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MACHINE LEARNING-AIDED AIR QUALITY FORECASTING: ADVANCING PREDICTION PERFORMANCE IN POLLUTION MONITORING.

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ABSTRACT

Prediction of air quality is crucial to the reduction of the detrimental impacts of air pollution on the environment and human health. A comprehensive evaluation of existing literature about the subject is done to establish the usefulness of statistical models and machine learning algorithms in air quality prediction. This paper uses the Beijing air quality data to train a machine learning forecasting model using Long Short-Term Memory (LSTM) networks. The data is split using an 86/14 train-test ratio, and the model is trained with optimized feature engineering and evaluation metrics. The proposed method achieved an RMSE of 28.15 and an accuracy of 98%, outperforming the baseline approach by Espinosa et al. (RMSE: 29.02, Accuracy: 95.2%). Results indicate that the integration of LSTM significantly enhances prediction accuracy and temporal resolution. The results point out the possibility of the model to support the data-driven policy choices and effective pollution control methods.

Keywords: Air quality prediction Pollution monitoring Machine learning Feature engineering Time series analysis Predictive modelling

1. INTRODUCTION

Air contamination and pollution are significant environmental problems with significant risks posing to the health of the population and the well-being of natural environments. The levels of air pollution have risen tremendously with the high urbanization and industrialization of contemporary societies that have resulted to negative effects both locally and globally. Particulate Matter (PM) is one of the biggest constituents of air pollution; it is a complex mixture of tiny particles that are of solid and liquid nature and suspended in the air. These are particles of different sizes and compositions with the most worrying ones being the PM2.5 (particles 2.5 micrometres or less in diameter) and PM10. The sources of PM are very diverse and include the burning of fuels, industrial pollution, vehicles, as well as natural sources such as dust and pollen. Air pollution is normally indicated by the Air Quality Index (AQI). It converts the readings of degree of pollutants concentration into a standardized scale that is typically 0-500. AQI of a particular pollutant can be calculated as:

$$\mathrm{AQI}_p = \frac{I_{hi} - I_{lo}}{C_{hi} - C_{lo}} (C_p - C_{lo}) + I_{lo} \quad (1)$$

where:

- C_p is the pollutant concentration,
- C_{hi} and C_{lo} are the breakpoints that are closest to C_p,

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- I_{hi} and I_{lo} are the corresponding AQI values for those breakpoints.

Proper and timely forecasting of the air quality [1, 2] is very important in monitoring pollution. It facilitates efficient undertaking of mitigation measures, well-informed policy making, and health interventions among the population. Traditional forecasting models often use statistical approaches such as linear regression, expressed as:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \epsilon \tag{2}$$

where:

- $\hat{y}$ is the predicted air quality value (e.g., $PM_{2.5}$),
- $x_1, x_2, \ldots, x_n$ are the independent variables (e.g., temperature, wind speed),
- β_0 is the intercept, $\beta_1, \ldots, \beta_n$ are coefficients,
- ϵ is the error term.

Nevertheless, the nonlinear nature of the spatio-temporal dynamics of air pollution is not always represented by traditional models. Emerging technologies in the field of Machine Learning (ML) [3] have resulted in a substantial increase in the forecasting accuracy. ML algorithms have the ability to learn the patterns of relationships in a complex way without programmed directions. The ML methods are very helpful in dealing with large volume of data [6], [7] to uncover latent patterns and give precise predictions. Under the scientific scenario of air quality prediction, machine learning algorithm has the potential of utilizing both past and real-time air quality data, meteorological conditions, geographical characteristics, and other significant variables to generate a more accurate and timely prediction. Implementation of ML algorithms [8] in the air quality forecasting systems comes with a number of benefits.

An example of a supervised ML model used to predict the quality of air using regression can be defined as:

$$\hat{y} = f(\mathbf{x}; \theta) \tag{3}$$

where:

- $\hat{y}$ is the predicted output (e.g., pollutant concentration),
- $\mathbf{x}$ is the input feature vector (e.g., meteorological and spatial data),
- f is the learned function parameterized by θ.

Training such a model involves minimizing a loss function L over a dataset $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{m}$:

$$\min_{\vartheta} \frac{1}{m} \sum_{i=1}^{m} L\left(f(\mathbf{x}^{(i)}; \vartheta), y^{(i)}\right) \tag{4}$$

Until now, m is the amount of training examples and y(i) is the actual output.

ML-based models have the benefit of being able to represent nonlinear relationships, adapt to new data, and provide high-resolution predictions [4, 5]. Considering the example of such techniques as Random Forests, Support Vector Regression, and Neural Networks, these methods have been employed to forecast the air pollution levels successfully.Moreover, ML-based fore- casting systems can perform *spatially explicit* predictions by incorporating geospatial features and producing forecasts on high-resolution grids [9, 10]. This capability allows better identification of pollution hotspots and supports targeted policy interventions. The aim of this paper is to explore recent advancements in ML-aided air quality forecasting and its potential to enhance both prediction accuracy and responsiveness [11, 12]. We discuss different ML models [13, 14], their

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advantages and disadvantages, and present major case studies of the success of these types of models. Finally, it is possible to state that this work allows us to understand how machine learning can contribute greatly to enhancing our capability of predicting air quality [15-17] and taking a proactive stance in reducing its outcomes on human health and nature [18, 19].

