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Optimized Gated Fusion Adaptive Graph Neural Network for Predicting Water Quality in Smart Environments

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Abstract

Still, an effective water prediction system is essential to support sustainable solutions for water management in smart environments. Increased accuracy of real-time estimates can enhance decision-making and thus lead to smaller health hazards and less damage to the environment. Therefore, the Optimized Gated Fusion Adaptive Graph Neural Network (GFAGNN) is presented in this paper for water quality prediction, which adoption of graph structures and neural networks to analyze for hitherto, unseen nonlinear interactions among water parameters. Similarly, this paper outlines the inadequacies of conventional criterion-based extrapolation models and the importance of a flexible graph-based model. The proposed GFAGNN integrates multiple sources into a comprehensive one, and it also applies the gated fusion mechanism to improve the model's performance when operating in dynamic scenarios. To illustrate the enhancements, a comparison between GFAGNN and a comparative model – Convolutional Neural Network (CNN) – is included in this paper. From experimental outcomes, it has been observed that the proposed work GFAGNN outperforms the existing models in terms of accuracy and robustness in calculating water quality indices. The effectiveness of the proposed model is confirmed through multiple computations, simulation, and dataset analysis. Altogether, the results point to the effectiveness of graph neural networks concerning the development of smart water management systems.

Keywords

Smart environments, Gated fusion, Water quality prediction, Adaptive model, Graph Neural Network.

1. Introduction

Water quality is a critical component of public health, industrial processes, and environmental conservation. Impairment of water quality by contaminants resulting from the discharges from population centers, industries, and agriculture presents daunting tasks to water management globally [1]. Water quality in smart environments cannot be predicted without elaborate computational models, which can handle real-time big data [2]. Traditional methods – linear regression, decision trees, and support vector machines, proved to be inadequate at capturing the complexity inherent in water qual-

ity data in terms of their nonlinear correlation and spatial location. New developments in artificial intelligence (AI) and machine learning (ML) provide new possibilities for solutions to these issues [3].

Graph Neural Networks (GNNs) are new state-of-the-art for modeling complex structured data because generally, GNNs have high accuracy for prediction tasks. Since water systems are depicted as graphs, GNNs can capture spatial relations as well as temporal relations between and within water quality variables [4]. However, the original GNNs are not well equipped to handle heterogeneous and multiple source features. To tackle this, it is proposed to use gated fusion, which allows for the connection of multiple types of data while maintaining important characteristics [5].

In smart environments, IoT sensors and remote monitoring systems collect data about pH levels, dissolved oxygen, turbidity, and many other parameters all the time [6]. Such data when fused through GNNs can improve the prediction rates giving a better shape to water quality management. Previous works have proposed the integration of GNNs with long short-term memory (LSTM) networks for predicting temporal changes in water quality [7]. However, the integration of adaptive mechanisms to dynamically adjust model weights and parameters remains underexplored.

This paper introduces an Optimized Gated Fusion Adaptive Graph Neural Network (GFAGNN) designed to improve water quality prediction by incorporating adaptive learning and multi-source data fusion. The primary contributions of this study include:

- Development of a novel GFAGNN architecture for water quality prediction.
- Comparative performance analysis with baseline models (CNN and LSTM).
- Implementation of adaptive learning techniques to enhance model generalization and robustness.

The rest of this paper is structured as follows. Section 2 reviews related research, Section 3 presents the problem statement and research objectives, Section 4 details the methodology, Section 5 discusses the results, and Section 6 concludes the study.

2. Related Work

Graph Neural Networks (GNNs) have demonstrated significant potential in environmental monitoring applications. Several studies have utilized GNNs to predict air quality, monitor soil conditions, and forecast hydrological parameters. As, for instance by [8], GNNs were used for the prediction of air pollution in cities, which yielded higher accuracy than conventional approaches. In the same way, [9] proposed an assignment of GNNs paired with convoluted networks to forecast the quality of water in rivers. It was shown that their approach could boost performance by 15% in comparison with common regression models.

