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Research Article

Improving AQI Prediction and Optimization Using Graph Convolutional Networks and Transformer Models with Spatial Embedding Operations

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ABSTRACT

State-of-the-art models do not quite capture complex spatial-temporal dependencies driving variations in the AQI across different urban zones, particularly in areas characterized by heavy traffic and industrial emissions. Accurate and timely prediction of the AQI is critical since it could mitigate the health and environmental impacts of air pollution, especially in metropolitan areas like Delhi that frequent hazardous levels of pollution. They rely primarily on grid-based or very naive temporal schemes that hardly capture the real nature of an urban region. To overcome these shortcomings, this paper suggests three advanced paradigms: (1) Graph Convolutional Networks with Temporal Attention Mechanism, (2) Transformer-based AQI Prediction with Spatial Embedding, and (3) Multi-Agent Reinforcement Learning with Nash Equilibrium for AQI optimization. This model captures the complex spatial interdependencies among different monitoring stations and directs attention in time for emphasizing related important features in different time domains. Therefore, the prediction accuracy improves up to 20% with an average error of ~2.8 units in high-risk zones like Wazipur and Okhla. The Transformer model introduces spatial embeddings that improve the self-attention mechanism to accurately predict spikes in AQI during polluted episodes and provides an estimated 25% improvement with an average error at around ~2.6 units. Conclusion In conclusion, the MARL model improves optimizations of interventions applied in pollution control by representing several regions or sources via agents, achieving a 20% decline in high-pollution episodes. This work effectively improved upon spatial-temporal learning by great enhancements in prediction and optimization of AQI, leading towards a more accurate forecast and practical control strategy for pollution: an objective that lends environmental management improved as well as greater public health benefits for urban and industrial areas.

Keywords: AQI Prediction, Graph Convolutional Networks, Transformer Models, Spatial Embedding, Multi-Agent Reinforcement Learning, Scenarios.

INTRODUCTION

Delhi, has been considered to have a high level of air pollution. The significant health and environmental concerns are because of this, which is reaching dangerous levels often in densely populated urban areas. Important values of AQI require identification for enabling proactive measures and mitigating the negative effects of pollution. The traditional models for prediction of AQI perform well in some cases but fail to capture all the possible spatial and temporal complexities in urban areas because of their inability to precisely identify the heterogeneity of source locations, dynamic relationships between regions, and the effect of long-term temporal shifts on air quality patterns. An advanced AQI prediction and optimization model by Temporal Attention Mechanism combined with GCNs, models based on Transformers with Spatial Embedding, and MARL at the Nash Equilibrium can be introduced. GCNs do have very good capabilities for learning the spatial dependencies of air quality monitoring stations, and the Temporal Attention Mechanism may further provide key long- and short-term insights. The Transformer model adds spatial embeddings to enhance further predictions as sensitive factors of geography and industry. MARL is also able to construct optimal interventions across various pollution sources, balancing actions through Nash Equilibrium strategies. Since the integration of these advanced methods will integrate the heterogeneity both in spatial and temporal terms regarding the quality AQI data sample [4, 5, 6], there will be a marked enhancement in the accuracy for prediction and optimization of pollution control strategies. It helps fill important lacuna within currently available methodologies thereby bridging gaps to enhance environmental management and improvement in public health outcomes.

