

Air Quality Prediction and Forecasting Using Machine Learning Algorithms: A Review

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Abstract

Precise prediction of air pollutant concentrations (PM_{2.5}, PM₁₀, NO₂, SO₂, O₃, CO) is important for public health and environmental protection. Over the last decade, machine learning (ML) and deep learning (DL) methods have been widely used to improve the accuracy of air quality predictions. This review synthesises results from 32 recent studies, including statistical, ML, DL, hybrid, and ensemble models, such as spatiotemporal and graph-based models. It emphasizes dominant methodologies, models for prediction, challenges, and avenues for future research, highlighting the expanding involvement of interpretable and hybrid ML approaches.

Keywords: *Air Quality Prediction, Machine Learning, Deep Learning, Hybrid Models, Ensemble Methods, PM_{2.5}, Spatiotemporal Forecasting, Graph Neural Networks*

1. Introduction

Air pollution is a global issue of particular concern, having direct consequences for human health, climate, and ecosystems. Reliable air quality forecasting enables early intervention and decision-making in policymaking. Conventional statistical models, though helpful, tend to miss intricate nonlinear spatiotemporal interrelations in pollutant concentrations. More recent advances in ML and DL have shown the potential to predict air pollutants like PM_{2.5}, PM₁₀, O₃, NO₂, and CO [1,4,5,6].

Berrocal et al. [1] contrasted statistical and ML approaches to exposure assessment and found that ML provided better spatial prediction. Systematic reviews by Agbehadji et al. [2] and Houdou et al. [3] highlighted the effectiveness of ML and DL for spatiotemporal prediction and explainable forecasting models. Models based on neural networks, such as ANN [4], LSTM [8,20], and CNN-LSTM [9,11], have effectively modeled temporal relationships in PM_{2.5} and other air pollutants. Hybrid models that integrate ML with statistical methods, such as Random Forest-ARIMA [14], also improve predictive performance while offering interpretability.

Current research has combined weather forecasting outputs (WRF) with ML models to enhance PM_{2.5} forecasting [7]. Ensemble approaches [10,13,15] make use of a combination of models to minimize the errors in predictions and strengthen robustness. Novel trends include the use of graph-based deep learning, attention mechanisms, and spatiotemporal transformers to capture the intricate dynamics of urban air pollution [24,25,28,30,31]. Additionally, the use of quantum-inspired optimization [26] and IoT-sensor data fusion [22] holds potential for real-time predictive systems.

Even with such improvements, challenges persist, such as data sparsity, temporal variability, spatial heterogeneity, and interpretability [32]. Scalable, real-time, and explainable air quality prediction models will be required in future research.

2. Research Methodology

This review thoroughly examines how machine learning (ML) and deep learning (DL) models are used to forecast and predict air quality. The research process includes selecting literature, categorizing models, identifying key metrics, and outlining analytical methods used in the studies.

2.1 Literature Selection

A wide search was conducted across databases such as Scopus, Web of Science, IEEE Xplore, MDPI, Springer, and PubMed. It focused on publications from 2015 to 2025 that address the prediction of air pollutants using ML/DL models. The keywords included “air quality prediction,” “PM_{2.5} forecasting,” “machine learning,” “deep learning,” “graph neural networks,” and “ensemble methods.”

We selected 32 studies for in-depth analysis [1–32]. These ranged from statistical models to classical ML models, DL structures, hybrid methods, and ensemble methods. The selection criteria were as follows:

- Availability of quantitative prediction outcomes (accuracy, RMSE, MAE, or R²)
- Focus on urban, regional, or global air pollution prediction
- Inclusion of both single-pollutant and multi-pollutant prediction papers.

2.2 Model Classification

The papers were grouped into four broad categories:

2.2.1 Statistical Models

Conventional statistical techniques, such as kriging and ARIMA, were primarily used for spatial interpolation and temporal trend analysis [1,14]. These techniques are helpful for baseline prediction but often fail to capture complex nonlinear and spatiotemporal relationships.

2.2.2 Machine Learning Models

ML methods were widely used for air quality prediction with meteorological, spatial, and historical pollutant data. Major algorithms included:

- Random Forest (RF) [1,6,14,15]
- Gradient Boosting Machines (GBM) [1,6]
- Support Vector Machines (SVM) [15,16]

Ensemble ML methods merged predictions from various models to improve robustness and reduce errors [10,13,15,23].

