8 hours. This observation is conducted two times in a week, resulting in a total of 104 observations in a year.

For effective implementation of above monitoring, CPCB has made an alliance with State Pollution Control Boards (SPCBs), various committees, and the NEERI (which is National Environmental Engineering Research Institute). For assessing the air pollution situation, identifying areas that need attention, and getting guidance to improve air quality, these are very helpful.

For continuously measuring of many criteria pollutants throughout the year, CPCB has installed a network of Continuous Ambient Air Quality Monitoring Stations (CAAQMS) in major cities of India. These stations make use of analyzers that stick to the United States Environmental Protection Agency Automated Federal Equivalent Method standards, for the monitoring of PM$_{10}$ and PM$_{2.5}$. These analyzers make use of principle of Beta ray attenuation for their working. These analyzers normally maintain a flow rate of 1 m$^3$/h during their operation.

2.3. Long Short-Term Memory Networks Model

LSTM is a type of Artificial Neural Networks (ANN) employed in the field of Artificial Intelligence (AI) and deep learning. RNNs represent a category of ANN that have received significant attention in recent times [13, 14]. RNNs, including LSTM networks, possess the ability to handle not just individual data points but also entire sequences of data. This distinctive feature makes LSTM networks particularly well-suited for the processing and prediction of sequential data.

As per research done in 2016 in China which had implemented three ML methods to forecast air quality due to PM$_{2.5}$ concentrations for different time periods. They have used different methods like multiple additive regression trees, deep feedforward NNs, and a hybrid model which is based on LSTM networks in which they found out LSTM to be most effective among all three for forecasting and controlling of air pollution [15].

Recurrent Neural Networks (RNNs) are a class of artificial neural networks which gained a lot of popularity in recent years. LSTMs are designed to remember sequential data, where the information at a given time step (t) shows dependency on the data of previous time step (t-1). Each neuron in an LSTM has three gates namely input, forget, and the output gate. The connections between neurons allow the information from the last time step to flow into the present time step. The gates in LSTMs enable the network to manage and overcome the challenges associated with long-term dependencies in the data. The memory blocks in LSTMs are interconnected across layers, forming a block structure. Each memory block consists of the gates mentioned above, that determine the current state of block. These gates have
the responsibility of either remembering or forgetting information during the training process. They achieve this through the use of a function called sigmoid function, which restricts the values between 1 and 0. By multiplying the data with 0, the LSTM forgets the information, while multiplication with 1 ensures that the information is remembered.

To make it clearer, let us have a look at the architecture of LSTM:

**Figure 2** Model Architecture of Long-Short Term Memory networks Model

- **Forget Gate:** The forget gate plays a crucial role in determining the relevance of information. It evaluates both the current input, denoted as \( x_t \), and the previous hidden state, represented as \( h_{t-1} \), by subjecting them to the sigmoid function. It produces values within the range of 0 to 1. This process helps in deciding whether certain information from the prior output is essential or not, with values closer to 1 indicating it is highly significant.

\[
f_t = \sigma(W_f[h_{t-1}, x_t] + b_f)
\]

where \( f_t \) denotes the forget gate at an instant of time \( t \), \( h_{t-1} \) denotes hidden vector from previous time step, \( x_t \) is used to represent the input at the current time step, \( b \) is the bias term, \( \sigma \) denotes the sigmoid function and \( W_f \) stands for the weight matrix which connects forget gate and input gate.

- **Input gate:** This gate executes a number of functions as mentioned. Firstly, it takes both \( x_t \) and \( h_{t-1} \) and feeds them into second sigmoid function. This sigmoid function transforms the values to fall within the range of 0 to 1. Simultaneously, the information from the current state and the hidden state is transferred through a hyperbolic tangent (tanh) function. The hyperbolic tangent function generates a vector, denoted as \( (\bar{c}_t) \), containing values that span from -1 to 1. The output values produced by these activation functions are then used for element-wise multiplication point-by-point.

\[
i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)
\]

\[
\bar{c}_t = \tanh(W_c[h_{t-1}, x_t] + b_c)
\]

where \( i_t \) represents input gate, \( W_i \) stands for the weight matrix which connects input and output gate, \( W_c \) stands for weight matrix of hyperbolic tangent operator connecting cell state information and network output, \( b_i \) denotes bias vector at time \( t \), \( b_c \) stands for bias vector at time \( t \) with respect to \( W_c \) and \( \bar{c}_t \) is value which is produced by tanh.

