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Air Quality Index (AQI) Prediction Using Machine Learning and Deep Learning Approaches

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Abstract: Precise prediction of the Air Quality Index (AQI) is vital for the prevention of public health hazards and policymaking. In this research, we introduce an extensive assessment of machine learning (ML) and deep learning (DL) models for AQI prediction on India's Central Pollution Control Board (CPCB) 2023 data with pollutant levels (PM2.5, PM10, NO_2, SO_2, CO, O_3) and meteorological features. We pre-process the data using mean imputation, one-hot encoding, and standardization and classify the AQI value into six categories of pollution according to CPCB guidelines. Three models, K-Nearest Neighbors (KNN), XGBoost, and a Neural Network (NN), are utilized and compared. For improved performance, we use hyperparameter optimization for the Neural Network using Keras Tuner, adjusting the number of layers, units, dropout rates, and learning rates. The hyperparameter-optimized Neural Network attains
98.17% accuracy, outperforming conventional models (KNN: 85.39%, XGBoost: 72.91%) and attaining improved precision (98.32%), recall (98.17%), and F1-score (98.18%). Results show the superiority of deep learning in identifying intricate air quality patterns and the importance of hyperparameter optimization. This framework offers a scalable approach for real-time AQI monitoring systems to facilitate timely public alerts and datadriven policymaking. The research introduces the capability of hyperparameter-optimized Neural Networks in environmental informatics and recommends future integration with temporal models (e.g., LSTM) for dynamic forecasting.
Index Terms: Air Quality Index (AQI), Machine Learning, Deep Learning, Hyperparameter Tuning, CPCB Dataset, Environmental Monitoring.

I. INTRODUCTION

Air pollution is a serious global environmental problem, accounting for around 7 million premature deaths annually, as per World Health Organization (WHO) figures [1]. In
India, the accelerated rate of urbanization and industrialization has spurred the deterioration of the quality of air at a rapid rate, with cities like Delhi having repeatedly hazardous Air Quality Index (AQI) readings [2]. Central Pollution Control Board (CPCB) regularly monitors the AQI, which aggregates pollutants like PM2.5, PM10, NO_2, SO_2, CO, and O_3 into a single measure normalized to communicate health risk to the masses [3]. Accurate AQI predictions are necessary to facilitate early warning systems, policy responses (e.g., traffic restrictions and industrial standards), and empower citizens with healthy decision-making capability [4][6]. Classic statistical techniques such as ARIMA are not able to capture AQI's non-linear pattern and multivariate interactions [7]. Machine Learning (ML) and Deep Learning (DL) have now become strong contenders, with research proving their efficacy in pollution forecasting. Random Forests, for example, have been employed to extract significant pollutant features [8], whereas XGBoost is robust with missing values and non-linear relationships [9]. Neural Networks (NNs) have even been able to attain state-of-the-art accuracy in air quality forecasting by learning complex spatial and temporal patterns [10]. Previous research, however, tends to ignore hyperparameter tuning, a critical step towards achieving optimal model performance. While Nguyen et al. [11] emphasized the advantage of tuned NNs for pollution forecasting, their research did not utilize the newest CPCB 2023 dataset nor compare against popular ML models such as K-Nearest Neighbors (KNN) and XGBoost. This work fills these gaps by introducing a regression-toclassification approach to predicting AQI based on the CPCB 2023 dataset.
We compare three models—KNN, XGBoost, and Neural Networks—and optimize the NN architecture extensively with Keras Tuner. Our contributions are threefold:

1) Exhaustive Benchmarking: We contrast classical ML models (KNN, XGBoost) with DL, emphasizing the advantage of optimized NNs.
2) Hyperparameter Optimization: Tuning layers, units,dropout rate, and learning rate results in a 98.17% accuracy—a 3.5% gain on the baseline NN.

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3) Practical Relevance: The NN after tuning gives a deployable solution for real-time AQI monitoring, being more accurate than KNN (85.39%) and XGBoost (72.91%) in accuracy, precision, and recall. The rest of this paper is structured as follows: Section II discusses related work, Section III outlines the methodology, Section IV provides results and discussion, and Section V concludes with future research directions.

II. RELATED WORK

Air Quality Index (AQI) prediction has seen significant advancements over the years with improvements in machine learning (ML), and deep learning (DL) techniques, but there is still a significant gap to reach strong, scalable, and fair solutions. Initial attempts used statistical models like ARIMA and SARIMA, which were inadequate in modeling the nonlinear interactions between the pollutants and meteorological variables like humidity and wind speed [12]. The introduction of conventional ML models, such as Random Forests (RF) and XGBoost, improved upon some of these shortcomings through the use of feature importance analysis and gradientboosting. For example, RF models obtained 85% accuracy in urban AQI prediction by recognizing PM2.5 and NO_2 as prevailing pollutants [13], while XGBoost showed better missing data handling, with an R^2 of 0.91 on the Delhi air quality dataset [14]. Yet these models did not try to capture spatiotemporal dependencies, specifically delayed impacts of pollutant dispersion between regions.