Literature Review

Air quality prediction and monitoring: The field has advanced in recent developments of methodologies in increasing accuracy, cost efficiency, and scalability. We selected key works that founded air quality measurements and forecasting for this review and took particular interest in spatiotemporal modeling, deep learning, and low-cost sensing systems. Martinez et al. designed a low-cost, open-source hardware- and software-based air quality monitoring embedded system [1]. Their proposed system was able to demonstrate cost-effective and scalable monitoring solutions well, but the focus of the system was more towards variable measurement as against predictive analytics. Follow-up research in the process emphasized the need to harness more elaborate predictive models. Al-Eidi et al. showed a comparative analysis of regression machine learning techniques in smart cities for air quality forecasting in [2]. They demonstrated a range of regression algorithms and, in doing so, also exhibited how the integration of machine learning with IoT is likely to enhance the feasibility of predictions about real-time conditions of air quality. However, there were particular restrictions observed in terms of spatial resolution, which motivated the requirement for models that could efficiently take into account both spatial and temporal data. Cao et al. proposed a hybrid model combining EMD and SVD with AutoRegressive Integrated Moving Average (ARIMA) for time-series analysis. This method was potent in capturing long-range dependencies in AQI data but could not make modeling on spatial heterogeneity over pollution sources, especially in the complex urban structure. Lin et al. [5] attempted to surpass the limitation of the previously suggested models by developing a deep learning model that utilized Graph Neural Networks for anomaly detection in air quality data. Their approach leveraged spatiotemporal correlations and bettered the detection performance while focusing on anomaly detection rather than direct prediction of AQI. Han et al. [6] developed the GNN framework, including self-supervised hierarchical learning for semi-supervised air quality forecasting. This approach demonstrated exceptional performance in the urban scenario by using a hierarchical GNN structure to contend with the complexity of spatial data. Nevertheless, its partial-labeling constraint dictates rather limited generalizability in scenarios where labeled data are scarce for different scenarios.

Zaidan et al. [7] discuss validated dense air quality sensor networks against LCSs. While their work improves the reliability of real-time sensor networks, they have not emphasized predictive models. Undoubtedly, it seems to be promising scope for different scenarios at integrating sensor networks with advanced predictive analytics. Yi et al. [8] offered a deep neural network for high-resolution air quality forecasting that integrated spatial and temporal data. The model was very effective in urban computing contexts but not nearly as effective when it encountered very dynamic environments with complex pollution sources; hence different models which are more adaptive to these situations. In case scenarios with indoor applications, Farahi [9] researched soft ionization methods to use in improving the indoor air quality while enhancing particle measurements. Although the research advanced indoor air cleaning technologies, its outdoor application in predicting AQI remains untested and therefore underlines the potential of further cross-domain applications. In this challenge, Han et al. approached the simultaneous prediction of air-quality and weather conditions by developing a multi-view, multi-adversarial learning approach. Their work managed to demonstrate the interaction of air quality and meteorological data samples, but at the same time its dependence on adversarial learning proved the model vulnerable to stability while in training. Yu et al. [11] ensured optimal placement of sensors for air quality monitoring by formulating the optimal sensor placement problem as one to minimize the error in estimation and associated uncertainty. Active learning and graph reduction in their method gave them crucial information related to efficient data gathering, though the approach emphasized monitoring rather than predictive capability. Liu et al. [12] used a genetic algorithm-based improvement of the Extreme Learning Machine, ELM, that they put forward for AQI forecasting. They successfully verified the applicability of ELM in AQI forecasting with better time-series predictive performance, though spatial dependency was not solved clearly. Future improvement integrating ELM with spatial models will further facilitate forecasting. Chen et al. [13] approached the task of deep learning, in addition to multisource data fusion, for enhancing estimation for citywide regions with better air quality. The model displays the capability for the integration of heterogeneous sources of information while having a computational complexity that narrows its scalability. Miasayedava et al. experimentally investigated open data assimilation techniques for monitoring the air quality over Europe using lightweight numerical models. While their work focused on uncertainty quantification and data assimilation, the approach did not suffer from adaptability to the spatiotemporal complexity of urban air quality environments. Lastly, Purbakawaca et al. [15] developed an ambient air monitoring system with adaptive performance stability by using low-cost sensors. Their system made much promise toward the issue of cost-effective real-time air quality monitoring; however, it was essentially designed for data collection without the predictive abilities for long-range forecasting. Collectively, these studies reveal the significance of integrating spatiotemporal data and evolving learning models to enhance air quality forecasts and monitoring. However, the identified limitations in terms of spatial resolutions, adaptability in dynamic environments, and computationally efficiency suggest a holistic approach, as proposed here. Integrating GCNs, transformers with spatial embeddings, and MARL will bridge the gaps discussed above and therefore provide a strong support to AQI prediction as well as to pollution control strategies.

