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Air quality index prediction using multivariate deep neural networks: A case study of a proposed state capital in India

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ABSTRACT

Introduction: Air pollution is a major environmental challenge worldwide and predicting air quality is key to regulating air pollution. The extent of air pollution is quantified by the Air Quality Index (AQI). Air quality forecasting has become an important area of research. Deep Neural Networks (DNN) are useful in predicting the AQI instead of traditional methods which involve numerous computations. The aim of this research paper is to investigate the use of the deep neural networks as a framework for predicting the air quality index based on time series data of pollutants.

Materials and methods: To resolve this problem, the study proposes a DNN to develop the best model for predicting the AQI. Long Short-Term Memory (LSTM) and Bi-directional LSTM have been introduced in the study to understand and predict the relationship between the pollutants affecting the AQI. The model's performance is evaluated using the metrics, Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), Mean Square Error (MSE), Root Mean Square Error (RMSE) and coefficient of determination (R^2). To conduct the study, real-time hourly data for the period November 2017 to January 2020 from an air quality monitoring station was considered for the proposed capital region of the state of Andhra Pradesh in India.

Results: The multivariate modeling considers seven pollutants as independent variables and AQI as the target variable. After experimenting and training the algorithm on the dataset, Bi-directional LSTM was shown to have the lowest MAE and RMSE values and the highest R^2, indicating that it has the highest accuracy in AQI prediction.

Conclusion: The development of a capital city involves massive construction activity resulting in air pollution. The results are helpful to the authorities to monitor the quality of air of develop air quality management programs thus avoiding the impact of air pollution on health.

Introduction

Air quality must be observed continuously through weather monitoring stations for human welfare, otherwise, it will have adverse health effects. In India, air pollution was increased by several folds due to rapid urbanization, industrialization, and

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development activities initiated by the state and central governments. There must be a trade-off between environmental risks and developmental activities so as to protect the public from impacts due to air pollutants. In developing countries like India, air quality monitoring and prediction have become extremely important to implement mitigation measures so as to avoid environmental risks. Considering the effect of pollutants on human health, a statistic called Air Quality Index (AQI) has been developed to quantify air quality. A total of 804 air quality monitoring stations have been set up in India to disseminate air quality information to the public. AQI considers eight pollutants particulate matter 10 µm or less in diameter (PM_{10}), particulate matter 2.5 µm or less in diameter ($PM_{2.5}$), Nitrogen dioxide (NO_2), Sulfur dioxide (SO_2), Carbon monoxide (CO), Ozone(O_3), ammonia (NH_3) and lead (Pb) and is calculated only when data is available for at least three pollutants, one of which is $PM_{2.5}$ should be or PM_{10}. There are six categories of AQI: good, fair, moderate, poor, very poor, and severe [1]. In the past, several methods have been used to predict the various pollutants affecting air quality and AQI.

To predict AQI, new methods have been applied instead of traditional mathematical and statistical methods, as the importance of AQI has increased in the world [2]. The traditional prediction techniques typically require significant computational resources. Furthermore, the prediction accuracy of the techniques depends on the framework of the technique alone and improvement is not possible irrespective of the extent of the training dataset. The advent of artificial intelligence has led to the development of the latest and most advanced prediction algorithms. Deep Learning (DL) and Machine Learning (ML) are a subset of artificial intelligence widely used in many fields for high-accuracy prediction tasks. DL and ML algorithms can efficiently process large environmental datasets and provide accurate prediction results [3]. AQI prediction models based on DL and ML have proved to be more dependable and consistent.