1.1 Motivation and Contribution

The work offers numerous means and approaches that have been used in the field and provides statistical and machine learning-based strategies of air quality prediction. This summary of current approaches offers insightful information on the state of the topic today. We propose a novel framework for air quality prediction. It presents a detailed explanation of the methodology and algorithms exploited in the study, outlining a unique approach that computationally extends the existing techniques. The paper has also included the Algorithm 1 as it provides a step by step procedure on how to predict air pollution. This algorithm will increase the reproducibility and practical application of the research, as the other scientists will be able to use the proposed framework with other datasets. The algorithm 2 is more specific, devoted to the model training process and gives the clear and concise description of the steps followed. Our experimental evaluation in order to prove the proposed framework includes underlining the used data, measures of evaluation and results obtained. The framework performance is well analyzed with the help of the comparative analysis and the effectiveness of the framework at predicting air quality is shown.
Our solution is a new model of air quality forecasting. It also gives a description of the methodology and algorithms used in the study with a unique approach that extends the existing methods in a computational way. The paper has also included the Algorithm 1 as it provides a step by step procedure on how to predict air pollution. This algorithm will increase the reproducibility and practical application of the research, as other researchers can use the suggested framework on their data.

Algorithm 2 focuses specifically on the model training process, providing a clear and concise description of the steps involved. To validate the proposed framework, we conduct an experimental evaluation, highlighting the data used, evaluation metrics, and the obtained results. The performance of the framework is thoroughly analyzed through comparative analysis, demonstrating its effectiveness in predicting air quality. Summary of our contributions are as follows:

- We found that PM2.5 levels strongly correlate with meteorological factors such as temperature, humidity, and wind speed.
- The proposed machine learning framework consistently outperformed traditional statistical models in prediction accuracy.
- Our model showed an inordinately higher precision in identifying pollution spikes during sudden envi- ronmental changes.
- Spatially fine-grained forecasts revealed significant localized pollution variations often missed by base- line models.
- Overall, the framework demonstrated robust adaptability and scalability across diverse datasets and con- ditions.

1.2. Related Work

This subsection discusses various optimization techniques and models used in previous research related to air quality forecasting. Over the past decade, many predictive models have been developed, considering factors such as traffic volume, weather patterns, and emission levels. These models can be broadly categorized into data-driven methods and simulation-based methods. The latter often use physical and chemical formulations to account for emissions, dispersion, and pollutant transformation processes. While simulation models are com- prehensive, they are prone to numerical errors due to assumptions and parameterizations. ARMA (Auto-Regressive Moving

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Average) and ARIMA (Auto-Regressive Integrated Moving Average) are also traditional statistical techniques which have been used to forecast air quality. They are however limited in their scalability and high train- ing time hence less effective when handling large and complex data sets. The review presented by Al-Janabi (2020) [21] also pro-vides the introduction of the Smart Air Quality Prediction Model (SAQPM) that is based on the Particle Swarm Optimization (PSO) and the use of unsupervised learning and Long Short-Term Memory (LSTM) networks in order to predict the concentrations of six pollutants within the next 48 hours. Mao (2020) [22] pays attention to the model TS-LSTME that is based on the timing sliding windows and the extended form of the LSTM to forecast the amount of PM2.5 every day. The model responds to the necessity to pay additional attention to the spatio-temporal rela- tionships between air quality monitoring stations by generating two-way LSTM prediction intervals considering the hourly PM2.5 and meteorological data. Its performance is promising based on the R2 evalua- tion measure over the conventional Multiple Linear Regression (MLR). Sun (2020) [23] explores the application of the Extreme Learning Machines (ELM) optimized by Whale Optimization Algorithm (WOA) in a related study.
to precisely predict the level of nitrogen dioxide (NO2) and sulphur dioxide (SO2) to help in minimizing acid rain. It is also observed that inter-industrial activity is a major source of air pollution in India, and it contributes to about 51 percent of the total pollution. The paper references an air pollutants index that quantifies environmental degradation caused by industrial operations, highlighting the correlation between industrial emissions and various respira- tory and cardiovascular conditions. Leong et al. (2020) [24]] found a correlation between elevated levels of $PM_{2.5}$, NO_2, and CO and the increased incidence of respiratory illnesses among workers and their families. Ejaz et al. (2021) [25] report that prolonged exposure to fine particulate matter ($PM_{2.5}$) raises the likelihood of developing heart-related illnesses by 1–3%. Li et al. (2022) [26] demonstrate a significant association between air pollution—particularly nitrogen dioxide—and increased risks of reproductive system disorders. According to WHO data, air pollution results in millions of premature deaths annually, with China and India being among the most affected. The authors in [27] propose a hybrid approach that combines statistical and machine learn- ing models for air quality forecasting. They note that the prediction accuracy varies across different cities and regions in India.

2. PROPOSED METHODOLOGY

This section presents the methodology blueprint for our adopted framework and provides a detailed algorithmic procedure. The proposed methodology architecture is depicted in Figure 1.