2.2.3 Deep Learning Models

DL models effectively captured intricate temporal and spatial relationships in pollutant time series. RNNs, LSTM, and GRU were used for forecasting PM_{2.5}, NO₂, and other pollutants [8,9,11,20]. CNN-LSTM hybrids used convolutional layers to extract spatial features and LSTM to model temporal relationships [9,11]. Graph Neural Networks (GCN, GAT) modeled spatial correlations between multiple monitoring sites [28,31]. Transformer-based spatiotemporal models utilized multi-head attention mechanisms to predict pollutant levels accurately [25,29,30].

2.2.4 Hybrid Models

Hybrid models combined the benefits of ML, DL, and statistical methods. Random Forest-ARIMA hybrids used both linear and nonlinear modeling for better interpretability [14]. BPSO-optimized deep learning models fine-tuned hyperparameters to improve prediction accuracy [17,26]. KSC-ConvLSTM models paired convolutional and recurrent networks with clustering methods to enhance spatiotemporal predictions [18].

2.3 Input Features and Data Sources

Most studies used a mix of:

- Air pollutant concentration: PM_{2.5}, PM₁₀, NO₂, SO₂, O₃, CO [4,5,6,7,8,20]
- Meteorological variables: Temperature, humidity, wind speed, solar radiation [6,7,22]
- Spatial and temporal data: Coordinates, timestamps, satellite data [5,7,28]
- IoT sensor data for local modeling, especially in campuses or urban areas [22,27]

WRF model simulations were combined with ML/DL models for better PM_{2.5} prediction [7].

2.4 Model Training and Evaluation

Models were trained using past air quality and meteorological data through cross-validation, train-test splits, and temporal validation. Performance measures reported in the studies include:

- Root Mean Square Error (RMSE) [7,9,11,17]
- Mean Absolute Error (MAE) [8,14,26]
- R² or coefficient of determination [6,20,27]
- Accuracy of AQI classification [14,21,32]

Ensemble and hybrid models outperformed single models across all performance measures [10,13,14,17,18,23,26].

2.5 Trends and Techniques Analysis

The review also examined trends in model development. Ensemble methods increase prediction reliability by utilizing groups of multiple learners [10,13,15,23]. Graph-based DL models represent complex spatial relationships among different locations [28,31]. Attention-based models improve focus on significant temporal or spatial features [25,26,29,30]. Hybrid and optimization-focused approaches enhance accuracy and interpretability [14,17,18,26].

This methodological design allows for a thorough evaluation of air quality forecasting methods, their strengths, weaknesses, and performance across different pollutants, datasets, and urban or regional scales [1–32].

3. Theory and Calculations

3.1 Air Quality Index (AQI) Calculation

Most studies predicting AQI or pollutant concentrations used the standard AQI formula based on pollutant concentration sub-indices:

$$AQI_p = \left(\frac{I_{Hi} - I_{Lo}}{BP_{Hi} - BP_{Lo}} \right) * (Cp - BP_{Lo}) + I_{Lo} \quad (1), (14), (21), (32)$$

Where:

Cp = observed pollutant concentration

BP_Hi / BP_Lo = breakpoint concentrations for the corresponding AQI category

I_Hi / I_Lo = corresponding AQI indices for the breakpoints

3.2 Long Short-Term Memory (LSTM) Networks

LSTM networks capture temporal dependencies in sequential pollutant data. Updates of the LSTM cell are given as:

$$\begin{aligned} ft &= \sigma(Wf \cdot [ht - 1, xt] + bf) \\ it &= \sigma(Wi \cdot [ht - 1, xt] + bi) \\ ot &= \sigma(Wo \cdot [ht - 1, xt] + bo) \\ Ct &= ft * Ct - 1 + it * \tanh \tanh (Wc \cdot [ht - 1, xt] + bc) \\ ht &= ot * \tanh \tanh (Ct) \end{aligned} \quad (8), (9), (11), (20)$$

Where: xt = input features at time t, ht-1 = previous hidden state, Ct-1 = previous cell state, ft, it, ot = forget, input, and output gates, W and b = weights and biases, σ = sigmoid activation

3.3 Gated Recurrent Unit (GRU)

GRU is a simplified recurrent network used in some studies for NO₂ and PM_{2.5} prediction:

$$\begin{aligned} zt &= \sigma(Wz \cdot [ht - 1, xt]) \\ rt &= \sigma(Wr \cdot [ht - 1, xt]) \\ \sim ht &= \tanh(W \cdot [rt * ht - 1, xt]) \\ ht &= (1 - zt) * ht - 1 + zt * \sim ht \end{aligned} \quad (20)$$

3.4 Convolutional Neural Networks (CNN) and CNN-LSTM Hybrids

CNN layers extract spatial features from multi-site pollutant data:

$$X^{(l+1)} = f(W^{(l)} * X^{(l)} + b^{(l)}) \quad (9), (11)$$

For CNN-LSTM hybrids, CNN outputs are passed into LSTM cells for temporal forecasting.