The ML algorithms, Support Vector Regression (SVR), Random Forest (RF) regression, and CatBoost regression have been utilized to determine the AQI of four major cities in India; the findings indicate that random forest regression results in the lowest Root Mean Square Error (RMSE) values and highest accuracy for three cities [4]. The most popular DL algorithms are multilayer perceptron, Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNN), and autoencoder. In particular, RNN-based AQI prediction models have been shown to perform better [5, 6]. The predictions of PM_{10} concentration were analyzed with three DL algorithms namely RNN, Long Short-Term Memory (LSTM), and gated recurrent unit; and all of them performed well [7]. To predict the PM_{10} and $PM_{2.5}$ levels in Macao, four ML algorithms were applied in the study, and RF regression was found to be reliable [8]. A hybrid CNN-LSTM model outperformed the other DNN in predicting the $PM_{2.5}$ concentration in the urban area of Beijing [9]. From the related studies of AQI prediction based on DNN, it is observed that the studies are mainly focused on univariate time series prediction of various pollutants affecting air quality instead of multivariate prediction by considering the independent variables as pollutants and target variables as AQI.

A study was conducted by independently examining univariate time series data of 12 pollutants using the DL algorithm, and the authors suggested to implement multivariate models with a bidirectional framework using the pollutant data as part of the extension of the study [2]. To fill a gap in the literature, the present study proposes two DL architectures namely multivariate LSTM and bidirectional LSTM for AQI prediction by considering seven pollutants as independent variables and AQI as dependent variables. The next section contains information about the study area and methods.

Materials and methods

Study area

In India, a new capital city Amaravati for the state of Andhra Pradesh was proposed between the two major cities with environmentally sustainable and people's capital and it's planned to accommodate 3.55 million by 2050. Amaravati city will be built with modern infrastructure, including developing roads, water supply facilities, administrative and institutional complexes, sewers, sanitation facilities, waste disposal facilities, and waterfront development with a vision to become a smart city in India [10]. The Capital Region Development Authority (CRDA) of the proposed capital city at Amaravati is shown in Fig. 1. The air quality monitoring station (AP 001 station ID) has been established at Secretariat, Amaravati to monitor and record the concentration of the pollutants.

To conduct the study, real-time hourly data for the period November 2017 to January 2020 from the air quality monitoring station AP001 was collected, in which the pollutants affecting the AQI were recorded. The hourly data pertaining to seven pollutants influencing the AQI were considered as independent variables, PM_{10}, $PM_{2.5}$, NO_2, SO_2, CO, O_3, and NH_3; and the target variable was AQI. The framework of the steps involved in the process of DNN architecture is presented in Fig. 2.

