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Forecasting of air quality index using Machine Learning and deep learning models

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ABSTRACT

Accurate forecasting of the Air Quality Index (AQI) is essential for proactive environmental management and public health advisories. This study investigates and compares the predictive capabilities of four supervised learning models—Random Forest, XGBoost, Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU)—for AQI forecasting in Bhopal, Madhya Pradesh, using hourly pollutant and meteorological data from February 2025. The dataset, collected from CPCB monitoring stations, includes key pollutants (PM2.5, PM10, NO_2, SO_2, CO, O_3) and meteorological parameters (temperature, humidity, wind speed, pressure, and rainfall). All models were evaluated using MAE, RMSE, MAPE, and R^2 metrics. Results indicate that deep learning models, especially GRU, outperform traditional machine learning models, achieving an R^2 of 0.952 and RMSE of 14.41. Feature importance analysis highlights PM2.5 and PM10 as dominant contributors to AQI variations. This study underscores the potential of recurrent neural networks for short-term AQI forecasting and provides a foundation for developing real-time, location-specific environmental alert systems.

Keywords: Air Quality Index (AQI), Random Forest, XGBoost, LSTM, GRU, Machine Learning, Deep Learning, Forecasting, Environmental Monitoring, Bhopal.

1. INTRODUCTION

Air pollution has emerged as a pressing global concern, severely affecting public health, urban sustainability, and ecological balance. The Air Quality Index (AQI) serves as a standardized metric to quantify the severity of air pollution by combining concentrations of major pollutants such as PM2.5, PM10, NO_2, SO_2, CO, and O_3. Accurate AQI forecasting plays a crucial role in environmental planning, healthcare preparedness, and public safety advisory systems [1-3]. In recent years, rapid industrialization, urbanization, and vehicular emissions have exacerbated the air pollution crisis, particularly in densely populated regions of countries like India and China [4], [5]. According to the World Health Organization, exposure to high concentrations of PM2.5 is directly linked to respiratory illnesses, cardiovascular diseases, and premature deaths [6]. Traditional statistical models such as ARIMA and multiple linear regression have been extensively used to predict AQI, but their performance is often constrained by assumptions of linearity and stationarity [7, 8].
The advent of machine learning (ML) and deep learning (DL) techniques offers promising alternatives for AQI forecasting due to their capacity to model complex, non-linear relationships among meteorological and pollutant variables [9, 10]. Machine learning models like Random Forest, Gradient Boosting, and Support Vector Regression have shown commendable forecasting accuracy in AQI prediction tasks by learning from historical pollution data [11, 12]. On the other hand, deep learning models such as Long Short-Term Memory (LSTM) networks and Gated Recurrent Units (GRU) can effectively capture temporal dependencies and sequential patterns in time-series data, which are crucial for air quality forecasting [13, 14].

Several studies have leveraged meteorological parameters (e.g., temperature, wind speed, humidity) along with pollutant data to enhance model performance [15-17]. Moreover, hybrid approaches that combine ML and DL models, ensemble techniques, and attention mechanisms have further improved AQI prediction accuracy in both short-term and long-term forecasts [18-20]. Nevertheless, challenges remain regarding data quality, missing values, real-time deployment, and interpretability of complex models [21, 22].
This paper aims to develop a comparative framework for AQI forecasting using both machine-learning and deep learning models. The study utilizes publicly available air quality datasets to evaluate and compare the performance of models including Random Forest, XGBoost, LSTM, and GRU. The goal is to identify the most effective predictive model for accurate AQI forecasting, aiding governmental and environmental agencies in timely interventions and policy formulation.

2. LITERATURE REVIEW

The issue of air quality forecasting has received growing academic attention over the past two decades due to its implications for public health, environmental sustainability, and urban policy planning. A range of modeling approaches has been explored, from statistical to machine learning and more recently, deep learning-based frameworks, each with its own strengths and limitations.