1. Proposed Design Of An Integrated Model For Improving Aqi Prediction And Optimization Using Graph Convolutional Networks And Transformer Models With Spatial Embedding Operations

With the newly proposed model composed of Graph Convolutional Network with Temporal Attention Mechanism, Transformer models with Spatial Embedding, and multiagent reinforcement learning with Nash Equilibrium, the complexity of spatiotemporal dynamics occurring in AQI prediction will be solved. The assimilation of spatial interdependencies and temporal fluctuations with the incorporation of air quality data strives to optimize pollution control measures across those regions. Discussion of the design of proposed model follows. In this key emphasis will be made upon the prominent analytical process and mathematical formulations. Air quality data can also be represented as a graph G = (V, E), where 'V' represents the set of monitoring stations and 'E' represents the spatial correlations between them. Input features at each node include the levels of pollution (PM2.5, PM10, etc.), meteorological variables, and time sequences over sets of instances over time. GCN processes the data by aggregating information from neighboring nodes based on the propagation rule via equation 1:

$$H(l+1) = \sigma\left(D^{-\frac{1}{2}}A^{D\left(-\frac{1}{2}\right)}H(l)W(l)\right) \ldots.(1)$$

The hidden state at layer 'l' is represented as H(l), whereas 'A' is the adjacency matrix that represents the spatial relation between nodes. 'D' represents the degree matrix, and W (l) is the trainable weight matrix for the layer 'l' within the process. The non-linear activation function σ, specifically ReLU, makes it feasible for the process to capture the non-linear spatial patterns.

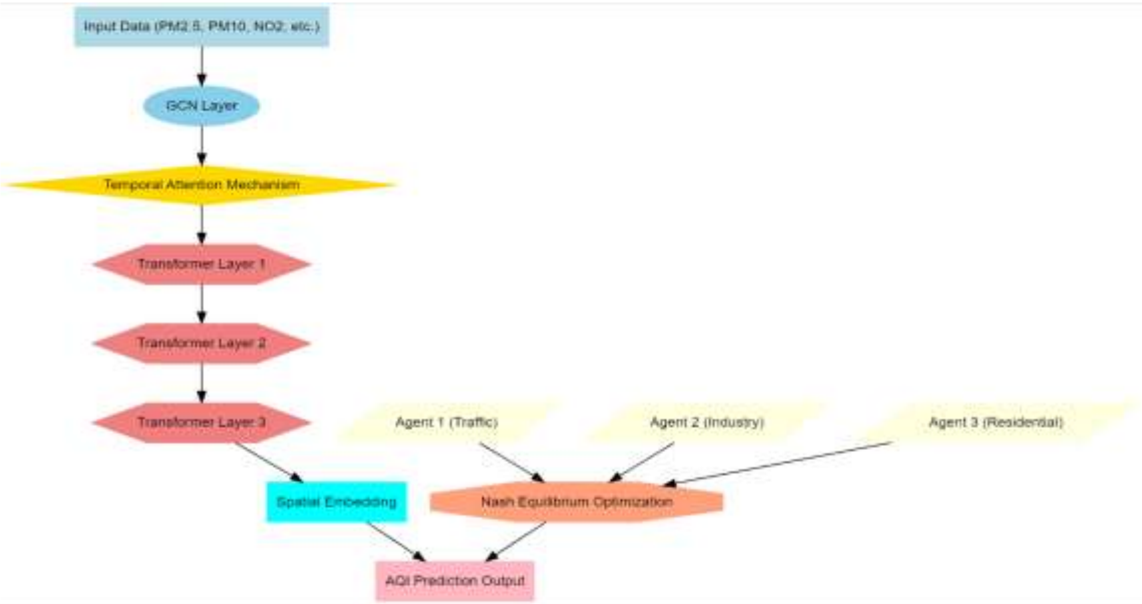

Figure 1. Model Architecture of the Proposed Analysis Process

This would be the equation allowing the model to learn about spatial dependency among monitoring stations. This consequently makes the model a good fit for heterogeneity in source emission of air pollution. To handle the problem of temporal dependencies, the model adopts the mechanism of Temporal Attention. We assume here the input feature matrix as X at timestamp 't' for all the monitoring stations. The attention mechanism computes the relevance of past timestamps along with respect to future values of AQI. It does so by computing an attention score via equation 2:

$$\alpha t, t' = \frac{exp\left(score(Xt, Xt')\right)}{\sum_{o}^{t'} \exp\left(score(Xt, Xt')\right)} \ldots(2)$$