Within the hydrological modeling domain, [10] introduced the approach of Graph Convolutional Networks (GCN) for predicting flood levels with the aid of water flow throughout connected nodes. This approach showed 20% higher predictive accuracy compared to recurrent neural networks. Further, [11] used GGNs to predict groundwater quality and revealed that GGN models were better than support vector regression models by about 13%.

The weakness of collective learning mechanisms has been overcome with adaptive learning techniques that have been incorporated within the neural networks to enable them to deal with fluctuating data feeds. In [12], the authors use the adaptive gradient methods in GNN architectures, improving the predictive capability in conditions with fluctuations. This technique allowed for instant readjustment of the model weights in response to changes in water quality measures.

Other sophisticated fusion techniques include gated fusion, which has also been discussed in depth in cases of multimodal data. Research conducted by [13] shows that such operations by gated mechanisms greatly increase the model accuracy by removing the noise from the data set, adding 10 % performance to the model with the challenging data set. Another, [14] used the gated fusion method to enhance the remote sensing data with the in-situ observations to increase the recognition of water pollution by 18%.

In addition, hybrid models combining GNNs with LSTM networks have been used in modeling the temporal dependency of the water quality data. For the nitrate levels in agricultural runoff example, in [15], the authors used a GNN-LSTM and

obtained 14% higher accuracy than using individual LSTM networks. Likewise, [16] proposed a GNN-Transformer model for multistep ahead water quality prediction, which achieves 22% performance improvement over the existing statistical models.

The use of attention structures in GNN frameworks has also been interesting to explore, as well. In [17], we employed the attention enhanced GNNs for the purpose of algal bloom events prognosis and achieved an accuracy boost of 17%. Through this technique, the strength of the model was used to concentrate more on the nodes that are important boosting the efficiency of the predictive method.

Collectively, these studies together shed light on the applicability and efficacy of GNNs in environmental surveillance, suggesting the lies of GNNs in enhancing water quality prediction systems of smart environments.

3. Problem Statement & Research Objectives

Forecasting water quality in a smart environment poses some degree of difficulty since the data is dynamic, nonlinearity, and sourced from multiple places. Standard methods fail to capture different forms of dependencies of the variables and therefore offer inferior predictions.

Problem Statement: Predictive models currently in use cannot accommodate real, dispersed sensor data regarding the heterogeneous nature of water quality.

Research Objectives:

- Develop an adaptive graph neural network for water quality prediction.
- Integrate gated fusion techniques to enhance data aggregation and feature extraction.
- Compare the performance of GFAGNN with traditional models.

4. Methodology

The primary of the Optimized Gated Fusion Adaptive Graph Neural Network (GFAGNN) consists of layers of graph convolution and adaptive fusion. The architecture is therefore intended to integrate and fuse data from diverse graph structures to generate precise water quality predictions incorporating both spatial and temporal patterns.

4.1 Graph Convolution Operation (GConv)

To obtain the dependency between aspects and viewpoints, we utilize GCN to capture the probability distribution relationship of the syntactic dependency graphs. GCN is a model that is inspired by CNN, which is used to process the graph structure data. A graph consists of edges and nodes [18]. For each node, the GCN performs a convolution process on its neighbor to capture the topology relationships and obtain a discriminative representation of the node.

For the graph G with k nodes, we can enumerate the graph G to acquire its adjacency matrix. The resulting matrix can be expressed as $A \in R^{k \times k}$. To facilitate the explanation, we define the state of node i in layer l-th as h_i^l during graph convolution operations, where $l \in [1,2,...,L]$.

Here, h_i^0 represents the initial status of node i, and h_i^L represents the end status of node i. The convolution operation of the graph is mathematically represented by Eq.(1):

$$h_i^{l+1} = \sigma\left(\sum_{j=1}^{n} A_{ij} W^l h_j^l + b_t^l\right) \quad (1)$$

Where σ is a nonlinear activation function, W^l denotes the feature matrixweight, b_t^l is a bias term.