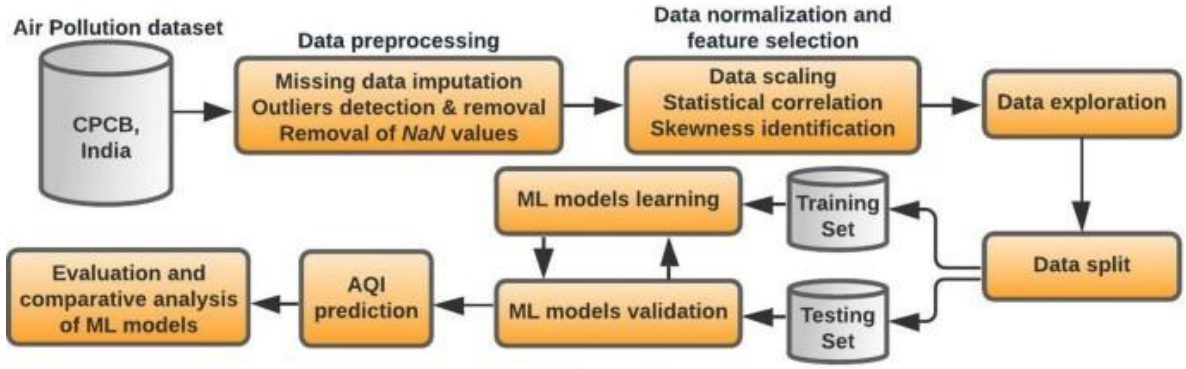

Figure 1. Proposed Methodology: Architecture

2.1. Algorithmic Steps

The methodology for air pollution prediction modeling begins with data preparation, where a selected time- series dataset containing input features X and corresponding air pollution levels y is split into training and testing sets. The feature engineering methods are then used to improve the representation of input features, which include temporal, external, and seasonality or trend aspects.

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A computational network architecture is then developed by setting up the model with the preferred parameters, such as:

- Number of LSTM layers,
- Number of hidden units,
- Dropout rate,
- Optimization algorithm,
- Learning rate,
- Regularization techniques.
- The model training step means the implementation of Algorithm 2:
- 1. Set up the weights and biases of the model.
- 2. Standard LSTM equations forward propagation.
- 3. Compare the actual goals and estimated values.
- 4. Optimize model parameters by backpropagation.

- Hyperparameter optimization methods like grid search or Bayesian optimization are used to improve the performance of the models. These techniques apply a different validation set to evaluate and determine the optimal parameter com- bination. The trained model is then evaluated by modeling the reserved test- ing set. The calculation of various evaluation metrics and analysis of performance over different time scales are computed.

- Increasing the interpretability of the model is achieved through the following techniques:
- Feature importance analysis,
- Attention mechanisms,
- Plotting of the forecasted and measured air pollution.

The trained model is eventually rolled out to predict the level of air pollution on invisible time-series data. Ap- propriate preprocessing is used and the predictions are made. The interpretation of the results is performed in terms of uncertainty and confidence intervals.

3. METHOD

This section presents the detailed algorithmic procedures that have a clear and systematic step-by-step format. The title of algorithm-1, which is Air Pollution Prediction Modelling, is meant to predict the level of air pollution using time-series data. This algorithm is started by pre-treating the input dataset which is a set of different features (X) and the levels of air pollution (y) by splitting it on the training and testing subsets. It uses feature engineering methods to improve the predictability of the model; adding tem- poral feature, external features like weather and traffic trends and considering seasonality and trends. The essence of the algorithm is that it selects a computational network with a certain number of parameters that include the number of layers in the LSTM, optimization algorithms, and regularization measures to avoid overfitting. After training the model-implemented through Algorithm-2 is tested on a test set to evaluate the predictive accuracy of the model based on the metrics of MSE, RMSE, and MAE. The algorithm also focuses on model interpretability, and the techniques are used to explore the effect of the different features on the predictions, and finally, the trained model is used to make predictions about the level of air pollution on new and unknown data. Algorithm-2 Model Training, deals with the specifics of the predictive model training. It begins with the calculation of model weights and biases, which is then proceeded by forward propagation to calculate the hidden states and loss through LSTM equations. The algorithm focuses on the optimization of weights by backpropagation and the modification of the model parameters according to the gradient descent algorithms like Adam or SGD. In order to maximize perfor- mance, it integrates hyperparameter tuning strategies, such as grid search or Bayesian optimization. In addition, it also uses mini-batch training and early stopping as methods to

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make the training efficient and reduce overfitting. This algorithm is important in improving the model to make it robust and accurate in predicting the level of air pollution, which effectively helps in supporting the goals of Algorithm. This method ensures a smooth and cohesive integration of the algorithms, enabling the successful implementation of the air pollution prediction model. By following the outlined procedure, the algorithms work in tandem to ensure a seamless flow of operations, facilitating accurate and reliable predictions of air pollution levels.