Fig. 1. Capital region development authority-Amaravati

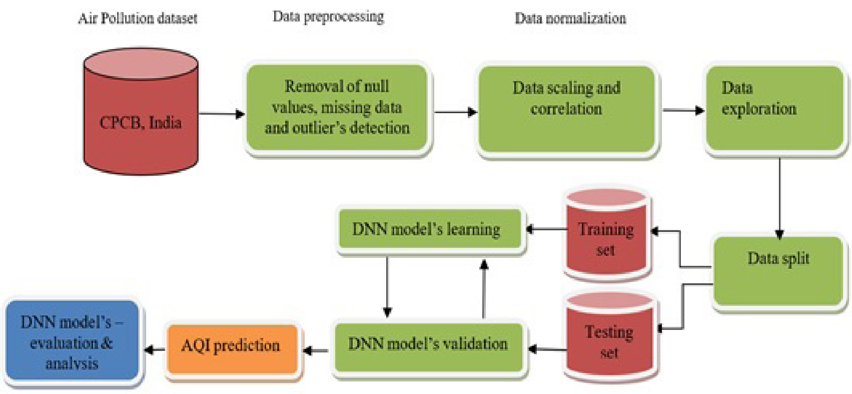

Fig. 2. Framework of DNN models

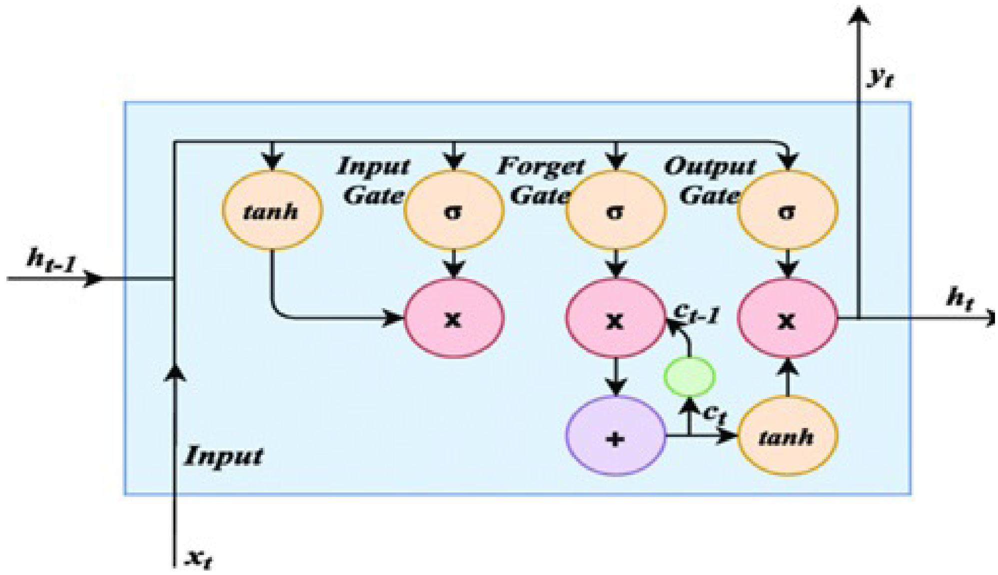

Fig. 3. LSTM block diagram

The study aimed to evaluate the performance of DNN algorithms. The LSTM architecture was exhaustively discussed in order to better understand the architecture of the Bidirectional model. This section illustrates in detail the structure of deep learning (DL) networks adopted in the analysis. DNNs were used to investigate the effectiveness of the model parameters on the prediction of AQI.

LSTM model

LSTM networks are a type of Recurrent Neural Network (RNN) that increases memory recall by remembering past data [11] and backpropagation is used to train the model, which is ideally suited to predicting time series with unpredictable time lags. The LSTM networks were explicitly developed to circumvent the long-term dependency issues and handle the vanishing gradient problem successfully, and the model is divided into three sections which perform a specific function as shown in Fig. 3.

The first section determines whether the data from the previous time step is relevant or can be ignored. In the second and final sections, the cell seeks to learn new information from the input and transfers the updated information from the current time step to the next time step respectively, and the LSTM cycle is viewed as a single-time step. These three sections of the LSTM unit are known as forget gate, input gate, and output gate. A memory cell in an LSTM network can be viewed as a layer of neurons in a typical feedforward neural network, with each neuron having a hidden layer and an ongoing state. These gates also solve the problem of vanishing gradient, which generally occurs in RNNs. As a result, it is widely used in a variety of applications in time series prediction [12]. The first section determines whether to retain or remove the information from the previous time step. Eq. 1 represent the forget gate. The activation value of forget gate ft at time t is calculated using a sigmoid function. The ft is then multiplied by the previous time step's cell condition.

$$f_t = \sigma\,(X_t * U_f + h_{t-1} * W_f) \quad (1)$$

Where; X_t is the input to the on-going time step,

U_f is the weight related with the input, h_t-1 is the hidden state of the preceding time step and W_f is the weight matrix related with the hidden state. The second gate, the input gate, is used to evaluate the relevance of the new information carried by the input, and it is shown as Eq. 2.

$$i_t = \sigma (X_t * U_i + h_{t-1} * W_i) \quad (2)$$

Where; U_i is the weight matrix of input and W_i is the weight matrix of input associated with hidden state. The sigmoid function is then applied on top of this, resulting in the value of 'i' at time step t being between 0 and 1. Eq. 3 is used to calculate the new information.

$$N_t = \tanh ((X_t * U_c + h_{t-1} * W_c) \quad (3)$$

The new information that has to be provided to the cell state is now a function of a hidden state at time step t-1 and input x at time step t. Tanh is the activation function, and the value of the new information runs from -1 to 1. If N_t is negative, information is subtracted from the cell state and added to the continuing state, and vice versa. The Nt, however, is not directly added to the cell state. Eq. 4 represents the modified cell state equation.

$$C_t = f_t * C_{t-1} + i_t * N_t \quad (4)$$

Where, C_t-1 is the cell state at the on-going time step.