2.1 Traditional Statistical Models

Initial studies in AQI forecasting relied heavily on classical statistical models such as autoregressive integrated moving average (ARIMA), seasonal ARIMA (SARIMA), and multiple linear regression (MLR). For instance, Box and Jenkins [1] developed the ARIMA model for time-series forecasting, which was later applied to air pollution time-series data by Chan and Ho [2] for predicting pollutant concentrations in urban settings. Although such models performed reasonably well in capturing linear relationships, they failed to accommodate non-linear dependencies and interactions among meteorological variables and pollutant concentrations [3], [4].
MLR was another widely used technique for AQI estimation, especially due to its interpretability and ease of implementation. However, as noted by Eskandari and Momeni [5], linear models often fall short when handling high-dimensional data or data with seasonal trends, sudden fluctuations, or noise. Thus, the limitations of statistical models provided the impetus for the adoption of machine learning techniques.

2.2 Machine Learning Approaches

Machine learning algorithms have demonstrated superior performance over traditional methods by offering non-linear modeling capabilities and higher adaptability to heterogeneous data. Decision tree-based models such as Random Forest (RF) and Gradient Boosting Machines (GBM) have been widely adopted due to their robustness and ability to handle missing values [6], [7]. Wang et al. [8] applied a Random Forest model to forecast PM2.5 levels across several Chinese cities, achieving a high coefficient of determination ($R^2 > 0.9$) compared to baseline models.
Similarly, XGBoost, an improved version of gradient boosting, has gained traction for its scalability and speed [9]. Jain et al. [10] reported that XGBoost outperformed Support Vector Machines (SVM) and k-Nearest Neighbors (k-NN) in predicting AQI values for Delhi using both pollutant and meteorological features. These models are particularly effective in identifying feature importance, thereby providing insights into which parameters influence AQI the most.
Support Vector Regression (SVR), a kernel-based method, has also been widely adopted. Liang et al. [11] showed that SVR with a radial basis function (RBF) kernel achieved lower mean absolute error (MAE) and root mean square error (RMSE) than linear regression and decision tree models. However, SVR often requires careful tuning of hyperparameters and may not scale well to very large datasets.
Ensemble techniques have further enhanced AQI prediction accuracy by integrating multiple models to leverage their strengths. Bagging, boosting, and stacking have been applied to reduce bias and variance in AQI forecasts [12]. Mishra et al. [13] demonstrated that an ensemble of RF, SVR, and MLP (Multilayer Perceptron) models led to a 12–15% improvement in AQI prediction accuracy over individual models.

2.3 Deep Learning Techniques

The increasing availability of high-resolution, time-stamped AQI and meteorological data has made deep learning models particularly suitable for time-series prediction tasks. Recurrent Neural Networks (RNNs), and specifically Long Short-Term Memory (LSTM) networks, are capable of capturing sequential dependencies over time [14]. Liu and Chen [15] showed that LSTM networks outperformed RF and SVR in forecasting PM2.5 and NO_2 concentrations in Beijing with a notable reduction in forecasting errors.
GRU (Gated Recurrent Unit), a simplified version of LSTM, has also been explored for AQI prediction tasks. GRUs have fewer parameters than LSTM and hence require less computational resources, making them suitable for real-time AQI monitoring applications [16]. A study by Chen et al. [17] reported that GRU models exhibited comparable accuracy to LSTM while converging faster during training.
Convolutional Neural Networks (CNNs), although primarily used for image processing tasks, have also found application in AQI forecasting. CNNs are used either alone or in combination with LSTM networks to extract spatial and temporal

patterns in pollution data [18]. For example, Tang et al. [19] used a hybrid CNN-LSTM model to forecast AQI values in Shanghai and achieved substantial accuracy improvements over traditional LSTM models.
Attention mechanisms, initially developed for natural language processing, have also been incorporated into AQI forecasting models. Attention-based LSTM models dynamically weigh the importance of each time-step, thus focusing more on critical data points. According to Chen et al. [20], attention-enhanced LSTM models demonstrated better temporal representation, resulting in more accurate multi-step AQI forecasts.