- **Cell State (CS):** The next phase involves determining and storing the results from the new state into the CS. This process begins with the previous CS, denoted as \( C_{t-1} \), being multiplied by the forget vector, \( f_t \). The values will be discarded from the CS if the outcome of multiplication is 0. Following this, the network accepts the
value of output which is generated from the input vector denoted as $i_t$, and carries out element-wise addition point-by-point. This addition operation updates the CS, resulting in a new CS, $C_t$.

$$C_t = f_t \times C_{t-1} + i_t \times \tilde{e}_t \ldots \ldots \ldots (4)$$

- Output gate: These are important for determination of value of upcoming hidden state. Initially, it takes the values of the previous hidden state and the current state and feeds them into a third sigmoid function as shown in Fig. 2. This sigmoid function transforms these values into a range between 0 and 1. Simultaneously, the freshly generated cell state, originating from the preceding cell state, is transmitted through a hyperbolic tangent (tanh) function. The result from both the sigmoid and tanh functions are then multiplied point-by-point. Depending on the ultimate outcome, the network determines what information should be retained within the hidden state, and which information should be discarded. This hidden state is subsequently used for making predictions.

$$o_t = \sigma \times W_o [h_{t-1}, x_t] + b_o \ldots \ldots \ldots (5)$$

$$h_t = o_t \times \tanh (C_t) \ldots \ldots \ldots (6)$$

where $o_t$ represents the output gate, $W_o$ stands for weight matrix of output gate, $h_t$ is output of LSTM and $b_o$ is bias vector with respect to $W_o$. Finally, the recently updated cell state and the newly revised hidden state are passed on to the subsequent time step, in the sequence. The procedure continues as the network processes data sequentially, enabling it to retain and update information as it progresses through the sequence of inputs.

In this work a LSTM model was developed and data of $PM_{2.5}$ was used to test and train the LSTM model. When the model was trained various errors like RMSE, MSE, $R^2$ and MAPE were calculated to check the performance of the model. When the obtained results met the expectations, the developed model was used for prediction of $PM_{2.5}$ for the next 30 days.

### 3. Results and discussion

#### 3.1. Time series analysis

Data from the official website of CPCB was taken for the monitoring station at DTU Delhi. Data was then preprocessed for any absurd values and the missing values were replaced by column mean. For getting an idea about variation of $PM_{2.5}$ in the city, various variation plots were drawn with the help of Python as shown in Fig. 3.

Daily variation follows a similar trend for every year from 2018 to 2022. From the annual variation plot, it can be seen that annual average of $PM_{2.5}$ was highest for the year 2018 (128.7 $\mu g/m^3$). The average value decreases for the year 2019 (116.3 $\mu g/m^3$) and 2020 (107.1 $\mu g/m^3$). Again, this value rises in the year 2021 (118.9 $\mu g/m^3$) and falls in 2022 (96.1 $\mu g/m^3$).

Monthly variation plot shows that $PM_{2.5}$ values are relatively higher in October to February, than other months of the year. From the Quarterly variation plot, it is clear that the highest level of $PM_{2.5}$ was obtained in 4th Quarter (October, November, December) (quarterly average 176.22 $\mu g/m^3$) i.e., in winter season, and lowest in Quarter 3 (July, August, September) (quarterly average 41.70 $\mu g/m^3$) i.e, in monsoon season.

The possible reason behind the increase in $PM_{2.5}$ level post monsoon could be high amount of biomass burning in northwestern Delhi and Punjab [16, 17]. Emissions originating from local sources are reported to have a great impact during the winter months. They contribute to more than 70% of the total $PM_{2.5}$ mass concentrations in Delhi during the wintertime [18]. The worst quality of air in Delhi was found during post-monsoon season due to burning of biomass in Punjab and Haryana [19].

The recurring and frequent occurrence of severe pollution episodes observed in Delhi can be attributed to two critical factors: high emissions and unfavorable weather conditions. Sometimes, they occur simultaneously and thus intensifies the problem. The major role in intensifying the frequency and severity of pollution concentration within this region is played by geographical location of Delhi since it is a landlocked and surrounded by landmasses instead of water. In winters, haze and smog are quite obvious in Delhi. These phenomena diminish visibility and aggravate level of pollution. During monsoon season, the level of $PM_{2.5}$ decreases due to precipitation by wash out process.
The data which was taken from the official website of CPCB for the period 2018-2022 was cleaned and preprocessed for any missing value. The missing values were replaced with the column mean. Data was then split into training and testing set. First four years of data i.e., 2018-2021 was taken for training and the data of year 2022 was used for testing the model and calculating various model performance parameters. We have taken different hyper-parameters (like no of epochs, window size learning rate, etc.) and different number of hidden neurons in our trial experiments. We used Adam optimizer and the loss function used is 'mean squared error', which is very common to be used for regression tasks. The model has three LSTM layers as hidden layers with varying numbers of units and a dropout layer after each LSTM layer to regularize the network and avoid overfitting. For evaluating how the LSTM model performs a K-Fold Cross-Validation was also done using the Keras Regressor from scikit-learn by putting no of folds is equal to 6. After that, the model was tested with data of 2022. Fig. 4 shows the plot for actual versus predicted values of PM$_{2.5}$ for the year 2022. It was given on daily basis.