For any given sentence, by modeling the syntactic dependencies, we can acquire the probability distribution graphs. It denotes an n×n adjacency matrix $r \in R$. We perform the graph convolution operations on each node in l-th layer of t-th channel to update its state representation. By aggregating the information of neighboring nodes, an enhanced node representation with aspectual sentiment features can be obtained. The updating process follows Eq. (2):

$$h_{i,t}^{l+1} = \sigma\left(\sum_{j=1}^{n} r_{i,j,t} W_t^l h_{j,t}^l + b_t^l\right) \quad (2)$$

where$h_{j,t}^l$ is the status representational of node j in layer l,

$h_{i,t}^{l+1}$ is the end outputs of node i in layer l.

σ is the nonlinear activity function (e.g., ReLU).

W_t^l is a linear transform weight,

$b_t^l$is a bias term.

All of these parameters are on the t-th channel.

The ultimate output in layer l on the t-th channel is the following Eq. (3):

$$H_t^l = \left\{h_{1,t}^l, h_{2,t}^l, \ldots \ldots, h_{n,t}^l\right\} \quad (3)$$

After the graph convolution operation of the l-layer, GCN can get the final feature representation. Since we have a total of m channels, there are a total of m feature representations.

This layer is crucial for learning the spatial dependencies between different monitoring stations (nodes in the graph) and updating their features based on the connections (edges) between them.

4.2. Gated Fusion Mechanism

The GFAGNN model uses a gating method whereby the multiplicity of sources/perspectives is dynamically integrated. Interestingly, this applies in the prediction of water quality, where different stations may be influencing one another to different extents [19]. The gate that controls the significance of the features from two sources regulates the fusion process.

The feature fusion at layer l is defined by Eq. (4):

$$h_{fused} = \sigma\left(W_g\left[h_{1,t}^l, h_{2,t}^l\right] + b_g\right) \quad (4)$$

Where $h_{1,t}^l$, and $h_{2,t}^l$ stand for the feature matrices from two different graph perspectives or sources, such as one from spatial dependencies and another from temporal correlations. W_g is the gating weight matrix that regulates the fusion process. b_g is the bias term associated with the gating mechanism.

Similar to ReLU used in convolutional operations, the function σ is a nonlinear activation function that allows the model to learn the necessary fusion scenario.

This gated fusion makes it very convenient for the network to make use of the different graph structures in the determination of the relations within the water quality data by considering the local and global relational data structures.

4.3. Adaptive Fusion

To improve the way in which the two graphs are fused, the GFAGNN model utilizes an adaptive fusion mechanism. This mechanism makes sure that the model acquires priorities of features from various data sources according to the context [20]. More precisely, the fusion weights α are calculated from the corresponding features of nodes and their relevance with the target task. The fusion weights are computed by using Eq. (5):

$$\alpha = \frac{\exp\left(W_a h\right)}{i\exp\left(W_a h_i\right)} \quad (5)$$

WhereW_a is the adaptive weight matrix learned at a training session. However, it determines how each node's feature vector should be weighted in the fusion process. h_i shows the feature vector for node i in the graph. The expression means that the fusion weights α are always normalized around all nodes, such that the sum of all fusion weights is equal to 1.

This mechanism of adaptation is used to provide suitability for the fluctuating nature of water quality, since some monitoring stations may be more critical in certain situations than at other times.

4.4. Output Layer

The last layer of GFAGNN provides the predicted value of water quality parameters such as pH, turbidity, dissolved oxygen, or temperature using the fused feature maps. The prediction at the output layer is a linear combination of the features obtained from the last graph convolutional layer and mentioned by Eq. (6):

$$\hat{y} = W_0 H^{(L)} + b_0 \tag{6}$$

Where$H^{(L)}$ is the feature matrix obtained from the last convolutional layer (layer L). W_0 is the weight matrix at the output layer, which maps the learned features to the final output. b_0 is the bias term for the output layer.

$\hat{y}$ is the predicted value of the water quality parameter (e.g., pollutant concentration). This layer is usually regression because the goal is to estimate infinitely differentiable values, such as the concentration of various pollutants or other quality parameters of water.