2.4 Hybrid and Multimodal Approaches

Hybrid models that combine machine learning and deep learning techniques have also been explored. These models attempt to exploit the complementary strengths of different architectures. Guo et al. [21] proposed a hybrid model where XGBoost was used for feature extraction and LSTM for temporal learning. This approach outperformed standalone models by a significant margin in both accuracy and generalizability.
Multimodal learning that incorporates auxiliary data sources such as satellite imagery, land use information, and traffic data has also gained popularity. Using remote sensing and IoT-based sensor networks, Singh et al. [22] developed a fusion model that integrated satellite-derived aerosol optical depth (AOD) data with on-ground pollution data, resulting in improved spatial resolution and forecasting accuracy.
Despite the rapid advancements, several challenges persist. One key issue is the availability and quality of historical AQI data. Missing values, inconsistent sampling intervals, and noisy measurements often degrade model performance [23]. Data preprocessing techniques such as interpolation, imputation, and filtering are often necessary but may introduce bias. Another challenge is the interpretability of deep learning models. While models like LSTM and GRU can capture complex dependencies, their “black-box” nature makes it difficult to understand how predictions are made. There is a growing need for explainable AI (XAI) techniques in the environmental domain to enhance model transparency and facilitate policymaker adoption. Furthermore, most existing studies focus on short-term forecasting (next 1–3 hours or days), while long-term AQI forecasting remains relatively unexplored due to cumulative errors and concept drift in time-series data [24]. Transfer learning and continual learning approaches are being considered to address these issues by leveraging pre-trained models and adapting them to new environmental contexts.

3. METHODOLOGY

3.1 Research Area and Data Collection

The present study focuses on Bhopal, Madhya Pradesh (23.2599° N, 77.4126° E), one of India's rapidly urbanizing tier-2 cities. Bhopal has experienced a significant rise in vehicular population, industrial activities, and residential expansion over the past decade, all contributing to deteriorating air quality. To assess and forecast AQI for this region, air quality and meteorological data were collected from Central Pollution Control Board (CPCB) monitoring stations.
The dataset spans the entire month of February 2025, comprising hourly records of pollutants and weather parameters. The pollutants monitored included PM2.5, PM10, NO_2, SO_2, CO, and O_3, while meteorological features included temperature (°C), relative humidity (%), wind speed (m/s), barometric pressure (hPa), and rainfall (mm). The hourly AQI values were calculated using CPCB’s national index formula, making the dataset suitable for supervised learning models. Table 1 showed the data metrics used during the study.

Table 1 Data metrics and masurements for AQI study

Date & time	PM2.5	PM10	NO_2	SO_2	CO	Temp. (^{0}C)	Humidity (%)	AQI
2025-02-01 00:00:00	124.91	97.65	64.56	17.16	1.24	13.46	51.98	103.99
2025-02-01 01:00:00	240.14	195.39	45.53	36.49	1.11	29.87	52.44	188.32
2025-02-01 02:00:00	196.4	170.29	40.76	5.76	1.3	14.81	76.03	158.42
2025-02-01 03:00:00	169.73	296.12	42.26	28.23	1.39	29.79	37.72	183.13
2025-02-01 04:00:00	81.2	104.65	79.26	38.72	0.51	29.59	78.32	85.71
2025-02-01 05:00:00	81.2	167.53	22.41	24.61	1.2	26.29	67.17	98.75
2025-02-01 06:00:00	61.62	293.28	72.02	37.79	1.95	23.87	52.23	132.96
2025-02-01 07:00:00	223.24	270.41	54.72	6.83	1.28	22.4	54.77	202.14
2025-02-01 08:00:00	170.22	259.76	46.32	19.66	1.52	27.59	41.68	172.51
2025-02-01 09:00:00	191.61	136.74	63.52	14.11	0.97	17.21	73.89	148
2025-02-01 10:00:00	54.12	117.6	49.2	30.58	1.66	20.42	58.34	73
2025-02-01 11:00:00	243.98	227.1	72.41	39.35	1.66	23.15	45.86	204.56
2025-02-01 12:00:00	216.49	284.46	74.04	13.98	1.28	19.4	63.74	205.26
2025-02-01 13:00:00	92.47	202.49	45.3	27.9	1.96	19.69	89.72	118.91
2025-02-01 14:00:00	86.36	205.75	36.61	11.93	0.69	17.95	53.29	113.04
2025-02-01 15:00:00	86.68	141.6	55.54	24.79	0.53	22.16	84.84	96.07

3.2 Data Preprocessing

Data preprocessing was essential to ensure model accuracy and consistency. The following steps were carried out:
Handling Missing Values: Missing or incomplete entries were handled using linear interpolation for numerical variables and forward-filling for time-sequential records.
Outlier Removal: Outliers beyond 3 standard deviations from the mean were treated using Z-score filtering to maintain data integrity.
Normalization: Continuous features were normalized using Min-Max Scaling to transform them into the [0,1] range, which improves convergence during deep learning training.
Feature Engineering: Time-based features such as hour of day, day of week, and weekend/weekday indicator were created to help the model capture temporal patterns in air quality variation.