**Figure 3** Variation of PM$_{2.5}$ at Delhi for the entire study period (a) Daily variation (b) Annual variation (c) Seasonal variation (d) Monthly variation, and (e) Quarterly variation

### 3.2. LSTM

The data which was taken from the official website of CPCB for the period 2018-2022 was cleaned and preprocessed for any missing value. The missing values were replaced with the column mean. Data was then split into training and testing set. First four years of data i.e., 2018-2021 was taken for training and the data of year 2022 was used for testing the model and calculating various model performance parameters. We have taken different hyper-parameters (like no of epochs, window size learning rate, etc.) and different number of hidden neurons in our trial experiments. We used Adam optimizer and the loss function used is 'mean squared error', which is very common to be used for regression tasks. The model has three LSTM layers as hidden layers with varying numbers of units and a dropout layer after each LSTM layer to regularize the network and avoid overfitting. For evaluating how the LSTM model performs a K-Fold Cross-Validation was also done using the Keras Regressor from scikit-learn by putting no of folds is equal to 6. After that, the model was tested with data of 2022. Fig. 4 shows the plot for actual versus predicted values of PM$_{2.5}$ for the year 2022. It was given on daily basis.
For checking the performance of the developed model various errors were calculated as shown in table 1. MSE was obtained as 1832.06, RMSE as 42.80, MAPE as 34.07 and $R^2$ as 0.514. It should be noted that lower value of RMSE shows that model is performing well. Value of $R^2$ will show how much correlation is there between actual and predicted values. Value close to one show that model is highly correlated and close to zero shows no correlation between actual and obtained values at all. Our model showed medium correlation.

Table 1 Various error values of developed LSTM Model

<table>
<thead>
<tr>
<th>S.no.</th>
<th>Error name</th>
<th>Obtained value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Mean Squared Error (MSE)</td>
<td>1832.06</td>
</tr>
<tr>
<td>2.</td>
<td>Root Mean Squared Error (RMSE)</td>
<td>42.80</td>
</tr>
<tr>
<td>3.</td>
<td>Mean Absolute Percentage Error (MAPE)</td>
<td>34.07</td>
</tr>
<tr>
<td>4.</td>
<td>$R$- Squared</td>
<td>0.514</td>
</tr>
</tbody>
</table>

Figure 4 Actual vs Predicted Graph for the year 2021 for testing of LSTM Model

Figure 5 Complete Graph showing Variation of PM$_{2.5}$ consisting of Obtained value and used value
After calculating this, the model was again used for forecasting the next 30 days value i.e., from 1 January 2023 to 30 January 2023. Fig. 5 shows the plot of obtained values merged with taken data of 2018-22. This plot shows the trend of data. Here, the values obtained were ranging from 282.6 µg/m³ to 130.9 µg/m³. These values are above the prescribed National Ambient Air Quality Standards for PM$_{2.5}$ set by CPCB. It indicates severe air pollution and poses a significant health risk. Hence, it is crucial for the authorities to take immediate actions to mitigate air pollution, identify the sources of pollution, and implement measures to improve air quality and bring it within acceptable limits.

4. Conclusion

Air pollutants, one of the major concerns, include harmful gases and PM which can adversely affect human health and environment. One of the criteria pollutants, PM$_{2.5}$ was analyzed for temporal variation at DTU, Delhi for the study period 2018-2022. Its Prediction for 30 days in 2023 was also done with developed LSTM model. Important results obtained in this work can be concluded as below:

- Variation plots were drawn to see the variation of PM over entire span of study. From variation plots in terms of daily variation, minimum value obtained was 1.00 µg/m³ and maximum value was 443.17 µg/m³ with a mean of 113.49 µg/m³. The annual plot showed that maximum annual average was obtained for the year 2018 (128.1 µg/m³) and minimum was for the year 2022 (96.1 µg/m³). From Monthly and Quarterly variations plots it was clear that during Winter season values obtained were on higher side and during monsoon it was lower comparatively.
- The possible reason behind higher pollutant level in winter season could be stubble burning in Punjab and Haryana, pollutant accumulation due to its trapping by cold air near the surface, its geographic location (since it is landlocked), etc. In monsoon season the values were lower comparatively due to precipitation.
- The LSTM model which was developed, showed MSE as 1832.06, RMSE as 42.80, MAPE as 34.07 and R$^2$ value as 0.514 between testing and training data. Then this model was used to predict the values for 1 January to 30 January 2023. Here, the values obtained were ranging from 282.6 µg/m³ to 130.9 µg/m³.

Measurement of concentration of air pollution with high degree of precision requires very expensive sensors. In future, particulate matter forecasting based on LSTM models will offer a practical solution for this and also help policy makers regarding this.

Compliance with ethical standards

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Disclosure of conflict of interest

No conflict of interest to be disclosed.

Statement of ethical approval

The present research work does not contain any studies performed on animals/human subjects by any of the authors.

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