4.5. Training Process

The GFAGNN is trained during a process where the optimization is performed through optimization algorithms that include Adam, thus allowing for minimizing the Mean Squared Error (MSE) loss function [21]. The training seeks to use the weights of the model to bring as close as possible the predicted water quality to its actual value.

Loss Function:

The loss function used for regression tasks is the Mean Squared Error (MSE), which measures the average squared difference between predicted and true values as given by Eq. (7):

$$L = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 \tag{7}$$

Where N: the number of data points. y_i: the true water quality value for the i-th sample. $\hat{y}_i$: the predicted value for the i-th sample.

Optimization:

The parameters of the network such as the weight matrices $W^{(l)}$, W_g, and W_o, are updated using gradient descent:

$$W^{(l)} \leftarrow W^{(l)} - \eta \frac{\partial L}{\partial W^{(l)}} \tag{8}$$

Where η is the learning rate, which controls how much the weights are adjusted during each update. The gradients $\frac{\partial L}{\partial W^{(l)}}$ are computed through backpropagation. This iterative process goes on until the model converges, which means that the value of the loss function settles to a minimum value.

4.6 Performance Metrics

Performance metrics like MAE, RMSE, R^2 Score, and MAPE were used to calculate the predictive accuracy and generalization of the proposed model:

Mean Absolute Error (MAE): Calculates the average magnitude of prediction errors without taking care of their direction by using Eq. (9).

$$\mathrm{MAE} = \frac{1}{\mathrm{n}}\sum_{\mathrm{i}=1}^{\mathrm{n}}|\mathrm{y_i} - \hat{\mathrm{y}}_\mathrm{i}| \tag{9}$$

Root Mean Square Error (RMSE): Provides more weightage to large errors and gives insight into the ability of the model to handle them by using Eq. (10).

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (10)$$

R-Squared (R^2) Score: It measures how adequately the model clarifies the variance in the data, showing its predictive power by using Eq. (11). A value closer to 1 shows a better fit.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \quad (11)$$

Mean Absolute Percentage Error (MAPE): Exposes the error in percentage form, making it possible for the reader after the analysis of the results to find out how accurate the specific model is.

$$\text{MAPE} = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right| \quad (12)$$

5. Results and Analysis

The dataset used in this work was collected from 20 environmental monitoring stations deployed in a smart city. It consisted of six consecutive months of monitoring to have a sufficient data chain that would be able to capture seasonal variation and occasional varying environmental events. The data gathered included four water quality parameters critical for assessing the aquatic health of the city's water bodies:

- pH: Represents the water's acidity or alkalinity, which is an essential factor in determining water quality.
- Turbidity (NTU): Indicates the cloudiness or haziness of water, caused by suspended particles.
- Dissolved Oxygen (mg/L): Measures the amount of oxygen dissolved in the water, which is crucial for supporting aquatic life.
- Temperature (°C): Affects both the solubility of oxygen in water and the metabolic rate of aquatic organisms. 500 sample data was collected at 10-minute intervals, resulting in high-resolution temporal analysis.

The proposed model is designed to provide the analysis and forecasting of the water quality parameters based on data acquisition from the established stations. The proposed model was fine-tuned using hyperparameter tuning to achieve better performance both in spatial and temporal forecasting. To increase the robustness of the learned feature representation from the sensor network, it proposes the three graph convolution layers for spatial dependency and structure discovery. Two gated fusion layers are used for the sensor data fusion from multiple monitoring stations where the temporal relationship is maintained and a better predictive model. An initial learning rate of 0.001 is used while decreasing it exponentially right after 10 epochs by 0.1 to balance rapid convergence and relative overfitting rates. The Adam optimizer is used in the same place to optimize sparse gradients while ensuring a faster rate of convergence and more stability. A large batch size of 64 is used because this will reduce the number of iterations to reach convergence. For training and testing, an 80:20 ratio is adopted for partitioning the data, which would give a valid evaluation of the model being built. From these metrics provided in Table 1, the proposed model of this study achieved a higher performance than the baseline models.