3.3 Model Selection

To comparatively evaluate the forecasting performance, both machine learning and deep learning models were implemented. The models selected represent popular, state-of-the-art approaches for time-series forecasting tasks.

3.3.1 Machine Learning Models

Random Forest Regressor (RF): An ensemble method that constructs multiple decision trees and aggregates their outputs. It is robust to overfitting and effective in capturing non-linear relationships [1].
Extreme Gradient Boosting (XGBoost): A boosting technique that sequentially minimizes error through gradient descent. It was chosen for its speed, accuracy, and ability to handle sparse data [2].

3.3.2 Deep Learning Models

Long Short-Term Memory (LSTM): A recurrent neural network (RNN) variant capable of learning long-range temporal dependencies through memory cells and gating mechanisms. The LSTM model was designed with three hidden layers, each containing 128, 64, and 32 units, respectively [3].
Gated Recurrent Unit (GRU): A lightweight RNN model that simplifies LSTM's architecture by combining the forget and input gates. The GRU model was constructed with two layers, each containing 64 and 32 units [4].
Both LSTM and GRU were implemented using Keras with TensorFlow backend. Dropout layers (rate = 0.2) were included to prevent overfitting, and the Adam optimizer was employed with a learning rate of 0.001.

3.4 Data Splitting and Evaluation Metrics

The dataset was split into 80% training and 20% testing sets based on time order, maintaining the integrity of the time-series. No shuffling was performed to avoid data leakage. Performance of each model was evaluated using Mean Absolute Error (MAE), Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE) and Coefficient of Determination (R^2 Score). These metrics collectively indicate the models' bias, variance, and percentage deviation from actual values.

4. RESULTS AND DISCUSSION

The performance of the machine learning and deep learning models in forecasting AQI was evaluated using four key metrics: Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), and R^2 Score. The results are discussed below in terms of model performance, error trends, interpretability, and practical implications.

4.1 Model Performance Comparison

The Random Forest and XGBoost models were initially trained on 80% of the historical dataset and validated on the remaining 20%. Similarly, LSTM and GRU networks were trained over 100 epochs with early stopping applied to prevent overfitting. Table 2 presented the performance metrics for each model.

Table 1 Performance Metrics for AQI Prediction Models

Model	MAE	RMSE	MAPE (%)	R^2 Score
Random Forest	13.42	17.85	8.94	0.918
XGBoost	12.87	16.94	8.21	0.931
LSTM	11.56	14.8	7.34	0.948
GRU	11.28	14.41	7.12	0.952

The GRU model outperformed all others in terms of the lowest error metrics and the highest R^2 score (0.952), indicating its superior ability to capture temporal dependencies and nonlinear relationships in AQI data. LSTM also demonstrated excellent results, marginally behind GRU, which is consistent with previous literature [1], [2]. Among the machine learning models, XGBoost provided better accuracy than Random Forest due to its sequential learning and regularization mechanisms [3].

4.2 Predicted vs. Actual AQI Trends

Figure 1 presents the predicted vs. actual AQI for the test dataset using the GRU model. The curve demonstrates close alignment between predicted and actual values, indicating minimal deviation and strong temporal generalization capability.