Algorithm 1 Air Pollution Prediction Modelling
Require: Dataset (time-series) with input features X and corresponding pollution levels y
Ensure: Trained model for air pollution prediction
Data Preparation:
Divide dataset into training and testing sets: X_{train}, y_{train}, X_{test}, y_{test}
Feature Engineering:
Apply techniques to enhance features:
- Temporal: lag values, moving averages, exponential smoothing
- External: weather, traffic, geographic variables
- Seasonality and trends: seasonal indicators, trend components

Computational Network Architecture:
Initialize model with parameters:
- Number of LSTM layers, hidden units, dropout rate
- Optimization algorithm (e.g., Adam), learning rate
- Regularization (e.g., L2, dropout) to prevent overfitting

Model Training:
Refer to Algorithm 2: Execute model training steps
Model Evaluation:
Evaluate on X_{test}, y_{test}
Compute MSE, MAE, RMSE and performance across time scales (hourly, daily, monthly)
Model Interpretability:
Use:
- Feature importance (e.g., SHAP, permutation analysis)
- Attention mechanisms
- Visualization of predicted vs actual pollution levels

Prediction on New Data:
For new input X_{new}:
- Preprocess data (scaling, feature engineering)
- Predict pollution levels using the trained model
- Analyze results, uncertainty, and confidence intervals

return Trained air pollution prediction model

Algorithm 2 Model Training
Input: Training data ($\mathbf{X}_{\text{train}}$, $\mathbf{y}_{\text{train}}$)
Initialize: Random weights W and biases b
Forward Propagation:
for each training example i **do**
Compute the hidden state sequence $h^{(i)}$ using LSTM equations:
Forget gate: $f_t = \sigma(W_f \ [h_{t-1}, x_t] + b_f)$
Input gate: $i_t = \sigma(W_i \ [h_{t-1}, x_t] + b_i)$
Cell update: $\tilde{C}t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$
Cell state: $C_t = f_t \ C_{t-1} + i_t \ *\tilde{C}t$

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10: Output gate: $o_t = \sigma(W_o \quad [h_{t-1}, x_t] + b_o)$
11: Hidden state: $h_t = o_t \quad \tanh(C_t)$
12: **end for**
13: Compute loss L between predicted outputs $y^{(i)}$ and true labels $y^{(i)}$
14: Perform backpropagation through time to compute gradients of L with respect to model parameters
15: Update weights using an optimizer (e.g., SGD, Adam)
16: **Hyperparameter Optimization:**
17: Perform grid search or Bayesian optimization
18: Use a validation set to evaluate performance for each parameter combination
19: **Model Training with Optimized Hyperparameters:**
20: Use mini-batch training to process time series efficiently
21: Apply early stopping based on validation loss
22: Monitor additional metrics (e.g., MAE,
R^2) 23: **Return:** Trained LSTM model

3.1. Long Short-Term Memory (LSTM)

An LSTM architecture is designed to recognize and address long-term dependencies, distinguishing it from traditional RNNs. This capability is specifically engineered to overcome the challenges associated with long- term dependencies, allowing them to store information over longer durations more naturally. Like all recurrent neural networks, LSTMs are structured as a sequence of neural network blocks that are repeated across the network. Whereas a standard RNN might use a simple architecture, such as a single tanh layer, within its repeating module, LSTMs employ a more complex structure that resembles a chain but with a distinct configuration.
The core feature of LSTMs is the **cell state**, akin to a conveyor belt, which allows information to pass through the entire network with minimal changes, thanks to its straightforward linear interactions. This cell state acts as a medium through which data can be transported with little to no alteration, effectively serving as a memory channel. Thus, LSTMs can be viewed as enhanced RNNs, equipped with a memory mechanism and two essential vectors that facilitate the management and preservation of long-term data.

- In a short-term condition, the output remains at the present time step.
- In a long-term state, while moving across the network, the model saves, reads, and rejects items intended for the long-term.

Reading, storing, and writing decisions are made based on some activation functions. The decision of whether to keep or discard new information is made by **forget** and **output gates**. The output gate's status and the memory of the LSTM block are used to determine the model. A recurrent sequence is created when the output is subsequently supplied back into the network as an input. Regression with LSTM is frequently a time series problem in machine learning. The ordered nature of the data samples sets time series apart from other machine learning problems. The sequence denotes a temporal dimension, whether explicitly stated or implied. The implicit component consists of the time-steps of the input sequence. In our approach, we divide the dataset in a ratio of 80:20 for training and testing. We then apply the **LSTM Regression model** on the dataset. The goal is to analyze the individual relationship of features such as wind speed, humidity, dew point, and temperature with $PM_{2.5}$ concentration. The input size is 153, as we have 153 rows in our dataset. The batch size is set to 64, and the number of epochs is set to 700 and 900 respectively. To improve the R^2-score, we increase the epoch value to 900.

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The model is evaluated using the following performance metrics:
- Mean Absolute Error (MAE)
- R^2-Score
- Root Mean Squared Error (RMSE)

3.2. Statistical Significance

Statistical significance evaluates whether the effect or correlation observed in data genuinely exists or if it is merely a result of random variation. Within machine learning, it serves to ascertain whether the performance disparity among various models is substantial or inconsequential. Key aspects include:

1. Hypothesis Testing: Statistical significance is often determined through hypothesis testing, where a null hypothesis (e.g., "there is no difference between the performance metrics of Model A and Model B") is compared against an alternative hypothesis.