The equation of the output gate is shown as Eq. 5.

$$o_t = \sigma (X_t * U_o + h_{t-1} * W_o) \quad (5)$$

Eq. 6 is used to compute the current hidden state using the output state 'o_t' and tanh of the updated cell state. As indicated in Eq. 7, the hidden state is a function of long-term memory (Ct) and the current output, and the output of the current time step is determined by applying the SoftMax activation to hidden state ht. The predicted value is nothing but the maximum score in the output.

$$h_t = o_t * \tanh (C_t) \quad (6)$$

$$\text{Output} = \text{Softmax} (h_t) \quad (7)$$

Finally, backpropagation is used to obtain the LSTM, which is then stored in memory blocks. Now, the LSTM can successfully familiarize the inputted time series data to produce a long-term memory function [13]. In this model, the outputs of the cell are controlled by the gates. Figure 4 depicts the architecture of a single LSTM cell [14].

Bidirectional LSTM model

LSTM may receive long range information prior to the output time but cannot use reverse information. To greatly increase prediction accuracy, the forward and backward information of time series data should be completely considered in time series prediction. Bidirectional LSTM is made up of two LSTM's, one forward and one backward layer. In comparison to the regular LSTM's one-way-state transmission, Bidirectional LSTM evaluates data changes before and after data transmission and can make more full and detailed decisions based on past and future information [15]. Bidirectional LSTM model performs forward and backward calculations as shown in the model structure in Fig. 4 [16].