3.5 Graph Neural Networks (GCN and GAT)

Graph-based deep learning is used to model spatial correlations between monitoring sites:

$$H^{(l+1)} = \sigma(D \sim^{-1/2} * A \sim * D \sim^{-1/2} * H^{(l)} * W^{(l)}) \quad (28), (31)$$

Where: $A \sim = A + I$ adjacency matrix with self-loops, $D \sim =$ diagonal degree matrix, $H^{(l)}$ = hidden layer representation, $W^{(l)}$ = learnable weight matrix

3.6 Transformer-based Spatio-Temporal Models

Attention-based transformers used multi-head attention to weigh temporal and spatial dependencies:

$$Attention(Q, K, V) = softmax((QK^T)/sqrt(dk))V \quad (25), (29), (30)$$

Where: Q,K,V = query, key, value matrices, dk = scaling factor

3.7 Hybrid Statistical + ML Models

Hybrid approaches combine ARIMA with ML models like Random Forest:

$$Linear\ component\ via\ ARIMA: y_t = \phi_1 * y_{t-1} + \dots + \phi_p * y_{t-p} + \epsilon_t \quad (14)$$

Nonlinear residuals captured by RF: $\epsilon^t = f_R F$ (lagged residuals, weather features)

3.8 BPSO Optimization for Model Hyperparameters

Particle Swarm Optimization (PSO) tunes weights/hyperparameters in hybrid DL models:

$$\begin{aligned} v_i(t+1) &= w * v_i(t) + c1 * r1 * (pbest_i - x_i(t)) + c2 * r2 * (gbest - x_i(t)) \\ &= x_i(t) + v_i(t+1) \end{aligned} \quad (17), (26)$$

Where: v_i = particle velocity, x_i = particle position, $pbest_i$ = personal best, $gbest$ = global best, $w, c1, c2$ = inertia and acceleration coefficients, $r1, r2$ = random numbers

3.9 Evaluation Metrics

Common metrics across studies for model validation:

$$\begin{aligned} RMSE &= sqrt((1/n) * \sum(\hat{y}_i - y_i)^2) && [7,9,11,17] MAE \\ &= (1/n) * \sum|\hat{y}_i - y_i| && [8,14,26] R^2 \\ &= 1 - \sum(\hat{y}_i - y_i)^2 / \sum(y_i - \bar{y})^2 && [6,20,27] \end{aligned}$$

Accuracy of AQI classification: [14, 21, 32]

4. Results and Discussions

Berrocal et al. (2019) Compared statistical and machine learning techniques for air pollution exposure estimation. Concluded that machine learning models, especially Random Forest and

Gradient Boosting, performed better than classical statistical models in terms of predictive accuracy.

Agbehadji et al. (2024) Explored machine learning and deep learning methods for spatiotemporal forecasting of air quality. Emphasized the need to integrate these approaches to enhance the predictive ability.

Houdou et al. (2024) Systematically evaluated interpretable machine learning methods for air pollution forecasting. Stressed the importance of models that strike a balance between accuracy and interpretability in order to improve decision-making in air quality management.

Xiao et al. (2015) Constructed an artificial neural network (ANN) model for PM_{2.5} pollution forecasting. Showed the promise of ANN in detecting nonlinear associations in air quality data.

Lary et al. (2015) Used machine learning to estimate concentrations of global PM_{2.5}. Demonstrated that machine learning models could accurately estimate PM_{2.5} concentrations over large regions.

Fan et al. (2023) Performed machine learning-based forecasting for ozone and PM_{2.5}. Made very substantial improvements in forecasting performance over conventional techniques.

Minh et al. (2021) Developed a PM_{2.5} forecasting system based on machine learning and WRF outputs. Obtained high accuracy in PM_{2.5} concentration predictions, which is appropriate for early warning systems.

Kristiani (2022) Utilized LSTM deep learning for short-term PM_{2.5} forecasting. Showed the ability of LSTM in extracting temporal patterns in air quality data.

Bai et al. (2024) Suggested a CNN-LSTM deep learning model for PM_{2.5} prediction. Demonstrated that the integration of CNN and LSTM enhanced prediction accuracy by extracting both spatial and temporal characteristics.

Ejohwomu (2022) Employed ensemble strategies for modeling and forecasting temporal PM_{2.5}. Established that ensemble models gave more reliable predictions than single models.

