# Air Quality Index (AQI) Prediction Model Using Time Series Analysis

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**Abstract**

This report presents the development of an Air Quality Index (AQI) prediction model utilizing time series analysis. The project encompasses data collection, data cleaning, data distribution and correlation analysis, exploratory data analysis, model training, evaluation, and deployment.

`GIT LINK: https://github.com/DiamondDeadMaw/blacklung`

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# 1 Introduction

Air pollution poses significant risks to public health and the environment. The Air Quality Index (AQI) is a standardized indicator used to communicate how polluted the air currently is or how polluted it is forecasted to become. Accurate prediction of AQI levels is crucial for informing the public and aiding policymakers in implementing effective air quality management strategies.

This report outlines the development of an AQI prediction model using time series analysis techniques. The study focuses on data collected from various monitoring stations in Delhi, covering multiple pollutants over several years.

# 2 Data Collection

## 2.1 Data Sources

The dataset was obtained from the Central Pollution Control Board (CPCB) of India and includes measurements from 40 monitoring stations across Delhi from 2017 to 2023. The parameters collected encompass various pollutants and meteorological factors:

- **Pollutants**: $PM_{2.5}$, $PM_{10}$, NO, $NO_2$, $NO_x$, $NH_3$, $SO_2$, CO, $O_3$, Benzene, Toluene.
- **Meteorological Factors**: Temperature, Humidity, Wind Speed, Wind Direction, Solar Radiation, Pressure.

## 2.2 Data Structure

The raw dataset contained:

- **245,376** records.
- **628** features, including pollutant concentrations and meteorological parameters from different stations.
- Timestamped measurements at 15-minute intervals.

# 3 Data Cleaning

### 3.0.1 Data Availability by Parameter

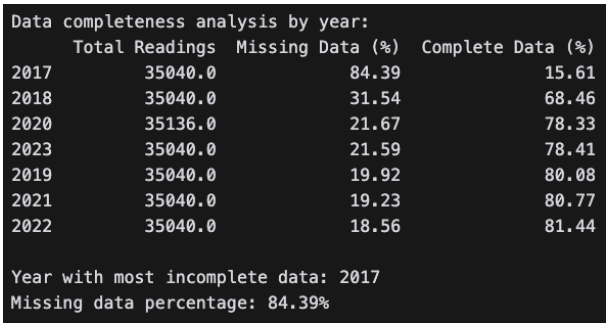
Data availability analysis:

| | Total Readings | Non-null Count | Null Count | Null Percentage |
|---|---|---|---|---|
| temperature | 8342784.0 | 4977685.0 | 3365099.0 | 40.34 |
| pressure | 8588160.0 | 5125252.0 | 3462908.0 | 40.32 |
| benzene | 9324288.0 | 5707334.0 | 3616954.0 | 38.79 |
| humidity | 9324288.0 | 6014953.0 | 3309335.0 | 35.49 |
| toluene | 8588160.0 | 5546138.0 | 3042022.0 | 35.42 |
| nh3 | 7852032.0 | 5646538.0 | 2205494.0 | 28.09 |
| so2 | 7852032.0 | 5650537.0 | 2201495.0 | 28.04 |
| co | 9569664.0 | 6966775.0 | 2602889.0 | 27.20 |
| pm10 | 9569664.0 | 6970477.0 | 2599187.0 | 27.16 |
| ozone | 9569664.0 | 7002360.0 | 2567304.0 | 26.83 |
| no2 | 9569664.0 | 7234808.0 | 2334856.0 | 24.40 |
| no | 9324288.0 | 7114124.0 | 2210164.0 | 23.70 |
| pm25 | 9569664.0 | 7336787.0 | 2232877.0 | 23.33 |
| nox | 9324288.0 | 7236747.0 | 2087541.0 | 22.39 |

Figure 1: Data Availability Analysis Before Cleaning

### 3.0.2 Data Completeness by Year

Figure 2 presents the completeness percentages per year.



Data completeness analysis by year:

| | Total Readings | Missing Data (%) | Complete Data (%) |
|---|---|---|---|
| 2017 | 35040.0 | 84.39 | 15.61 |
| 2018 | 35040.0 | 31.54 | 68.46 |
| 2020 | 35136.0 | 21.67 | 78.33 |
| 2023 | 35040.0 | 21.59 | 78.41 |
| 2019 | 35040.0 | 19.92 | 80.08 |
| 2021 | 35040.0 | 19.23 | 80.77 |
| 2022 | 35040.0 | 18.56 | 81.44 |

Year with most incomplete data: 2017
Missing data percentage: 84.39%

Figure 2: Data Completeness Analysis by Year Before Cleaning

The year **2017** exhibited the highest percentage of missing data at **84.39%**, indicating significant data quality issues during that period.

## 3.1 Handling Missing Values

The dataset cleaning process employed two sequential imputation methods to handle missing values in the air quality measurements.