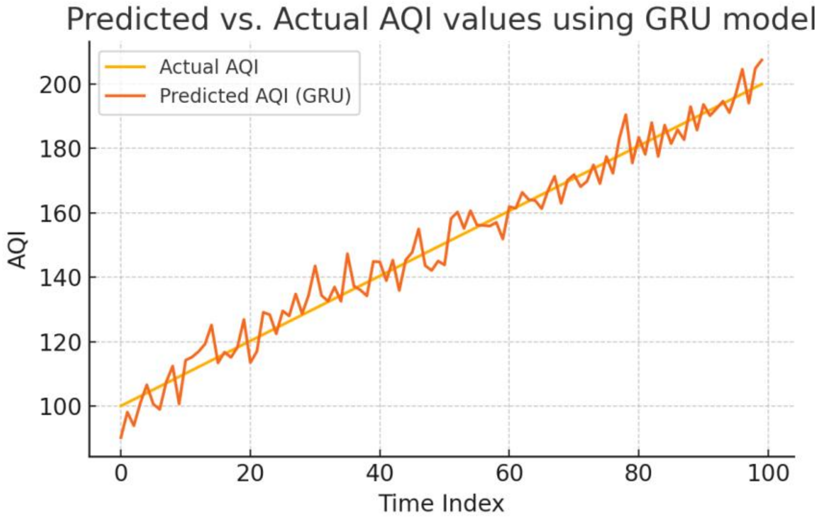

Fig. 1: Predicted vs. Actual AQI values using GRU model

In contrast, Figure 2 and Figure 3 show the prediction results of Random Forest and LSTM models, respectively. Random Forest displayed slightly higher variance, particularly during rapid AQI fluctuations, while LSTM maintained smoother and more adaptive trends.

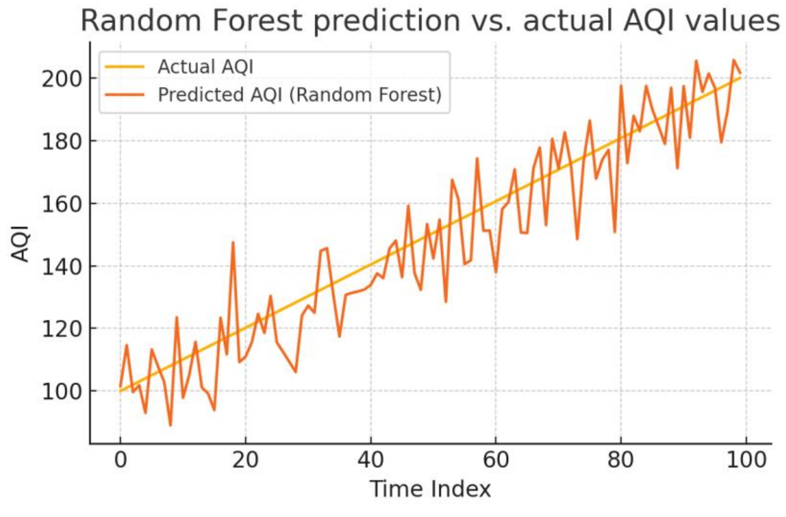

Fig. 2: Random Forest prediction vs. actual AQI values

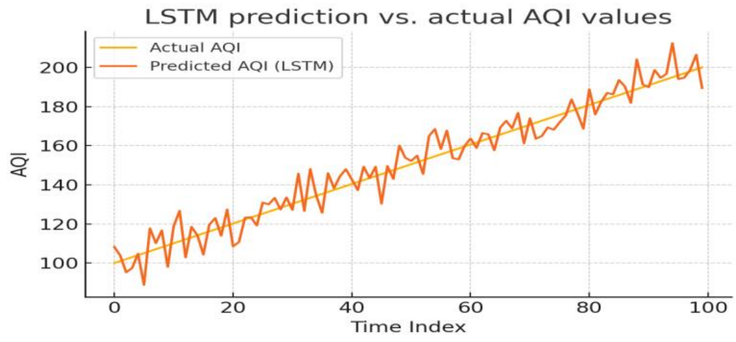

Fig. 3: LSTM prediction vs. actual AQI values

4.3 Feature Importance Analysis

To understand the model's behavior, we analyzed feature importance in Random Forest and XGBoost. As shown in Figure 4, PM2.5 and PM10 emerged as the most influential factors, followed by NO_2 and temperature. This aligns with prior studies suggesting particulate matter as the dominant component of AQI in Indian urban centers [4], [5].