Utku (2025) Designed a deep learning-based hybrid model of CNN-RNN for PM_{2.5} prediction. Attained enhanced prediction performance through the use of both convolution and recurrent neural networks.

Karimian (2019) Assessed various machine learning methods to PM_{2.5} prediction. Determined the strengths and limitations of several models, offering future research insights.

Özüpak et al. (2025) Performed a comparative study of machine learning models for air quality prediction. Emphasized the promise of ensemble approaches to improve predictability.

Yenkikar et al. (2025) used a hybrid random forest and ARIMA model for interpretable AQI prediction. Obtained high precision with model interpretability.

Balogun et al. (2022) surveyed machine learning models for air quality forecasting. Presented a detailed description of different models and their usage in air quality forecasting.

Masih et al. (2025) Constructed a machine learning-based air quality forecasting model for Guangdong. Showcased the feasibility of machine learning models for practical air quality observation.

Sawah et al. (2025) Improved prediction of air quality with a hybrid BPSO model. Attained higher prediction accuracy through optimized parameters for the model.

Chen et al. (2025) Suggested a hybrid deep learning method for air pollution forecasting with KSC-ConvLSTM. Demonstrated very high improvement in prediction accuracy over conventional approaches.

Study (2023) Utilized deep learning methods for the prediction of air quality. Attained very high accuracy in forecasting different air pollutants.

Study (2023) Applied machine learning methods in NO₂ air quality prediction through LSTM and GRU. Shown the performance of these models in predicting NO₂ concentrations.

Das (2025) Constructed an air quality prediction model for AQI monitoring. Attained real-time predictive capability appropriate for air quality management systems.

Panaite et al. (2024) Improved air-quality predictions in university campuses via machine learning. Attained enhanced accuracy in predictions with incorporation of local data sources.

Özüpak et al. (2025) Developed ensemble approaches to improve air quality prediction. Obtained improved prediction accuracy through model ensembling.

Zhang et al. (2024) Enhanced deterministic 3-day air pollution predictions based on machine learning models. Obtained tremendous improvements in forecast accuracy.

Awang et al. (2025) Developed an innovative ST-iTransformer model for forecasting spatio-temporal ambient air pollution. Illustrated the capability of the model to identify intricate spatiotemporal relationships.

Kumar et al. (2024) Made predictions on air quality index with an attention hybrid deep learning model. Improved accuracy of prediction by including attention mechanisms.

Geng et al. (2025) Designed FuXi-Air for urban air quality prediction using emission-meteorology-pollutant multimodal machine learning. Exhibited high accuracy for urban air quality prediction.

Panja et al. (2024) Made use of Extremely Spatio-Temporal Graph Convolutional Networks (E-STGCN) for air quality prediction. Demonstrated remarkable improvements in prediction accuracy.

Liu et al. (2024) utilised time series decomposition and a convolutional sparse self-attention mechanism transformer model for air quality prediction. Attained extremely high accuracy in short-term AQI predictions.

Zhang et al. (2024) Improved air quality prediction using a new spatio-temporal model combining graph convolution and multi-head attention mechanisms. Attained substantial prediction accuracy improvements.

Wang et al. (2024) Designed a graph attention recurrent neural network model for PM2.5 prediction. Obtained high precision in long-term forecasting of PM2.5.

Das (2025) Established an air quality prediction model for monitoring AQI. Obtained real-time prediction abilities appropriate for air quality management systems.

Table 1: Comparison Table

S.No	Reference	Model Type	Pollutant(s)	Dataset Source	Key Result / Finding
1	Berrocal et al., 2019 [1]	ML	PM2.5, PM10	Urban / Regional	ML models (RF, GBM) outperformed statistical models in spatial prediction accuracy.
2	Agbehadji et al., 2024 [2]	ML / DL	PM2.5, NO ₂ , O ₃	Urban / Spatiotemporal	Highlighted effectiveness of ML and DL in spatiotemporal forecasting; emphasized integrating approaches.
3	Houdou et al., 2024 [3]	Interpretable ML	PM2.5, PM10, NO ₂	Urban	Stressed need for interpretable models balancing accuracy and explainability.
4	Xiao et al., 2015 [4]	ANN (DL)	PM2.5	Urban	ANN captured nonlinear associations; promising for PM2.5 forecasting.
5	Lary et al., 2015 [5]	ML	PM2.5	Global	ML accurately estimated PM2.5 over large regions.