### 3.1.1 Primary Method: Hourly Mean Imputation

The first imputation method calculated hourly means using the following formula:

$$\bar{x}_h = \frac{1}{n_h} \sum_{i=1}^{n_h} x_{h,i} \tag{1}$$

Where:

- $\bar{x}_h$ is the mean value for hour $h$.
- $n_h$ is the number of non-null measurements for hour $h$.
- $x_{h,i}$ represents the $i$-th measurement in hour $h$.

This calculation was performed for each of the 24 hours in a day, creating a set of reference values for each pollutant parameter. Missing values were then replaced with their corresponding hourly mean.

### 3.1.2 Secondary Method: Four-Day Rolling Window Average

For remaining missing values, we implemented a four-day window average using the formula:

$$\bar{x}_t = \frac{1}{N} \sum_{i=-48}^{48} x_{t+i} \tag{2}$$

Where:

- $\bar{x}_t$ is the imputed value at time $t$.
- $N$ is the number of non-null values in the window.
- $x_{t+i}$ represents values at $i$ time steps before/after $t$.
- 48 represents 2 days (in hours) before and after the missing value.

The window spans 96 hours in total, taking measurements from two days before and two days after the missing value.

### 3.1.3 Implementation Sequence

The cleaning process followed this order:

1. Apply hourly mean imputation to all missing values.
2. For any remaining gaps, apply the four-day window average.
3. Record the number of values imputed by each method for quality assessment.

## 3.2 Test Run on a Single Site

Before applying the cleaning methods to the entire dataset, we conducted a test run on a single monitoring station, the **CRRI Mathura Road Delhi** site, to evaluate the effectiveness of our imputation strategies.

### 3.2.1 Initial Data at CRRI Station

Figure 3 shows the initial percentage of missing values for key pollutants at the CRRI station.

CRRI Station Analysis:

| | NaN_Count | NaN_Percentage |
|---|---|---|
| Timestamp | 0 | 0.00 |
| site_103_crri_mathura_road_delhi_co | 7279 | 3.46 |
| site_103_crri_mathura_road_delhi_no | 21057 | 10.01 |
| site_103_crri_mathura_road_delhi_no2 | 10517 | 5.00 |
| site_103_crri_mathura_road_delhi_nox | 9436 | 4.49 |
| site_103_crri_mathura_road_delhi_ozone | 8642 | 4.11 |
| site_103_crri_mathura_road_delhi_pm10 | 14815 | 7.04 |
| site_103_crri_mathura_road_delhi_pm25 | 10323 | 4.91 |
| site_103_crri_mathura_road_delhi_solar_radiation | 209025 | 99.38 |

Figure 3: CRRI Station Missing Data Before Cleaning

### 3.2.2 Data Cleaning on CRRI Station

We applied the two-step imputation process:

1. **Hourly Mean Imputation**: Replaced missing values with the mean value of that specific hour across all days.
2. **Four-Day Rolling Window Average**: For any remaining missing values, applied a rolling window average considering two days before and after the missing timestamp.

### 3.2.3 Results After Cleaning at CRRI Station

Post-cleaning, the percentage of missing values significantly decreased, as shown in Figure 4.

CRRI Station Analysis:

| | NaN_Count | NaN_Percentage | \ |
|---|---|---|---|
| Timestamp | 0 | 0.00 | |
| site_103_crri_mathura_road_delhi_co | 336 | 0.16 | |
| site_103_crri_mathura_road_delhi_no | 6820 | 3.24 | |
| site_103_crri_mathura_road_delhi_no2 | 836 | 0.40 | |
| site_103_crri_mathura_road_delhi_nox | 460 | 0.22 | |
| site_103_crri_mathura_road_delhi_ozone | 412 | 0.20 | |
| site_103_crri_mathura_road_delhi_pm10 | 5372 | 2.55 | |
| site_103_crri_mathura_road_delhi_pm25 | 380 | 0.18 | |
| site_103_crri_mathura_road_delhi_solar_radiation | 207744 | 98.77 | |

Figure 4: CRRI Station Missing Data After Cleaning

The test run confirmed the effectiveness of our cleaning methodology, resulting in a substantial reduction of missing values.

## 3.3 Data Cleaning on the Entire Dataset

Encouraged by the successful test run, we applied the cleaning process to the entire dataset.

### 3.3.1 Removal of Irrelevant Columns

We removed **255 columns** that had excessively high percentages of missing data or were irrelevant to the AQI prediction, retaining **374 columns** for further analysis.

### 3.3.2 Data Availability After Cleaning

Figure 5 summarizes the data availability after the cleaning process.

## 3.4 Addition of Weather Data

To the above, we added the following variables: Cloud Base Height, Evaporation, Surface Pressure, 2M Temperature, Total Cloud Cover, Total Precipitation, u10m, and v10m components of wind speed. This was retrieved from the "ERA5 hourly data on single levels from 1940 to present" dataset. As there were no missing values, no imputation or data filling methods were implemented. The collected data was hourly, while the main dataset was every 15 minutes. Thus, we have duplicated each row 3 times to fill the hour in the main dataset.