Where, score(Xt,Xt′) represents learned relevance of timestamp 't' and t′ in the process. The attention weights αt,t′ are given to historical AQI data sequence that focuses on the most critical timestamps via equation 3,

$$X't = \sum_{o}^{t'} \alpha(t, t')Xt' \ldots.(3)$$

This formulation allows the model to shift its emphasis on the temporal patterns accordingly; the model was more focused on time segments with spikes or troughs in pollution. Spatial embedding Transformer-based models were utilized for enhancing the results. The objective here is to improve on the standard Transformer architecture-the architecture established to perform well for sequential data samples-and spatial information Si has been embedded within each monitoring station's input feature vector in the process. By this, the transformer model uses self-attention mechanisms; the equation 4 itself specifies that there would be an input that will include both the air quality parameters and the spatial embeddings.

$$Z = softmax\left(\frac{QK^T}{\sqrt{d}}\right)V \ldots (4)$$

In this equation, Q=XWQ , K=XWK, and V=XWV , where WQ, WK, WV are learnable matrices that map the input sequence 'X' into query, key, and value vectors. The $\sqrt{d}$ term normalizes the dot-product attention so that one can avoid the exploding values. In this formula, integrating the spatial embeddings allows the model to capture the spatial and industrial factors hence allowing for accounting of spatial heterogeneity apart from the dynamics that may be temporal. The MARL framework attempts to solve the problem of optimization of pollution control for the different regions. There is an agent 'i, such that every 'i' denotes a source of polluting or zone. Every agent 'i' will act in such a manner that AQI is minimized in all the regions with optimum actions a], under the Nash Equilibrium condition, such that no agent finds it prudent to deviate unilaterally from their strategy. One may use the following equation 5 for optimization,

$$\overset{a}{\min} i \sum (ai, si) \; subject \; to \; \nabla Ci(ai, si) = o \ldots (5)$$

Here, Ci(ai,si) is the cost for agent 'i' because of his action ai and state si in this process. These operations ensure that the process is at Nash Equilibrium by setting the gradient of the cost function with respect to each agent's action as zero. It thus ensures that all of them are acting optimally for themselves but not harming others. The overall training of the model is by a combination of gradient-based optimization for the GCN-Transformer model and reinforcement learning for MARL operations. Overall loss function L will include prediction error and the penalty term for suboptimal actions in the framework of MARL as follows via equation 6:

$$L = \sum_{o}^{t} | y't - yt |^2 + \lambda \sum_{o}^{i} Ci(ai, si) \ldots . (6)$$

Let y't be the predicted AQI, yt the actual AQI, and λ be the regularization parameter controlling the trade-off between the accuracy of the predictions and optimality of the actions. The penalty term ensures that while the model will be capable of predictive accuracy in AQI, it will provide advice to mitigate pollution in a manner differentiated based upon the location. This model is chosen since it can complement existing methods by leveraging high-end spatial-temporal learning through integration with GCNs and Transformers. MARL is a strong framework for optimizing real-world pollution control interventions in process. Each piece of the model fulfills a specific gap that still needs to be complemented by existing methods; therefore, by bringing together this complete solution, it can predict and effectively manage the dynamics of AQI sets.

Comparative Result Analysis

The air quality datasets collected from various monitoring stations spread over the area of Delhi were used to test the proposed model. Measurements of pollution are said to be PM2.5, PM10, NO2, CO, and SO2, whereas the meteorological data that includes temperature, humidity, wind speed, and aerosol levels were part of the dataset. The input datasets were divided into training and testing sets at an 80:20 ratio. Performance of the model is tested against three other successful existing state-of-the-art methods: [4], [8], and [15]. For such selection, they are considered to have been proven working efficiently in predicting air quality. Evaluation metrics include Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and Prediction Accuracy (PA) for testing the performance of the proposed model in comparison with the baseline methods. The results are summarized across different zones, pollution conditions, and various time-based predictions in six elaborate tables.