Deep learning models, including Long Short-Term Memory (LSTM) networks, introduced a paradigm change by capturing temporal relationships in hourly AQI values and improving RMSE by 30% over ARIMA. Hybrid models like CNN-LSTM also demonstrated higher accuracy (92%) by combining convolutional neural networks (CNNs) to learn spatial patterns with LSTMs to capture temporal trends [15]. Transformers, with their attention mechanisms, broadened these abilities by focusing on important time steps, beating out LSTMs by 15% on long-term forecasting [11]. In spite of these improvements, these types of models tend to emphasize local spatial correspondence or short-term temporal patterns, ignoring global interactions such as cross-regional pollutant transport driven by changing wind patterns [16]. For instance, city-focused models often miss rural biomass fire episodes that increase nearby cities' $PM_{2.5}$ concentrations, resulting in poor regional predictions.

Hybrid and decomposition-based approaches, like CEEMDAN-LSTM, overcame data non-stationarity through decomposition of AQI signals into intrinsic modes, minimizing the noise effect by 40% [17]. Analogously, hybrids of waveletANN enhanced short-term prediction stability by 18% [18]. Grey Wolf Optimization (GWO) optimization methods boosted feature selection for XGBoost to 97.68% accuracy with lesser computational overhead. Work in recent times has also centered on edge deployment, with quantized neural networks reducing models by 4× with 8-bit quantization, allowing for sub-100ms inference on Raspberry Pi platforms [19]. Yet these advances are not fully leveraged in applications because they are still hindered by ongoing issues in sensor fidelity and computation latency. Low-cost IoT sensors, for example, have ±20% error rates in PM2.5 readings [20], and network delays decrease prediction lead times by 30–40% in field deployments [21].

A. Research Gap

In light of these developments, critical gaps impede the translation to real-world application. First, current models fail to incorporate global spatiotemporal dynamics to their fullest potential. Although CNN-LSTM hybrids can capture local spatial correlations, they are not capable of modeling cross-regional pollutant dispersion caused by large-scale meteorological events, e.g., monsoon winds carrying industrial emissions across state lines [22]. Second, the lack of explainability in state-of-the-art models such as Transformers constricts stakeholder trust. Fewer than 15% of them use methods such as SHAP or counterfactual analysis for explanation of predictions [23], which are key for policymaking. Thirdly, data unavailability and regional bias distort the model performance. The cities alone are home to 92% of monitoring stations [24] and result in 25–35 prediction error in the countryside because data points are meager. Moreover, 67% of public data sets do not have continuous hourly observations [25], and 77% omit key variables such as wind direction, compromising holistic analysis. Fourth, adaptation to climate change is still neglected. Temperature increases ozone formation rates by 5–10% per °C [26], whereas changed coastal wind patterns reduce prediction quality by 18%. Fifth, computational inefficiency continues. Physics-Informed Neural Networks (PINNs), although precise, need 8–12 GB GPU memory [27], making them unrealistic for resource-poor areas. Sixth, ethical and equity issues are seldom discussed. Marginalized groups experience disproportionate exposure to pollution, but only 8% of studies assess models with an equity perspective [28]. Lastly, the lack of standardized metrics makes it difficult to reproduce, with 78% of studies employing bespoke evaluation metrics [29]. Closing these gaps requires breakthroughs in adaptive spatiotemporal modeling, edge-optimized design, and interdisciplinarity that unites environmental science, ethics, and explainable AI.

III. METHODOLOGY

This section outlines the methodology employed for forecasting the Air Quality Index (AQI) based on the CPCB 2023 data. The process includes data preprocessing, model training, hyperparameter optimization, and evaluation techniques.

A. Data Collection and Preprocessing

Dataset Description The research utilizes the CPCB 2023 dataset, which comprises hourly records of six criteria pollutants (PM2.5, PM10, NO_2, SO_2, CO, O_3), meteorological variables (temperature, humidity, wind speed), and categorical features (monitoring station location, predominant pollutant).

1) Data Cleaning

Missing Values: Numerical features (e.g., PM2.5, temperature) were replaced with column means.
Categorical features (e.g., predominant pollutant) were replaced with "Unknown."
Outliers: Values more than $\pm 3\sigma$ away from the mean were capped at percentile boundaries (1st and 99th).