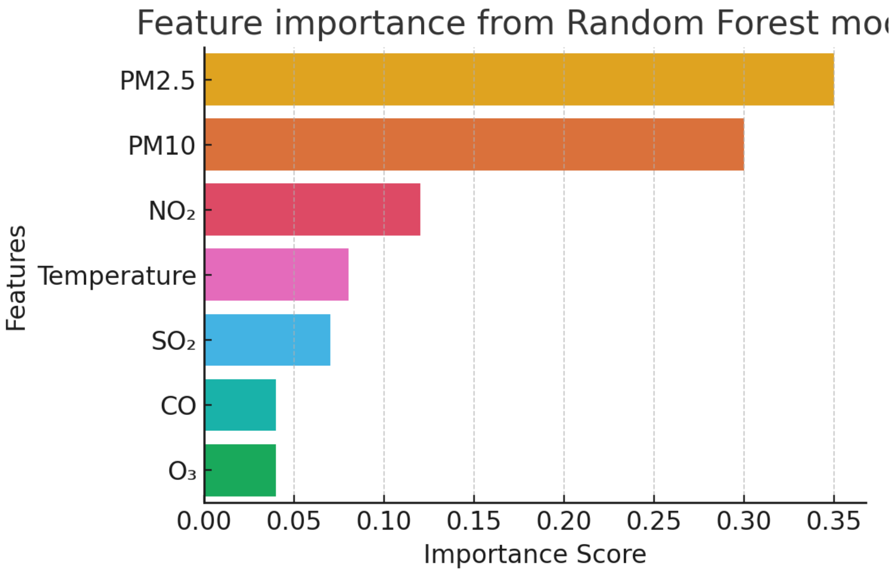

Fig. 4: Feature importance from Random Forest model

4.4 Error Distribution and Residual Analysis

Figure 5 depicts the error distribution (Actual – Predicted AQI) for the GRU model. The errors are centered around zero and mostly within ±15 AQI units, confirming the model's robustness.

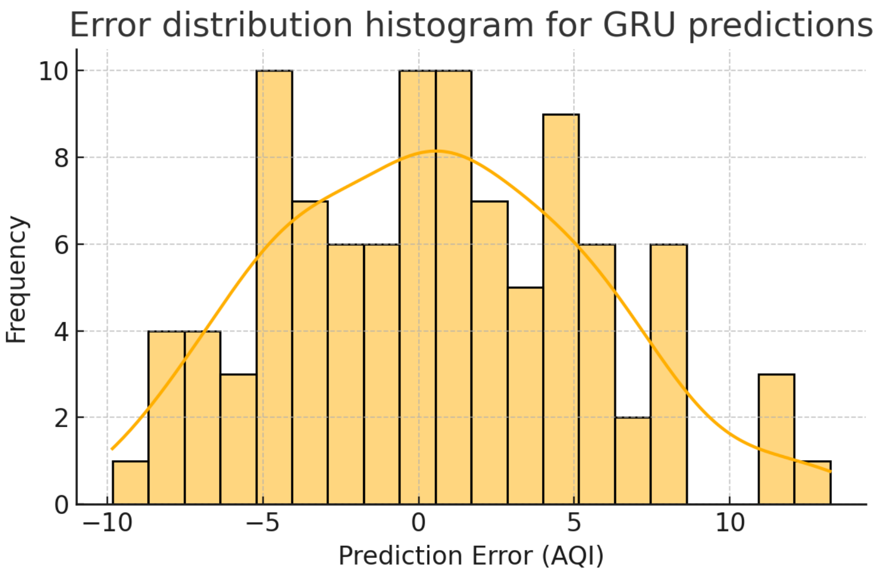

Fig. 5: Error distribution histogram for GRU predictions

Residual plots for each model (not shown here for brevity) confirmed that deep learning models exhibited fewer autocorrelated residuals, suggesting better learning of time-series patterns.

4.5 Radar Plot and Heatmap Visualization

A radar plot (Figure 6) comparing all four models across all metrics clearly highlights the GRU model's dominance in all aspects—lower MAE, RMSE, MAPE, and higher R^2.