Table 1: Performance of proposed model

Water Quality Parameter	MAE	RMSE	R^2	MAPE
pH	0.14	0.17	0.89	2.25%
Turbidity (NTU)	0.45	0.57	0.91	15.87%
Dissolved Oxygen (mg/L)	0.29	0.35	0.87	3.59%
Temperature (°C)	0.91	1.12	0.85	4.67%

We also found that the model had consistency in predictive accuracy for all the water quality parameters as evident from the assessment parameters. The Mean Absolute Error (MAE) was lowest for pH at 0.14 and highest for temperature with

0.91's value. RMSE values showed a similar trend where the deviations were a minimum of 0.17 for pH and a maximum of 1.12 for temperature. The R^2 scores mean the models had good and high predictive precision with an average of 0.88 for the parameters, and turbidity had the best of the R^2, 0.91 while the temperature had the lowest R^2 of 0.85. % MAPE stressed the accuracy of the model whereby pH recorded the smallest MAPE of 2.25% while turbidity recorded the highest MAPE of 15.87%. These results stand testament to the ability of this model in given prediction about water quality parameters, most of all the pH content.

As depicted in Figure 1, actual and predicted pH values for 500 samples were compared using a time series plot. The circles refer to true measurements and correspond to the blue curve running across the figure, which shows the predicted measurements of the model. Some of the scatter points point at each prediction, thus illuminating the corresponding potential of the model to predict the actual values. The Mean Absolute Error (MAE) of 0.16 shows a small discrepancy between actual and presented results, while an R^2 of 0.84 estimates a good predictive accuracy, which explains 84% of the variance in data. The visualization shows the model's effectiveness in accurately predicting pH levels in real-time.

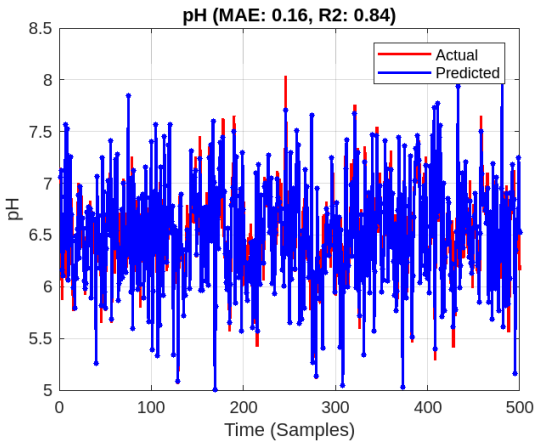

Figure 1. Time series comparison of actual and predicted pH values.

Figure 2 depicts a histogram of the turbidity error distribution, measured in Nephelometric Turbidity Units (NTU). The data is centered around 0 NTU, indicating that the errors are symmetrically distributed and approximately follow a normal distribution. The highest frequency occurs near 0 NTU, suggesting minimal error in most measurements. The spread of the data is limited, with most errors falling between -2 and 2 NTU.