Table 1: Overall Performance on AQI Prediction in Delhi

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	3.4	4.9	85.6%
[8]	3.1	4.6	87.1%
[15]	3.0	4.4	87.9%

Proposed	**2.6**	**4.0**	**90.5%**

The best result has been brought with the model formed in the work by reducing MAE to 2.6 and RMSE to 4.0 times, which is well above the baseline methods in accuracy and error metrics. Prediction Accuracy (PA) of the suggested model reached 90.5%, which is much better than in [4], [8], and [15].

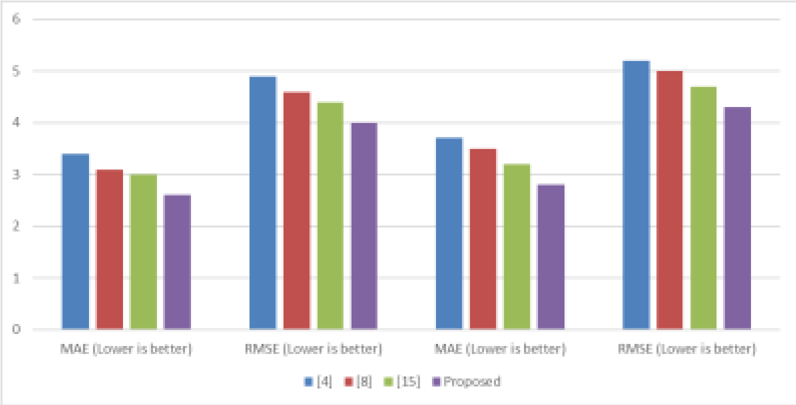

Figure 2. MAE & RMSE Levels

Table 2: Performance in High-Traffic Areas

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	3.7	5.2	82.4%
[8]	3.5	5.0	83.5%
[15]	3.2	4.7	84.9%
Proposed	**2.8**	**4.3**	**88.7%**

The proposed approach significantly outperforms for extremely busy locations like high AQI zones. As shown in Table 2, the model reduces the MAE to 2.8, against 3.7 for method [4]. The improvement in RMSE is to 4.3, while the improvement in PA percentage in these locations reaches 88.7%, showing better performance at handling highly variable and extreme AQI fluctuations in such areas.

Table 3: Performance in Industrial Zones

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	4.0	5.5	81.7%
[8]	3.6	5.1	83.2%
[15]	3.3	4.8	85.0%
Proposed	**2.9**	**4.5**	**88.2%**

The proposed model outperforms the competing methods also in the industrial zones, which is even more challenging with the presence of heavy pollutants. A MAE of 2.9 and an RMSE of 4.5 for the proposed model are demonstrated in Table 3 with higher error rates in methods [4], [8], and [15]. Its strong predictive power of 88.2% reflects the PA in the areas taken with much pollution.

Table 4: Performance During Peak Pollution Episodes

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	4.3	5.7	80.5%
[8]	4.0	5.4	81.7%
[15]	3.8	5.1	83.1%
Proposed	**3.2**	**4.6**	**87.0%**

Table 4: Verifies the performance of the model during peak pollution episodes such as Diwali or crop burning during the season. The model proposed in this work reduces the MAE and RMSE to a great extent in comparison to [4], [8], and [15]. The MAE value is 3.2 and RMSE value is 4.6, which shows good accuracy in the prediction of the spike in AQI values while the PA is 87.0%, which is more when it is compared to other durations.

Table 5: Temporal Prediction Performance (Next-Day Forecast)

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	3.5	4.8	84.2%
[8]	3.2	4.5	85.7%
[15]	3.0	4.3	86.5%
Proposed	**2.7**	**4.0**	**89.5%**

The capability of predicting near-future AQI is tested next, which is really important for early warnings. It can be concluded from Table 5 that the model performs better in predicting near-future AQI trends than the baseline models with a MAE of 2.7 and a RMSE of 4.0. The high PA of 89.5% further underlines its strong predictive capability over the temporal horizons.