6	Fan et al., 2023 [6]	ML	PM2.5, O ₃	Urban	Significant improvement over conventional methods in pollutant forecasting.
7	Minh et al., 2021 [7]	ML + WRF	PM2.5	Urban / Regional	High accuracy in PM2.5 predictions; suitable for early warning systems.
8	Kristiani, 2022 [8]	LSTM (DL)	PM2.5	Urban	LSTM effectively extracted temporal patterns for short-term PM2.5 forecasting.
9	Bai et al., 2024 [9]	CNN-LSTM (DL)	PM2.5	Urban	CNN-LSTM improved accuracy by capturing spatial and temporal features.
10	Ejohwomu, 2022 [10]	Ensemble (ML)	PM2.5	Urban	Ensemble methods provided more reliable temporal PM2.5 forecasts than single models.
11	Utku, 2025 [11]	CNN-RNN Hybrid (DL)	PM2.5	Urban	Hybrid deep learning model enhanced PM2.5 prediction performance.
12	Karimian, 2019 [12]	ML	PM2.5	Urban	Compared ML models; identified strengths and limitations for PM2.5 forecasting.

13	Özüpak et al., 2025 [13]	ML Ensemble	PM2.5, PM10, NO ₂	Urban	Ensemble strategies improved prediction accuracy compared to single ML models.
14	Yenkikar et al., 2025 [14]	Hybrid (RF + ARIMA)	AQI	Urban	Hybrid model achieved high precision and interpretability for AQI prediction.
15	Balogun et al., 2022 [15]	ML Survey	PM2.5, PM10	Urban / Regional	Surveyed ML approaches for air quality forecasting; summarized model performance.
16	Masih et al., 2025 [16]	ML	PM2.5	Guangdong	Demonstrated ML feasibility for practical air quality observation.
17	Sawah et al., 2025 [17]	Hybrid BPSO ML	PM2.5	Urban	Optimized hybrid model improved PM2.5 prediction accuracy.
18	Chen et al., 2025 [18]	Hybrid DL (KSC-ConvLSTM)	PM2.5	Urban	High prediction accuracy; combined clustering with convolutional and recurrent networks.
19	MDPI Study, 2023 [19]	DL	PM2.5, NO ₂ , O ₃	Urban	Deep learning models achieved high accuracy for multiple pollutants.

20	Sustainability Study, 2023 [20]	LSTM / GRU (DL)	NO ₂	Urban	LSTM and GRU effectively predicted NO ₂ concentrations.
21	Das, 2025 [21]	ML / Real-time	AQI	Urban	Developed AQI monitoring model with real-time predictive capability.
22	Panaite et al., 2024 [22]	ML	PM2.5	University campus	Local IoT data improved accuracy of campus-level air quality predictions.
23	Özüpak et al., 2025 [23]	ML Ensemble	PM2.5, PM10	Urban	Ensemble ML approaches enhanced prediction robustness and accuracy.
24	Zhang et al., 2024 [24]	ML	PM2.5, PM10	Urban	Improved 3-day deterministic air pollution forecasts using ML.
25	Awang et al., 2025 [25]	ST-Transformer (DL)	PM2.5, NO ₂	Urban	Spatiotemporal transformer captured complex dependencies for accurate forecasts.
26	Kumar et al., 2024 [26]	Attention Hybrid DL BPSO	AQI	Urban	Attention mechanisms + quantum-inspired PSO improved AQI prediction accuracy.
27	Geng et al., 2025 [27]	Multimodal ML	PM2.5, PM10, NO ₂ , O ₃	Urban	FuXi-Air model integrated emission, meteorology, and pollutants for

					urban AQ prediction.
28	Panja et al., 2024 [28]	E-STGCN (Graph DL)	PM2.5	Urban	Graph convolutional networks captured spatiotemporal correlations; improved accuracy.
29	Liu et al., 2024 [29]	Transformer DL	AQI	Urban	Convolutional sparse self-attention transformer improved short-term AQI prediction.
30	Zhang et al., 2024 [30]	Graph, Multi-Head Attention DL	PM2.5	Urban	Enhanced prediction accuracy by combining graph convolution with attention mechanisms.
31	Wang et al., 2024 [31]	Graph Attention RNN (DL)	PM2.5	Urban / China	Achieved high precision in long-term PM2.5 forecasting.
32	Das, 2025 [32]	ML / Real-time	AQI	Urban	Real-time AQI prediction model suitable for management systems.

5. Conclusion

Machine learning and deep learning methods have revolutionized air quality forecasting, making it precise, explainable, and real-time. Hybrid and graph-based models, ensemble methods, and attention mechanisms show great promise. Scalability, data sparsity, and the integration of multiple pollutants are areas that need to be focused on in further research to improve environmental regulation and public health practices.

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