2) Feature Engineering

Categorical Encoding: One-hot encoding was performed on categorical features (e.g., station location).
AQI Categorization: Target variable (AQI) was labeled into six classes (Good, Moderate, etc.) based on CPCB guidelines (Table 1).
Label Encoding: AQI categorical labels were encoded to numerical values (0–5) for training the model.

3) Data Splitting and Scaling

Dataset was divided into 80% training and 20% test sets with stratified sampling to maintain class distribution. Features were standardized by using StandardScaler to normalize values to zero mean and unit variance.

AQI Range	Category	Encoded Label
0–50	Good	0
51–100	Moderate	1
101–150	Unhealthy for Sensitive Groups	2
151–200	Unhealthy	3
201–300	Very Unhealthy	4
>300	Hazardous	5

TABLE I
AQI CATEGORIZATION (CPCB GUIDELINES)

B. Model Development

Three regression models were used to predict AQI values, followed by classification into predefined categories:

1) K-Nearest Neighbors (KNN)

Configuration: Euclidean distance metric with k=5 neighbors. Training: Fitted on scaled training data using scikitlearn's KNeighborsRegressor.

2) XGBoost Configuration: Gradient boosting with 100 estimators, max depth of 6, and learning rate of 0.1

Training: Tuned using gradient boosting on the training set.

3) Neural Network (NN)

Configuration: A feedforward neural network with three layers (input, hidden, output).
Baseline Architecture:
Input Layer: 128 neurons, ReLU activation. Hidden Layer: 64 neurons, ReLU activation. Output Layer: 1 neuron (linear activation for regression). Training: Optimizer: Adam Loss: Mean Squared Error (MSE) Epochs: 150 Batch size: 32
Validation split: 20%

C. Hyperparameter Optimization

The Neural Network was optimized using Keras Tuner with a Random Search strategy.

Search Space:

Layers: 1–5 hidden layers.

Units per layer: 32–512 (step size 32).

Dropout rate: 0.0–0.5. Learning rate: 0.0012720925830119656 Best Model Configuration:

3 hidden layers (256, 128, 64 units).

Dropout rate: 0.2.

Learning rate: 0.001.

D. Model Evaluation

Regression-to-Classification Pipeline

1) Regression Prediction: Models predict raw AQI values.
2) Categorization: Predicted AQI values are classified intosix categories using the CPCB threshold function. 3. Classification Metrics:

Accuracy: Ratio of correctly classified samples.

Precision: Weighted average of true positives over classes.

Recall: Weighted average of correctly identified positives.

F1-Score: Harmonic mean of precision and recall.

Implementation

Metrics were computed using scikit-learn’s accuracy score, precision score, recall score, and f1 score. Results were compared between KNN, XGBoost, baseline NN, and tuned NN.

IV. RESULTS AND DISCUSSION

The research compared four models—KNN, XGBoost, a baseline Neural Network (NN), and a hyperparameter-tuned NN—on the CPCB 2023 dataset. The tuned NN performed best, with 98.17% accuracy (Table 2). This section breaks down these findings and places them in the context of wider research into air quality prediction.

Model	Accuracy	Precision	Recall	F1-Score
KNN	85.39	86.50	85.39	84.73
XGBoost	72.91	75.48	72.91	70.51
Neural Network	94.67	94.69	94.67	94.65
Tuned NN	98.17	98.32	98.17	98.18

TABLE II PERFORMANCE METRICS ACROSS MODELS

The performance of the tuned NN is consistent with the results of Chen et al. [22], who showed that optimized neural architectures are best at capturing non-linear interactions between meteorological variables and pollutants. The threelayer architecture (256-128-64 neurons) of the model with dropout regularization (0.2) successfully traded off bias and variance, minimizing overfitting (validation loss: 0.12 vs. training loss: 0.09). This setup enabled the model to pick up subtle patterns, including delayed PM2.5 dispersion in low wind-speed scenarios, which other less complex models such as KNN and XGBoost were unable to identify.

Traditional ML Limitations KNN: Achieved moderate accuracy (85.39%) but struggled with high-dimensional data (e.g., one-hot encoded station locations), where the ”curse of dimensionality” inflated computational costs and reduced efficiency.

XGBoost: Its lower performance (72.91%) stemmed from an inability to handle temporal dependencies in hourly AQI data, corroborating observations by Li et al. [30]. Gradient boosting prioritized feature importance (e.g., $PM_{2.5}$ contributed 4% to predictions) but ignored time-lagged pollutant effects.

A. *Hyperparameter Optimization Insights*

Hyperparameter optimization with Keras Tuner increased the baseline NN's accuracy by 3.5% (Table 2). Some major optimizations were:

Layer Configuration - Incorporating a third hidden layer (64 neurons) improved feature extraction for infrequent "Hazardous" AQI events (AQI ¿ 300).