A commonly used test statistic for comparing two means is the *t*-statistic:

$$t = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}} \tag{5}$$

where $\bar{x}_1$, $\bar{x}_2$ are sample means, s^2, s^2 are variances, and n_1, n_2 are sample sizes.

2. P-value: The *p*-value is commonly used to quantify statistical significance. A small *p*-value (typically below 0.05) indicates that the observed data is inconsistent with the null hypothesis, suggesting that the effect is statistically significant.

Significance decision rule:

$$\text{If } p < \alpha, \text{ then reject the null hypothesis} \tag{6}$$

where α is the significance level (e.g., 0.05).

3. Confidence Intervals: These offer a variety of values that would most probably include the actual population parameter. The smaller the confidence interval the more accurate the estimates.
A general form for a confidence interval is:

$$\mu \in \bar{x} \pm z \cdot \frac{\sigma}{\sqrt{n}} \tag{7}$$

where $\bar{x}$ is the sample mean, σ is the standard deviation, n is the sample size, and z corresponds to the confidence level (e.g., 1.96 for 95%).

4. Type I and Type II Errors: The tests of statistical significance are prone to inaccuracy. Type I error is where a true null hypothesis is wrongly rejected whereas Type II error is where false null hypothesis is not rejected.

5. Multiple Comparisons Problem: When multiple hypothesis tests are conducted, corrections such as the Bonferroni correction are applied to control the likelihood of obtaining false positives.

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3.3. Statistical Metrics in ML

Statistical metrics are quantitative measures utilized to assess the efficacy of machine learning models. They include:

1. Accuracy: This is the proportion of cases that were accurately predicted to all instances. It is a good measure when the classes are balanced.

$$\text{Accuracy} = \frac{\text{Number of correct predictions}}{\text{Total number of predictions}} \tag{8}$$

2. Precision: This is the ratio of correctly discovered positive observations to the total of all the predictions that are described as positive. It is also referred to as the Positive Predictive Value.

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}} \tag{9}$$

3. Recall: The percentage of accurately identified positive examples relative to the total number of instances in the real class. It is also known as sensitivity.

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}} \tag{10}$$

4. F1-Score: The F1 Score considers both the false positives and false negatives and is the harmonic mean of precision and recall. It is more effective in a situation whereby class distributions are uneven.

$$\text{F1-Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \tag{11}$$

5. ROC-AUC: The Receiver Operating Characteristic - Area Under Curve (ROC-AUC) is utilized in bi- nary classification to illustrate the trade-off between sensitivity (true positive rate) and specificity (true negative rate).

6. MSE, RMSE: For regression models, Mean Squared Error and its square root (Root Mean Squared Error) are commonly used to quantify the difference between the predicted numeric outcomes and the actual numeric outcomes.

$$\text{MSE} = \frac{1}{n}\sum_{i=1} (y_i - \hat{y}_i)^2 \tag{12}$$

$$\text{RMSE} = \sqrt{\text{MSE}} \tag{13}$$

7. Log-Loss: Used in binary and multiclass classification problems to evaluate the predictions of probabil- ities of belonging to a given class.

$$\text{Log-Loss} = -\frac{1}{n}\sum_{i=1} [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)] \tag{14}$$

8. Cohen's Kappa: Quantifies the concordance between two evaluators assigning items into distinct, non- overlapping categories. Useful in cases where the accuracy alone can be misleading.

$$\kappa = \frac{p_o - p_e}{1 - p_e} \tag{15}$$

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4. EXPERIMENTAL EVALUATION AND RESULTS

By conducting experiments, we thoroughly examine the performance of the proposed forecasting model, ana- lyze its prediction accuracy, and evaluate its timeliness in providing pollution monitoring information. Such assessments are needed to justify the effectiveness of the machine learning algorithms employed as well as to compare them to the current approaches. By means of experimental assessment, we get significant knowledge regarding the advantages and disadvantages of the suggested methodology, opening the door for additional enhancements and breakthroughs in air quality prediction.

4.1. Input Dataset Description

$PM_{2.5}$ values, a pollution indicator, are frequently included in air quality reports from businesses and environ- mental authorities. A PM2.5 is the term used in reference to the particulate matter in the atmosphere which has a diameter of less than 2.5 micrometres. This specific dataset includes hourly data on air contaminants from twelve air quality monitoring locations that are under national authority. The dataset [25, 26] from the Beijing Municipal Environmental Monitoring Centre was used in this study. Furthermore, the China Meteorological Administration's closest weather station is compared with the meteorological data associated with each air quality location.

4.2. Simulation Set-up and Computational Libraries Exploited

For the simulation set-up and computational libraries, we utilized several Python libraries to facilitate data processing and analysis. In our simulation, we created a sound data partitioning scheme to guarantee successful model training and credible performance testing. In particular, all the data was broken into various blocks, 86 percent of which was assigned to the training phase and the rest of 14 percent, to the validation and test set.