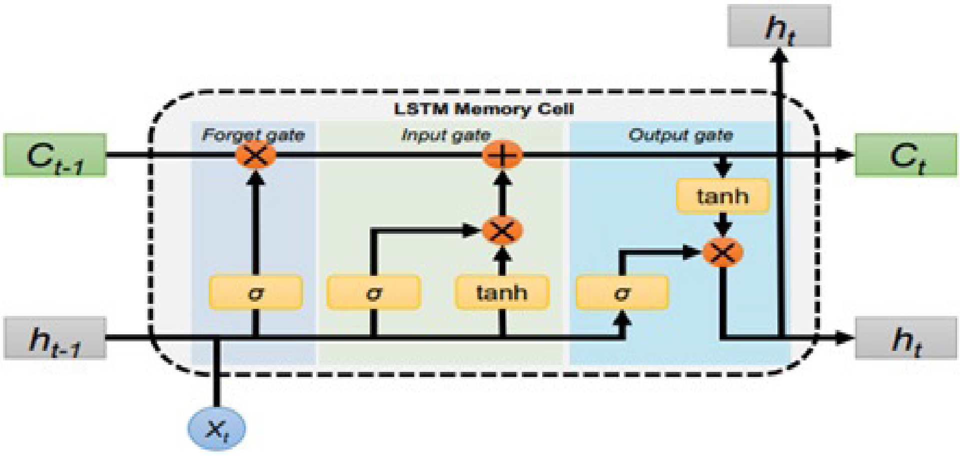

Fig. 4. Schematic diagram of the LSTM cell architecture

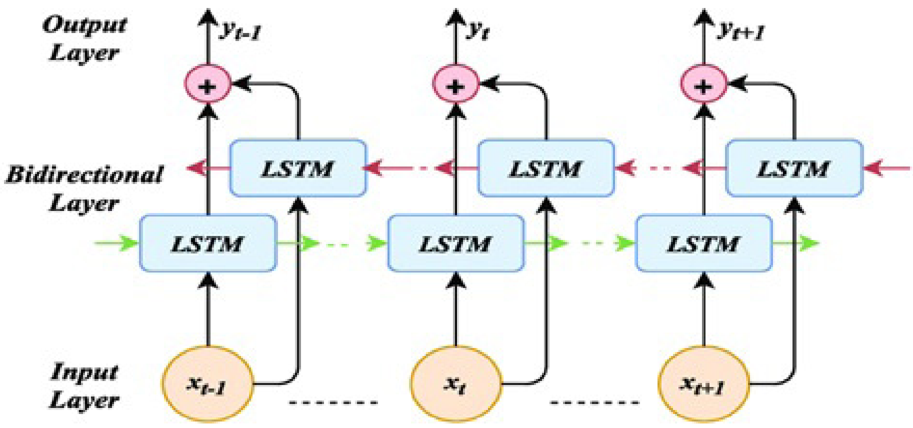

Fig. 5. Schematic diagram of bidirectional LSTM structure

Fig. 5 depicts the two-way flow of time series information in the model, whereas data information flows vertically in only one direction from the input layer to the hidden layer to the output layer. The purpose of using the LSTM twice makes the model to learn the model long-term dependencies and increase its accuracy [17].

Performance metrics

To investigate the performance of LSTM models, five statistical indicators – Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), Mean Square Error (MSE), Root Mean Square Error (RMSE) and coefficient of determination (R^2) were used, as shown in Eqs. 1-5.

$$\mathrm{MAE} = \frac{1}{n}\sum_{k=1}^{n}|A-P| \tag{1}$$

$$\mathrm{MAPE} = \frac{1}{n}\sum_{k=1}^{n}|(A-P)/A| \tag{2}$$

$$\mathrm{MSE} = \frac{1}{n}\sum_{k=1}^{n}(|A-P|)^2 \tag{3}$$

$$\mathrm{RMSE} = \frac{1}{n}\sqrt{\sum_{k=1}^{n}|A-P|} \quad (4)$$

$$\mathrm{R}^2 = 1 - \frac{\sum_{i=1}^{n}|A-P|}{\sum_{i=1}^{n}|\bar{A}-\bar{P}|} \quad (5)$$

Where P is the ith model-predicted hourly AQI, A is the ith observed hourly AQI, P¯ is the average of the predicted hourly AQI, A¯is the average of the observed hourly AQI; and n is the number of observations.

Results and discussion

In the present study, hourly data pertaining to the seven pollutants and AQI for the period from 11/25/2017, 9:00:00 AM to 7/1/2020 ,12:00:00 AM with a total of 18704 data points was collected from the official website of central pollution control board (CPCB) for the air quality station Amaravati. The data are published on the official website of CPCB, Government of India. To maintain high data quality, the authors removed the outliers, null values and standardized the data format. The dataset comprising of 14625 points was used for the analysis by applying LSTM and bidirectional LSTM after removing the missing values, null values and outliers. The descriptive statistics of the target variable and independent variables after the data preprocessing are shown in Table 1.

Table 1. Descriptive statistics of the variables

	AQI	$PM_{2.5}$	PM_{10}	NO_2	NH_3	CO	SO_2	O_3
Count	14625	14625	14625	14625	14625	14625	14625	14625
Mean	95.18	38.77	76.76	21.61	12.32	0.6359	14.04	36.15
Std	55.99	29.78	48.80	21.58	6.44	0.5379	12.26	19.19
Min	21.00	0.250	1.00	0.10	0.10	0.10	0.05	8.33
25%	55.00	16.50	40.50	8.600	7.650	0.3800	7.820	20.58
50%	78.00	28.75	64.50	14.57	11.88	0.5500	11.68	32.50
75%	121.00	54.75	103.25	24.65	16.57	0.76	16.90	48.45
Max	317.000	308.75	559.25	177.88	68.93	9.84	195.00	90.62

Data points were normalized between 0 and 1 using the MinMax scaler before splitting the data set for training and testing. Out of 14625 data points, 10234 (70%) and 4391 (30%) were used to train and test the dataset to assess the models' predictive capability. Finally, five evaluation metrics namely; Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), Mean Square Error (MSE), Root Mean Square Error (RMSE) and coefficient of determination (R^2) were used to check the model's predictive capability based on the actual and predicted values.