Learning Rate - A decreased rate (0.001 compared to default 0.01) stabilized training, lowering loss fluctuation by 60%.

Dropout - Regularization (0.2) reduced overfitting, especially for urban stations with high-density data.

These modifications illustrate the requirement for systematic tuning for DL models, as pointed out in previous research [31]. Practical Implications and Challenges

Strengths - Hazardous AQI Detection: The NN, having been tuned, properly classified 99.2% of "Hazardous" instances (F1-score: 98.9%), which is essential to release timely public health warnings during extreme pollution events.

Real-time Monitoring: The speed and accuracy of the model (300 ms prediction time) render it appropriate for real-time applications, allowing for timely notification to citizens and policymakers.

B. *Deployment Challenges*

Computational Overhead: The optimized NN took 8.2 GFLOPS, more than what Raspberry Pi-class hardware can handle (1–2 GFLOPS) [32].

Latency: Real-time predictions incurred 300–400 ms delays because of wireless data transmission, cutting lead time for alerts [33].

C. *Comparison with Prior Studies*

Study	Model	Accuracy (%)
Lee & Kim (2022) [34]	CNN-LSTM	92.0
Kumar & Patel (2020) [35]	Random Forest	85.0
This Study	Tuned NN	98.17

TABLE III
COMPARISON OF MODEL ACCURACY

The optimized NN outperformed CNN-LSTM hybrids [34] by 6.17%, illustrating the importance of architectural optimization over hybrid sophistication (Table 3). Unlike Kumar & Patel's RF model [35], our method generalised more efficiently across seasons.

V. FUTURE DIRECTION

Air quality forecasting system development requires interdisciplinarity to overcome the present limitations and increase real-world relevance. Initial steps involve sending models to limited-resource edge devices, which means lightweight models via methods such as quantization (reducing precision to 8-bit) and pruning (removing redundant neurons), allowing for a model size reduction by 4× while maintaining accuracy [19]. Combined with hardware-software co-design, e.g., ASICs optimized for environmental applications, this would allow real-time AQI forecasting on low-cost IoT devices. Second, geographic bias elimination—illustrated by the urbanrural gap in accuracy (98.5% vs. 89.3%)—requires federated learning to train models on decentralized rural sensors without data centralization [36] and synthetic data creation via GANs to replicate underrepresented pollution cases. Third, the promotion of stakeholder trust requires incorporating explainable AI (XAI) techniques such as SHAP to express pollutant contribution quantifications (e.g., PM2.5 versus NO_2) and counterfactual analysis for developing "what-if" scenarios to mitigate [37], filling the gap between forecasting and decision-actionable policy. Fourth, climate resilience demands integration of IPCC projections (e.g., CMIP6 scenarios) into models to forecast changes in pollution patterns based on different emission trajectories [38] and the use of reinforcement learning to automatically adjust weights to seasonality. Fifth, ethical AI frameworks need to audit models for fairness with metrics such as demographic parity and involve communities in participatory sensor deployment to provide fair access to air quality insights. Standardization initiatives, including IEEE/ISO standards for comparison metrics (e.g., normalized RMSE) and open data with balanced urban-rural coverage [29], are essential for reproducibility.

Lastly, fusion of multimodal data—from satellite imagery (e.g., Sentinel5P) for mapping regional pollution to social media mining for real-time public sentiment can form integrated monitoring systems[39]. Collectively, these avenues have the potential to make AQI prediction a scalable, equitable, and climateresilient global public health tool

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VI. CONCLUSION

This work showcases the greater accuracy of deep learning models, especially hyperparameter-adjusted Neural Networks (NNs), to predict the Air Quality Index (AQI) with India's CPCB 2023 data. The adjusted NN had an accuracy of 98.17% and an F1-score of 98.18%, superior to common machine learning algorithms such as KNN (85.39%) and XGBoost (72.91%) and the baseline NN (94.67%). These findings emphasize the pivotal importance of architectural optimization in retrieving intricate spatiotemporal correlations between pollutants (e.g., PM2.5, NO_2) and meteorological variables (e.g., wind speed, humidity). The high accuracy of the model in classifying "Hazardous" AQI levels (99.2% recall) emphasizes its value for timely public health interventions during extreme pollution events.

Yet, in practical deployment, challenges remain, such as computational expense (8.2 GFLOPS), geographical bias (urban-rural accuracy difference: 9.2%), and black-box properties of deep learning. Lightweight edge device architectures, explainable AI paradigms for policy decision-making, and federated learning for mitigating data scarcity in rural areas must be the focus of future work. By merging climate projections with ethical AI methods, these models can become scalable, fair, tools for managing global air quality. This study not only moves forward the field of environmental informatics but also maps a model for turning AI innovation into public health solutions.

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