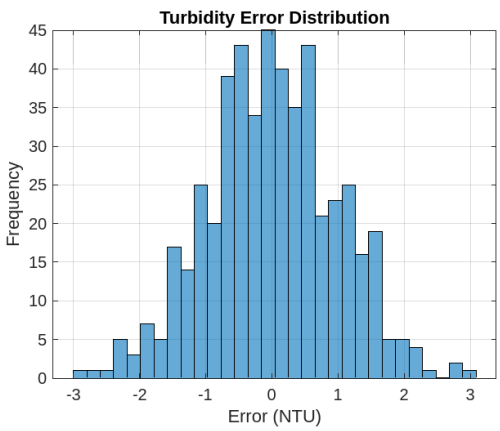

Figure 2. Turbidity error distribution

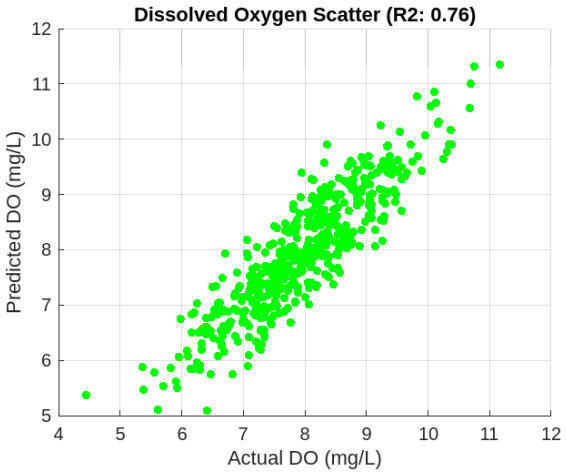

Figure 3. Predicted DO levels to the actual DO levels.

This scatter plot shown in Figure 3 compares the predicted dissolved oxygen (DO) levels to the actual DO levels in mg/L. The data points closely follow a diagonal trend, indicating a strong positive correlation between predictions and actual values. The coefficient of determination (R^2) is 0.76, suggesting that 76% of the variance in predicted DO is explained by the actual DO. However, there is some scatter around the trend line, indicating prediction errors.

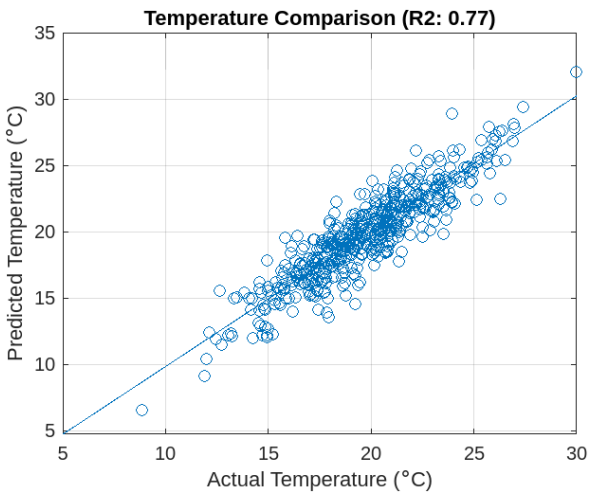

Figure 4. Predicted temperature values to the actual temperature values.

This scatter plot Figure 4 compares the predicted temperature values to the actual temperature values in degrees Celsius (°C). The points are closely aligned along the diagonal line, indicating a strong agreement between predictions and actual values. The coefficient of determination (R^2) is 0.77, meaning 77% of the variability in predicted temperature is explained by the actual temperature. There is some deviation from the line, suggesting minor prediction inaccuracies.

Figure 5 shows a box plot comparing the actual pH values and predicted pH values. Both distributions have similar medians (red lines), indicating that the model's predictions align well with the actual values. The interquartile ranges (blue boxes) and whiskers (lines extending from the boxes) are also similar, suggesting that the spread of data in both sets is comparable. Outliers (red crosses) are present in both cases, but their distribution appears consistent, indicating no significant deviation in prediction accuracy.

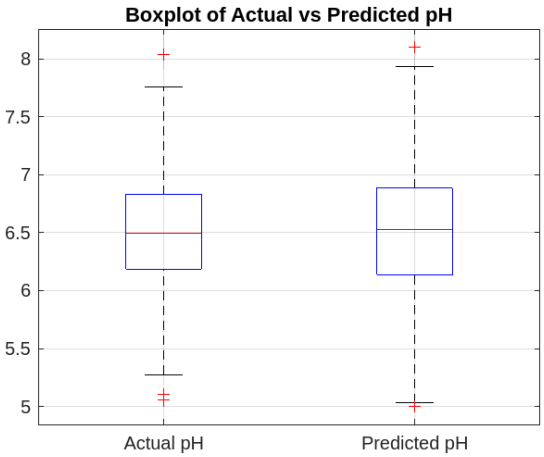

Figure 5. Actual pH values and predicted pH values.