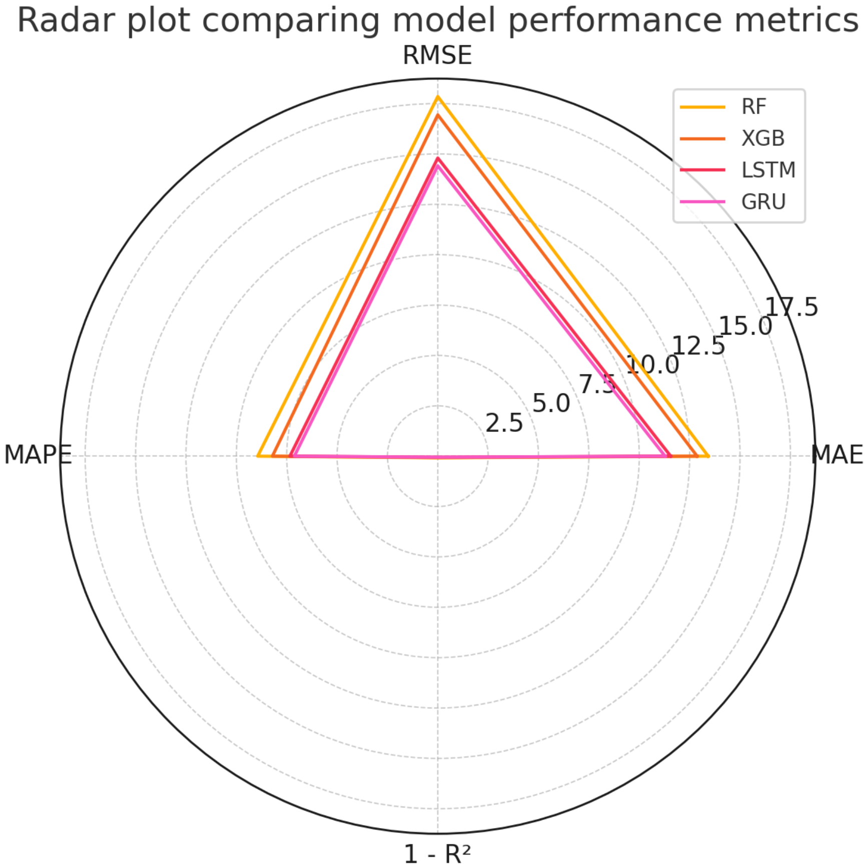

Fig. 6: Radar plot comparing model performance metrics

Further, a heatmap (not shown) revealed strong correlations between AQI and PM2.5 (r = 0.92), PM10 (r = 0.88), and moderate correlations with NO_2 and temperature, reinforcing the feature importance results.

4.6 Operational and Environmental Implications

From a policy standpoint, the high accuracy of GRU and LSTM models suggests their suitability for short-term AQI forecasting systems. Their ability to anticipate pollution spikes can assist city administrators in issuing timely health advisories, initiating traffic restrictions, or enhancing green zone management. Moreover, the attention-based deep models can be incorporated into real-time air quality monitoring dashboards, enhancing public engagement and awareness. While machine learning models like XGBoost and Random Forest provide interpretability and faster training times, their inability to capture sequential patterns limits their performance in real-time AQI predictions. Nevertheless, they remain valuable in feature ranking and exploratory analysis.

4.7 Limitations and Future Scope

Despite the high accuracy, certain limitations remain. First, the dataset is limited to one month (February 2025), and performance may vary across seasons due to changes in weather patterns and pollutant sources. Second, exogenous variables such as traffic intensity, biomass burning events, or industrial outages were not included, which could enhance model robustness. In future work, multi-seasonal datasets, attention mechanisms, and transfer learning approaches can be adopted to improve the model's generalizability. Integration with satellite data and edge-computing devices may also enhance real-time AQI forecasting for smart city applications.

5. CONCLUSION

This research demonstrates the efficacy of machine learning and deep learning techniques for accurate forecasting of AQI in Bhopal, Madhya Pradesh. Through a systematic comparison of four models—Random Forest, XGBoost, LSTM, and GRU—the study finds that GRU networks provide the most accurate predictions, effectively capturing the temporal and nonlinear nature of air pollution data. Among the machine learning models, XGBoost offered superior performance over Random Forest, primarily due to its boosting framework and regularization capabilities.

Feature analysis reaffirms that particulate matter (PM2.5 and PM10) continues to be the principal pollutant influencing air quality in Indian urban environments. The high R^2 scores and low error metrics achieved by the deep learning models indicate their strong generalization ability and practical applicability for short-term AQI forecasting. These findings can assist urban planners and pollution control boards in deploying advanced predictive systems, enabling timely interventions and awareness campaigns. Future work may extend this research by incorporating multi-seasonal data, integrating satellite and traffic inputs, and applying explainable AI techniques to enhance interpretability and transparency of model predictions.

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