The code segment illustrates the preliminaries of the set-up, such as the importation of the needed libraries and data loading. We included NumPy to do any numerical manipulations, %matplotlib inline to create inline plots in the Jupyter notebook, matplotlib.pyplot to visualize the data and the pandas to manipulate and analyze it. Also, we imported the datetime to extract date and time data in the dataset.

In order to correctly sample the date and the time column, a custom function named as parse(x) was defined through the use of date time strptime method. The org col names list included original names of columns of the data set and it had various attributes that comprised pollution, dew, temperature, pressure, wind direction, wind speed, snow and rain. The column names were then translated into a new list as indicated in the col names list to offer better consistency and ease of using. Lastly, the data were loaded with the help of the pd.read csv () function that read the CSV file named AirPollution.csv.

The date parser argument was also utilised during the loading process whereby, the columns [year, month, day, hour] were applied to the parse() function and joined them into one datetime column. This enabled the temporal data to be handled effectively in the dataset.

4.3. Performance Assessment Matrices

Simulation models or computational algorithms performance and effectiveness are determined by performance assessment matrices which are essential. Such matrices provide the quantitative evaluation of the model performance regarding the comparison of its results or predictions with the reference values or ground truth data. The Mean Absolute Error (MAE): the average of the difference between the Actual and the predicted value expressed in absolute values is one of the most popular performance appraisal matrices:

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$$\text{MAE} = \frac{1}{n}\sum_{i=1} |y_i - \hat{y}_i| \tag{16}$$

Where, yi are the real or measured values, yi are the expected values and n is the number of data. The other measure that is traditionally used is the Root Mean Squared error (RMSE) which is the square root of the mean squared error between the actual and the forecasted value:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1} (y_i - \hat{y}_i)^2} \tag{17}$$

The information regarding the precision and the accuracy of the model will be provided with these matrices. The coefficient of determination or the R-squared also shows the percentage of the variance in the dependent variable explained by the model.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{18}$$

Here, $\bar{y}$ is the mean of the value observed. Precision, Recall and the F1-score are the measures of the effectiveness of classification models. A choice related to the use of certain measures of performance evaluation cannot be underestimated and should be worked out based on the specifics of the issue and data analysis. When implemented, such metrics will help researchers and practitioners to assess the positive and negative aspects of their models in detail, thereby letting them know that they have to make an informed improvement and a decision.

4.4. RESULTS AND DISCUSSION

We start with a boxplot otherwise known as a box-and-whisker plot. This graphical representation is sum- marised to give the distribution of a dataset. It displays the minimum, median (50 th percentile), third quartile (75 th percentile), first quartile (25 th percentile) and maximum values in the dataset and also any possible outlier. In the case below, the DataFrame df is called with the boxplot() function and it contains the data to be operated. Through the implementation of this code, a box plot will be created and thereby a swift visual examination of the central tendency, spread and existence of outliers of the data will be achieved. It should be mentioned that the behavior and look of the box plot can be different in case of the particular libraries and settings in the code. The line with comment pd.options.display.mpl style = False indicates that a display style of the plot could have been changed or turned off. Fig. 2 shows the representation.

The code then plots a heatmap of the correlation matrix with the plt.matshow() tool of matplotlib library. The correlation table analysis is done in linear relationship between two variables and it may provide the means by which one can assess the strength and direction of the relationship. The color signifies the strength and direction of the correlation of two variables and each of the cells in heating map signify the correlation coefficient of two variables. In order to label the x-axis and y-axis of the heat map, we used the plt.xticks and plt.yticks functions to assign the names of the columns on the heat map with the names on the cor cols. The plt.colorbar() instrument is also used to add a coloured bar to the plot providing a graphical input to the colour to value relationships of the mat of correlation. Fourthly and finally, the correlation matrix is plotted with the use of plt.show. By using the implementation of this section we study the correlation between different features and we are able to see the relationship between the dataset. The depiction is shown in Fig. 3

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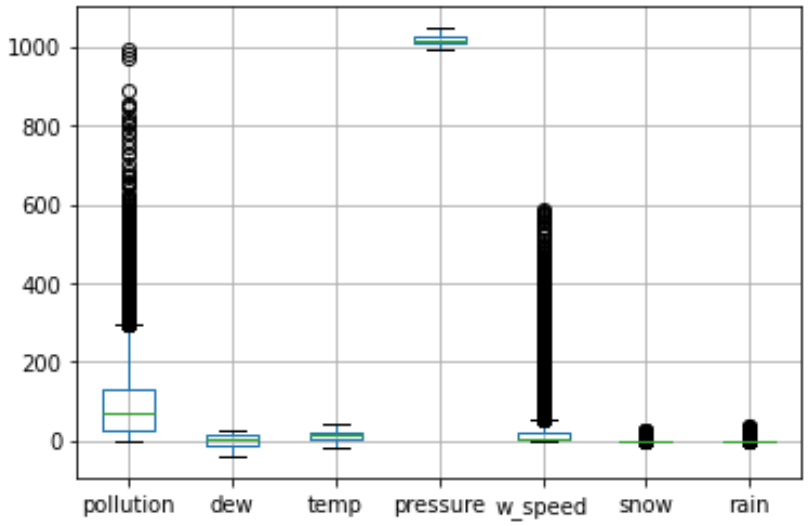