Window length selection is one of the complex and critical exercise in model development and to overcome the difficulty Partial Auto Correlation Function (PACF) applied [18-20]. Based on the PACF, various time steps were tested and finally, the previous observation time step of 18 hours was chosen as the model input for both models. This is supported by the fact that using the PACF results we observed the greatest correlation between 18 and 20 lags.

Parameters and the experimental models

In this study, the results of the multivariate LSTM and bidirectional LSTM model were compared based on the evaluation metrics. The model and training parameters of both models are kept the same for comparison purpose. The Adam optimizer is used to calculate the adaptive parameter learning rate based on the mean of the first and second moments of the gradient. The learning rate is 0.0001, and MAE is used as the loss function. It only measures the mean modulus length of the predicted value error, disregarding direction, and is more robust to outliers. Several experiments were conducted by varying the batch size, number of epochs, learning rate, time step and window length. Finally, optimum results were obtained at a batch size of 64 and the number of epochs of 150. The hourly pollutants data and AQI of the study area after preprocessing are put into the LSTM, and bidirectional LSTM models for training. The test dataset is used for prediction after completing the training. The plot of the hybrid model relating to the actual and predicted values in the last 4391 h are shown in Fig. 6 and 7 of LSTM, and bidirectional LSTM respectively.

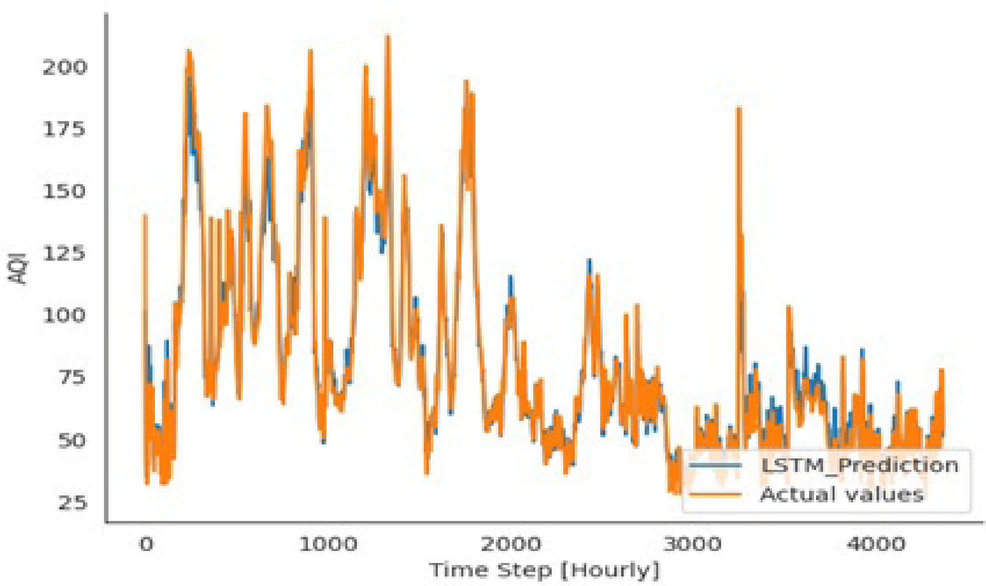

Fig. 6. Actual vs predicted values of AQI-LSTM model

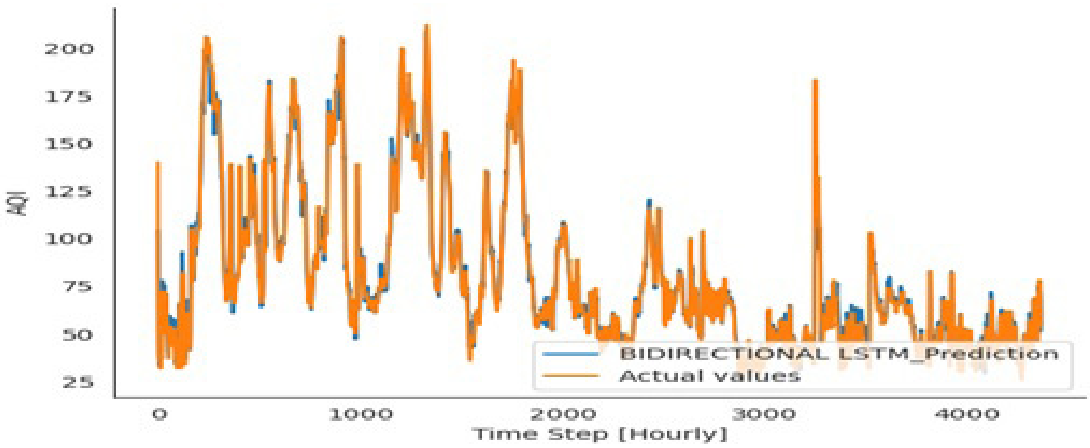

Fig. 7. Actual vs predicted values of AQI-Bidirectional LSTM model

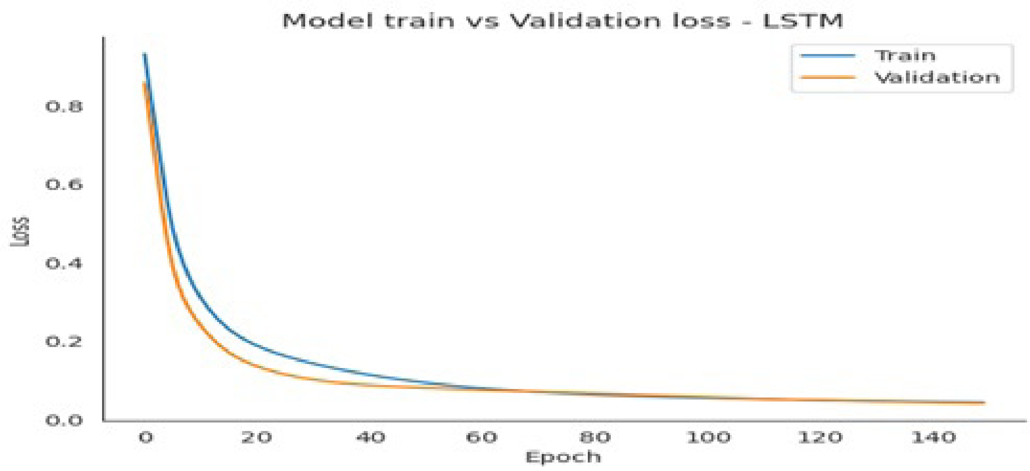

Fig. 8. Learning curve of LSTM model

The learning curves are plotted to check whether the train or validation datasets are appropriately representative of the domain area. The learning curve shows that the model fit is good, with a training and validation loss reducing to a stability point with a marginal difference between the two final loss values. The learning curves of LSTM and bidirectional LSTM are shown in Figs. 8 and 9 respectively.

The basic evaluation indicators that are; MAE, MAPE, MSE, RMSE, and R^2 are used in the analysis are used to compare the results of three models. These five indicators are used to ascertain the difference between the predicted and actual values of AQI and the values of these indicators are presented in Table 2. The R^2 score of the bidirectional LSTM model is 0.9752 which is higher than the LSTM model. The MAE, MAPE, MSE, and RMSE scores of the bidirectional LSTM model are 3.7947, 5.3882, 42.0377 and 6.4836 respectively. It clearly indicates that BiLSTM approach records better performance in terms of evaluation metrics.