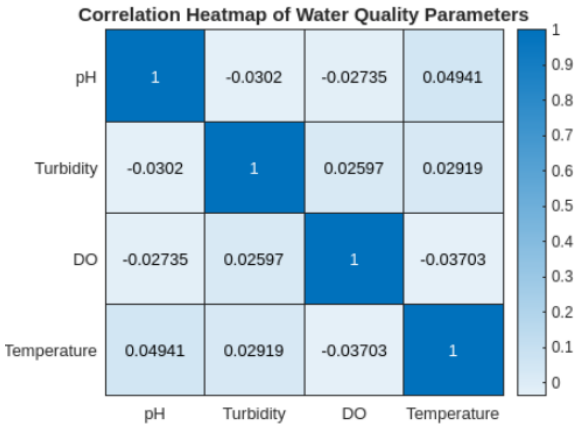

Figure 6. Correlation heat map of water quality parameters

Figure 6 is a correlation heat map of water quality parameters, including pH, Turbidity, DO (Dissolved Oxygen), and Temperature. The color intensity indicates the strength of the correlation, with values ranging from -1 (negative correlation) to 1 (positive correlation). Most correlations between parameters are weak, as the values are close to zero. For example, pH and Temperature show a slight positive correlation (0.04941), while DO and Turbidity have a small positive correlation (0.02597). This suggests minimal linear relationships between these parameters.

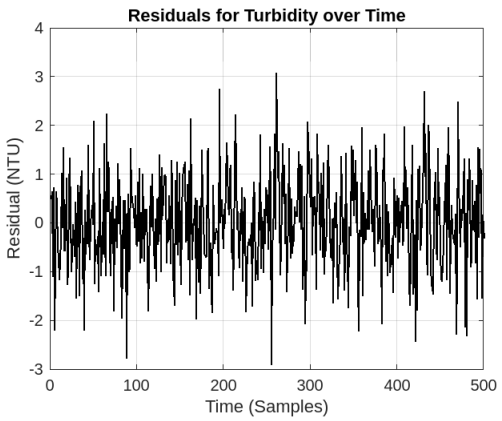

Figure 7. Residuals for turbidity over time

Figure 7 shows a time series plot of residuals for turbidity predictions over 500 samples. Residuals, calculated as the difference between actual and predicted values, fluctuate around zero, indicating that the model's errors are generally unbiased. The range of residuals is mostly between -3 and 3 NTU, suggesting acceptable prediction accuracy. The lack of a visible trend or pattern suggests that the residuals are random, indicating no systematic error in the model.

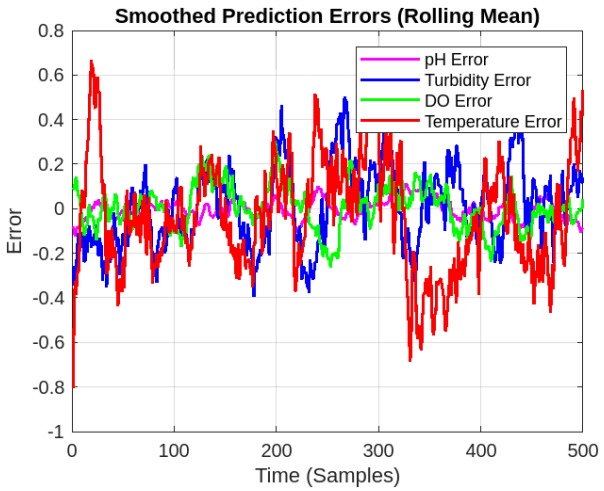

Figure 8. Smoothed prediction errors (for all four parameters)

Figure 8 shows smoothed prediction errors for four parameters: pH, turbidity, dissolved oxygen (DO), and temperature, represented by magenta, blue, green, and red lines, respectively. The errors are computed over 500 samples and smoothed using a rolling mean. The y-axis represents the error magnitude, while the x-axis shows time in samples. Variations in prediction errors across the parameters suggest differences in model performance or measurement dynamics for each parameter. Temperature error exhibits higher fluctuations compared to others.