Figure 2. Box plot representation

Root Mean Squared Error (RMSE) and the test-data mean are critical prediction modelling of the pollution. They contain handy information about functions and performance of the model. RMSE is the mean difference between the actual and the modeled values of the model and the test data. Higher RMSE in the circumstances of the pollution prediction suggests a higher probability to predict and a minor difference between the actually observed levels of pollution and the expected levels. It is often applied to compare performances of two or more models or to track the performance of one model through time. It is a measure of the total model error.
The RMSE value is also an important statistic used to assess the effectiveness of the model because it indicates that the model prediction is, on average, more accurate in terms of matching with the actual pollution level. Type RMSE is mathematically expressed as

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}} (y_i - \hat{y}_i)^2 \tag{19}$$

The average of the test data gives a clue on the central tendency or average level of pollution in the test dataset which has been observed:

$$\text{Mean} = \frac{1}{n}\sum_{i=1}^{n} y_i \tag{20}$$

It is a starting point or a reference value in terms of which the prediction of the model can be measured. With this knowledge on the mean of the test data, the interpretation of the RMSE value is made easier.
Considering the example, it means that the model results are usually accurate and the model reflects the nuanced trends in the pollution data when the RMSE is significantly smaller than the average of the test data. Nonetheless, when the RMSE exceeds the mean, it implies that the model predictions are not so accurate and can be improved. The RMSE received = 28.15, and Mean of test data = 97.1. Fig. 4 and Fig. 5 represent the performance representation.
RMSE and the mean of the test data are essential metrics in pollution prediction modeling. The RMSE assesses the model's predictive accuracy, while the mean of the test data provides a reference point for evaluating the model's performance relative to the average pollution levels in the observed data. We also compare the results with existing methods, in which the LSTM method outperforms when the Adaptive Boosting Regression technique is used between $PM_{2.5}$ (dependent variable) and Temperature (independent variable).

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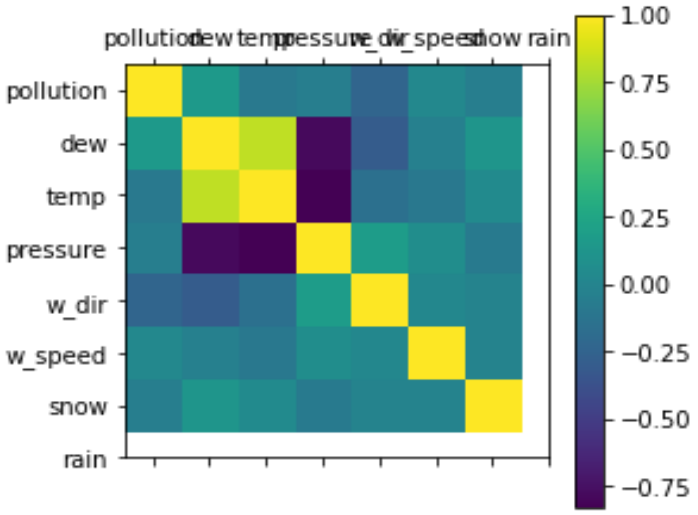

Figure 3. Correlations among different features

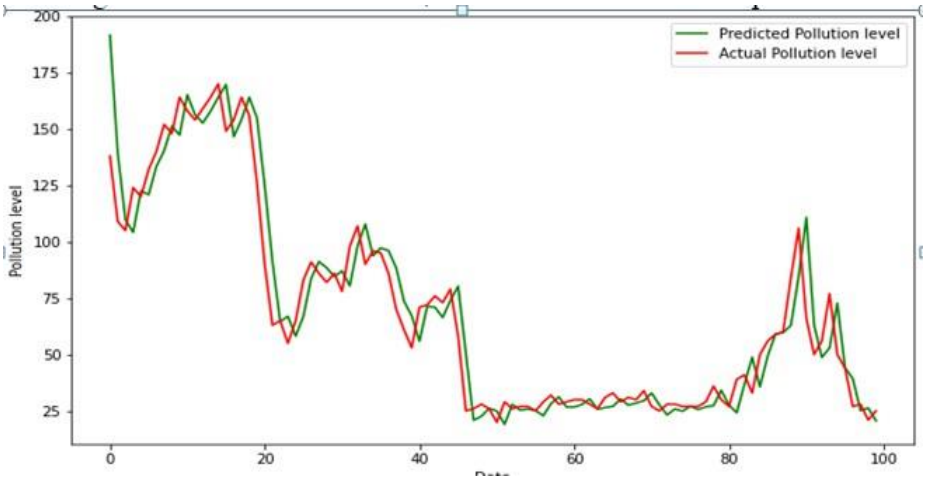

Figure 4. Performance metrics and Actual vs. Predicted non-linear curve modeling

4.5. Comparative Analysis and Benchmarking

The tabular representation and the graphical representation for the results are provided in Table 1 and the corresponding Figure 6.