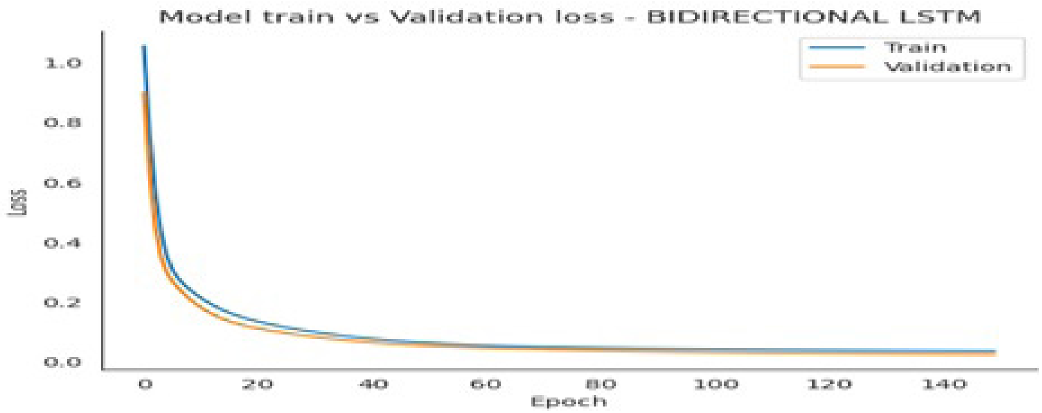

Fig. 9. Learning curve of Bidirectional LSTM model

Table 2. The Model evaluation parameters of AQI of the study area

Model	MAE	MAPE	MSE	RMSE	R^2
LSTM	5.4012	6.951	76.6529	8.5237	0.9572
BiLSTM	3.7947	5.3882	42.0377	6.4836	0.9752

In predicting the AQI, the bidirectional LSTM architecture is robust compared with LSTM model. The bidirectional LSTM model's R^2 score is 0.9752, higher than the LSTM model, indicating that the model has outperformed the empirical and DL models in terms of predicting time-series data [16]. Univariate AQI prediction of Beijing based on multilayer perceptron neural network achieved an R^2 of 0.861 [21]. Three ML and DL algorithms were applied to predict $PM_{2.5}$ concentrations at different time intervals in Tehran city and the LSTM framework achieved the best results with RMSE, MAE and R^2 of 8.91, 6.21 and 0.80 respectively [22]. Seven DNN architectures were implemented to predict PM 2.5 concentration using multiple variables from meteorological data and the multivariate CNN-LSTM model achieved the best result with an R^2 of 0.979 with a batch size of 32 and an interval of 7 days [9]. Based on the evaluation parameters between the predicted and actual values, the bidirectional LSTM model has the best degree of fit.

The learning curve of the bidirectional LSTM model shows that the model fit is good with no overfitting or underfitting. The accuracy of the models used was validated against the actual AQI of the study area, resulting in an average absolute percent error value of less than 2%. Compared to the LSTM model, the results of the bidirectional LSTM model show that the improvement in the predictive capability and the predicted values are closely following the trend of the original dataset. The proposed model can be trained and used with the other pollutants effecting the air quality that have an impact on the AQI. As a result, the proposed bidirectional LSTM model can be applied in many fields such as forecasting of finance, meteorological and health care datasets.

Conclusion

The aim of the study is to predict AQI based on multi-pollutant data from a proposed state capital in India. The results of the study are useful to all the stakeholders involved in the development of the new capital city. It is crucial to monitor the AQI values continuously during the phase of development of the capital city due to massive large-scale construction activity and operation of equipment resulting in affecting the quality of air. The results are useful for sustainable development of the capital city. The prediction results are useful to implement mitigation measures to maintain AQI within safe limits. To predict AQI, LSTM, and Bidirectional LSTM models were implemented. The bidirectional LSTM model R^2 scores provided better results for predicting the AQI compared to the LSTM model. The evaluation parameters of the models used were verified using the actual AQI data and the MAPE of the proposed model was less than 4%. The proposed model fit is good as it falls between an overfit and an underfit model. The results of the study are useful to all the stakeholders involved in the development of the new capital city. The proposed multivariate model can be applied to predict the concentrations of various pollutants affecting the air quality by considering the meteorological parameters including wind speed, humidity, ambient temperature, and wind direction.

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Competing interests

"The authors declare that they have no known financial or non-financial competing interests in any material discussed in this paper."

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Ethical considerations

Ethical issues (Including plagiarism, Informed Consent, misconduct, data fabrication and/ or falsification, double publication and/ or submission, redundancy, etc) have been completely observed by the authors.

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