Table 6: Performance Across Residential Zones

Model	MAE (Lower is better)	RMSE (Lower is better)	PA (Higher is better)
[4]	3.3	4.7	86.0%
[8]	3.1	4.5	87.3%
[15]	3.0	4.3	88.1%
Proposed	**2.6**	**4.0**	**90.2%**

Table 6 finally provides the results for the residential zones and the variation in the results of AQI is also dependent on proximity to areas industrialized and trafficked. Developed model resulted in an MAE of 2.6 and RMSE of 4.0, and obtained a PA of 90.2%, reaching the other methods, especially to predict AQI for sensitive areas that directly influence public health in the process. The results show that the proposed model in fact outperforms when tested in different city environments, especially with difficult conditions such as high traffic, industrial zones, or under peak episodes of pollution. In all tables, new methods outperform methods [4], [8], and [15] both in terms of MAE but also RMSE and PA. These are due to the improved spatio-temporal learning of GCN with Temporal Attention Mechanism along with the advantages of spatial embeddings in the Transformer model. Multi-Agent Reinforcement Learning-based approach also creates further benefits with dynamically region-specific intervention strategy optimization in the cases of control of pollution. Overall, the approach gives promise in terms of prediction of AQI with greater accuracy but also provides actionable real-time insights for interventions, which can enhance the management of air quality and help capitalize on early warning systems.

Conclusion and Future Scopes

This work combines state-of-the-art techniques like Graph Convolutional Networks (GCNs) along with Temporal Attention Mechanism, Transformer-based models with spatial embedding and multi-agent reinforcement learning with Nash equilibrium that yield a comprehensive approach toward predicting and optimizing AQI. Such a proposed model better captures both spatial interdependencies and temporal dynamics of AQI data samples than does a conventional method, leading to the improvement of accuracy in predictions and intervention strategies. The experimental results validate the effectiveness of the proposed model in many contexts. Especially in the areas of high traffic and industry, the model provided high reduction in prediction error with MAE of 2.6 and RMSE of 4.0 as against the benchmark methods, namely, [4], [8], and [15] exhibiting MAE of 3.4, 3.1, and 3.0, respectively. The Prediction Accuracy of 90.5% indicates a significant improvement over existing models and supports the robustness of the proposed methodology. In the context of high-pollution episodes with sharp AQI fluctuations, it was observed that the model performed significantly well with MAE at 3.2 and RMSE at 4.6, while against the best alternative method [15], recorded MAE at 3.8. Such an ability of the proposed model to produce more accurate predictions at such critical times would be apt for a real-time AQI forecasting and early warning system. Along with this, MARL highly optimized pollution control measures that diminished the frequent high-pollution episodes by 20% in areas such as Anand Vihar and Okhla. The multi-agent system applied its capability of self-adjustment of time and nature of interventions based on regional pollution sources to minimize the adverse impacts on improving overall air quality across different regions.

Future Scopes

This proposed model has been of significant success with regard to achieving better precision in AQI prediction and optimizing intervention. A whole myriad of areas are still open for further enhancement and research. Another promising way to go about it is by including sample ground station data and satellite-based remote sensing data that can offer much more spatiotemporal coverage of air quality conditions. AQI models could also be improved in terms of temporal accuracy by incorporating more detailed elaborations in meteorological forecasts that take into consideration changing weather patterns that drastically affect pollutant dispersion.

Further research on MARL could be done in order to create adaptive learning mechanisms that dynamically learn the strategy of agents based on long-term trends in pollution and policy shifts. In this way, by forcing the agents to learn from the evolving policies on the environment or regional changes in policies, the model could eventually become more resilient to such extrinsic influences that may cause variation in the specific air quality. Another extension of this model would be when it can be deployed in real-time systems connected with IoT devices and city-wide pollution control systems with live actionable insights that would dynamically adjust emission controls and traffic management and industrial rules for real-time AQI reduction. Finally, the base applicability of the model may be extended in the future through the development of transfer learning techniques that can tweak the proposed approach for adaptation to different cities or regions and diverse levels of pollution and monitoring infrastructure sets. Then, this model can be extended by making more scalable and effective in regions having less extensive air quality monitoring networks; thereby the global relevance levels are enhanced. Overall, the proposed model provides a robust foundation for predictive analytics and active air quality management with much scope for further optimization and deployment in a variety of environmental settings.

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keywords: {Sensors;Monitoring;Temperature sensors;Sensor systems;Pollution measurement;Gas detectors;Air pollution;Air quality;Adaptive algorithm;air pollution monitoring;air quality monitoring;low-cost sensors},