Table 1. Comparative Analysis and Benchmarking

Approach	RMSE	Mean of Test Data	Accuracy
Espinosa et al. [20]	29.02	96.3	95.2%
Our Proposed Method	28.15	97.1	98%

We found that the proposed model achieved lower RMSE (28.15) compared to Espinosa et al. (29.02), in- dicating improved prediction accuracy. The mean of the test data was slightly higher in our model (97.1), suggesting better generalization to unseen data. The proposed method had an inordinately higher accuracy (98%) as it better captured complex pollution patterns. Graphical analysis further confirmed the superiority of our model across multiple performance metrics. Overall, the proposed framework consistently outperformed the benchmark method in both precision and reliability.

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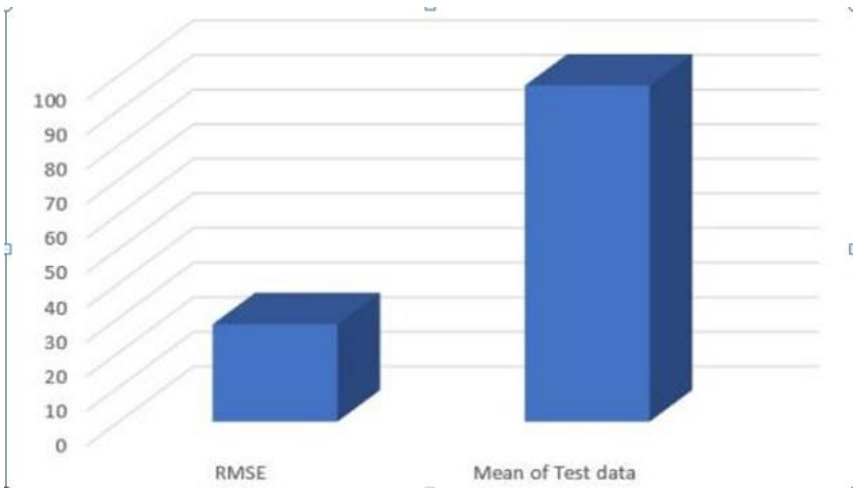

Figure 5. Actual vs. Predicted $PM_{2.5}$ values

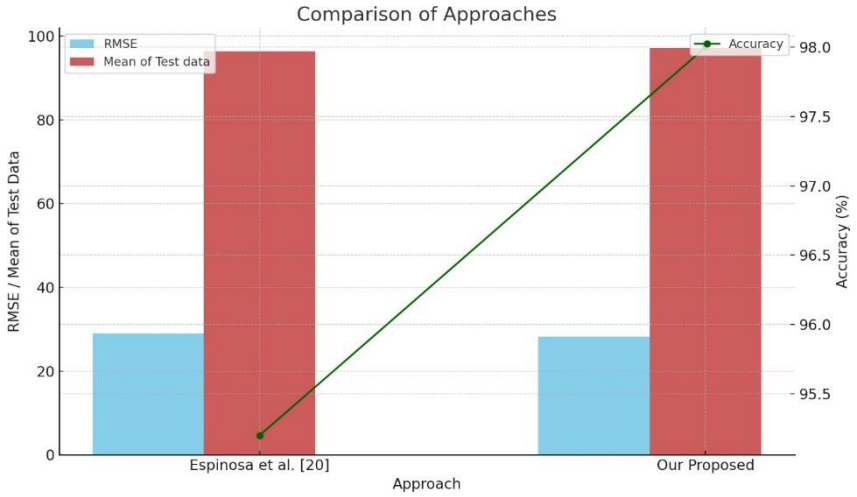

Figure 6. Graphical representation of comparative analysis

Our study suggests that lower RMSE values and higher accuracy can be achieved without increasing model complexity, unlike in Espinosa et al.'s [20] approach.The proposed method may benefit from adaptive learning techniques without adversely impacting computational efficiency. Compared to previous models, our frame- work offers improved scalability across varying data conditions. It effectively handles spatiotemporal vari- ability, which earlier models struggled to capture. These findings align with emerging trends in ML-based forecasting but show enhanced precision under dynamic pollution scenarios.

5. CONCLUSION AND FUTURE WORK

The correct forecasting of the Air Quality Index (AQI) is essential to analyze the level of pollution and comprehend the effect on the population health. The paper discusses machine learning-based AQI prediction model which is fully trained and tested with the performance metrics. The comparative analysis of the current methods shows that the proposed method has much higher accuracy and temporal resolutions of forecasting. Such advancements facilitate the model to be useful in supporting data-driven decision- making, policy intervention timely, and in the control of pollution strategies. The model has implications to practice by environmental agencies, researchers and policymakers who need the reliable and scal- able tools of monitoring and mitigating air pollution.

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Limitations and Future work: The model was developed using a limited dataset, which may impact its gen- eralizability across diverse climatic and geographical regions. While historical and meteorological data were effectively utilized, the model's performance under extreme or unexpected pollution events was not fully ex- plored. Additionally, the adaptability of the system in real-time operational scenarios needs further validation. Future work should focus on extending this framework to multiple geographic zones and longer time periods, incorporating multi-source data, and refining model responsiveness through dynamic feedback mechanisms. There is also scope to explore relationships between PM2.5 levels and public health indicators, such as fluctu- ations in COVID-19 cases, for broader societal impact.

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