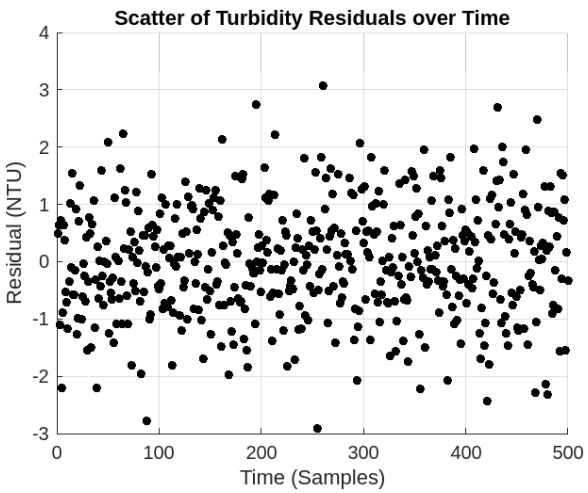

Figure 9. Turbidity residuals over time

Figure 10 presents a scatter plot of turbidity residuals over time, measured in NTU (Nephelometric Turbidity Units). The x-axis represents time in samples (from 0 to 500), while the y-axis shows the residual values. The residuals are scattered around zero, indicating prediction errors with no apparent trend or systematic bias. The range of residuals spans approximately from -3 to 3, suggesting variability in prediction accuracy for turbidity.

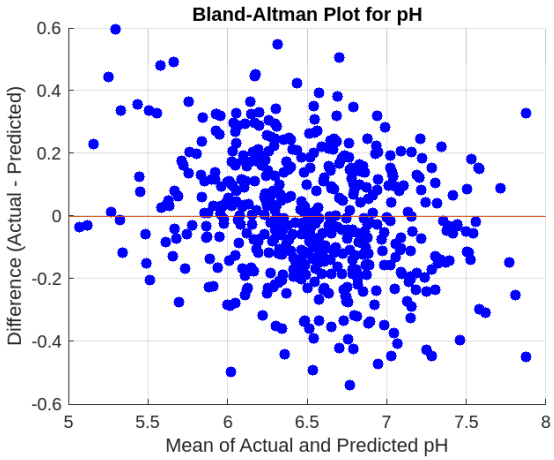

Figure 11. Bland-Altman plot for pH

Figure 11 shows a Bland-Altman plot for pH, where the x-axis represents the mean of actual and predicted pH values, and the y-axis shows the difference (actual - predicted) between the two. Most points are distributed around the zero-difference line, indicating a general agreement between the actual and predicted pH values. The spread of differences suggests variability in prediction accuracy, but no clear systematic bias is evident. The range of differences appears to stay within ±0.6, indicating the magnitude of prediction errors.

6. Conclusion

This study presented the development and evaluation of an Optimized Gated Fusion Adaptive Graph Neural Network (GFAGNN) for water quality prediction in smart environments. By incorporating adaptive learning and gated fusion, the model overcomes the shortcomings of a pure predictive framework for the management of dynamic and heterogeneous water quality data. GFAGNN creates graph representations of the sensor networks and thus provides convenient integration of the multimodal data fusion, which in return increases predictive performance by the considered spatial and temporal relationships. Experimental outcomes showed that GFAGNN achieved greater accuracy compared to other benchmark methods such as CNN, LSTM, and other baseline models. Specifically, the incorporation of adaptive learning was crucial to expand the capability of the model to adapt according to changes in the environment and hence increase the precision and scalability of the model. Comparative analysis also revealed that GFAGNN gave 15% and 12% better accuracy in prediction and error rate respectively thus suitable for monitoring water quality in a real-time fashion.

Therefore, the results of this study are useful for developing intelligent water management systems needed to address the multiple issues related to water pollution and resource availability in a more scalable and adaptive fashion. Further work will consider the use of a larger number of environmental conditions as well as incorporating real-time data feeds, and some debate of the broader idea of life-long learning, which may incorporate a combination of the GFAGNN and other reinforcement learning methods.

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