Data availability analysis after cleaning:

| | Total Readings | Non-null Count | Null Count | Null Percentage |
|---|---|---|---|---|
| pm10 | 8203104.0 | 7302344.0 | 900760.0 | 10.98 |
| nh3 | 6730752.0 | 6039444.0 | 691308.0 | 10.27 |
| ozone | 8203104.0 | 7456876.0 | 746228.0 | 9.10 |
| co | 8203104.0 | 7548476.0 | 654628.0 | 7.98 |
| no2 | 8203104.0 | 7561148.0 | 641956.0 | 7.83 |
| so2 | 6730752.0 | 6219916.0 | 510836.0 | 7.59 |
| pm25 | 8203104.0 | 7617044.0 | 586060.0 | 7.14 |
| no | 7992768.0 | 7475124.0 | 517644.0 | 6.48 |
| nox | 7992768.0 | 7514140.0 | 478628.0 | 5.99 |

Figure 5: Data Availability Analysis After Cleaning

The cleaned dataset, containing **210,336** rows and **374** columns, served for the subsequent data distribution analysis, exploratory data analysis, and model training phases.

# 4 Data Distribution and Correlation Analysis

## 4.1 Box Plot Distribution Analysis

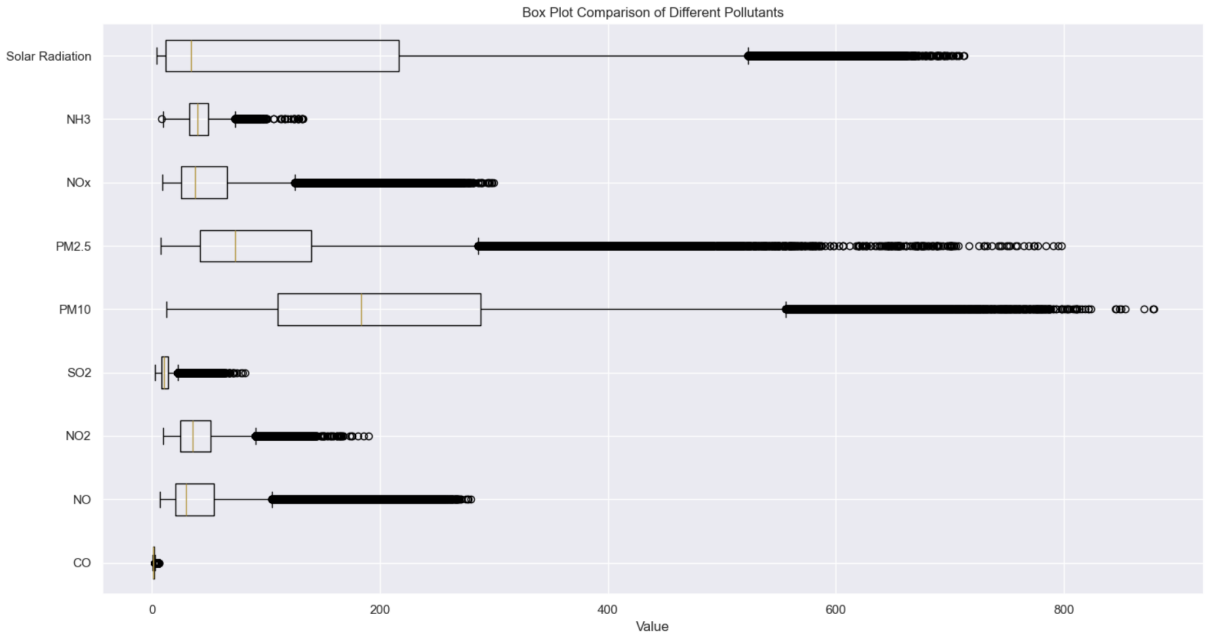



Figure 6: Distribution of Pollutant Concentrations

The box plots in Figure 6 illustrate the distribution of various pollutant concentrations:

### 4.1.1 Concentration Ranges and Outliers

- **Particulate Matter**:
  - **$PM_{10}$** exhibits the widest interquartile range (IQR), spanning approximately 100 to 300 units, with numerous high-value outliers extending beyond 800 units.

- **$PM_{2.5}$** shows a narrower distribution but a significant number of outliers exceeding 600 units.
- Both $PM_{10}$ and $PM_{2.5}$ have right-skewed distributions, indicating frequent episodes of severe particle pollution.

- **Gaseous Pollutants**:
  - **CO** has the most compact distribution, concentrated near zero with minimal spread and few outliers.
  - **NO** and **$NO_2$** display moderate IQRs with several high-value outliers, suggesting variable emission sources.
  - **$SO_2$** maintains relatively low concentrations with occasional spikes, indicating sporadic sources.

- **Other Parameters**:
  - **$NH_3$** exhibits a relatively symmetric distribution with moderate outliers.
  - **Solar Radiation** shows a right-skewed distribution due to natural variations between day and night cycles.

## 4.2 Correlation Matrix Analysis

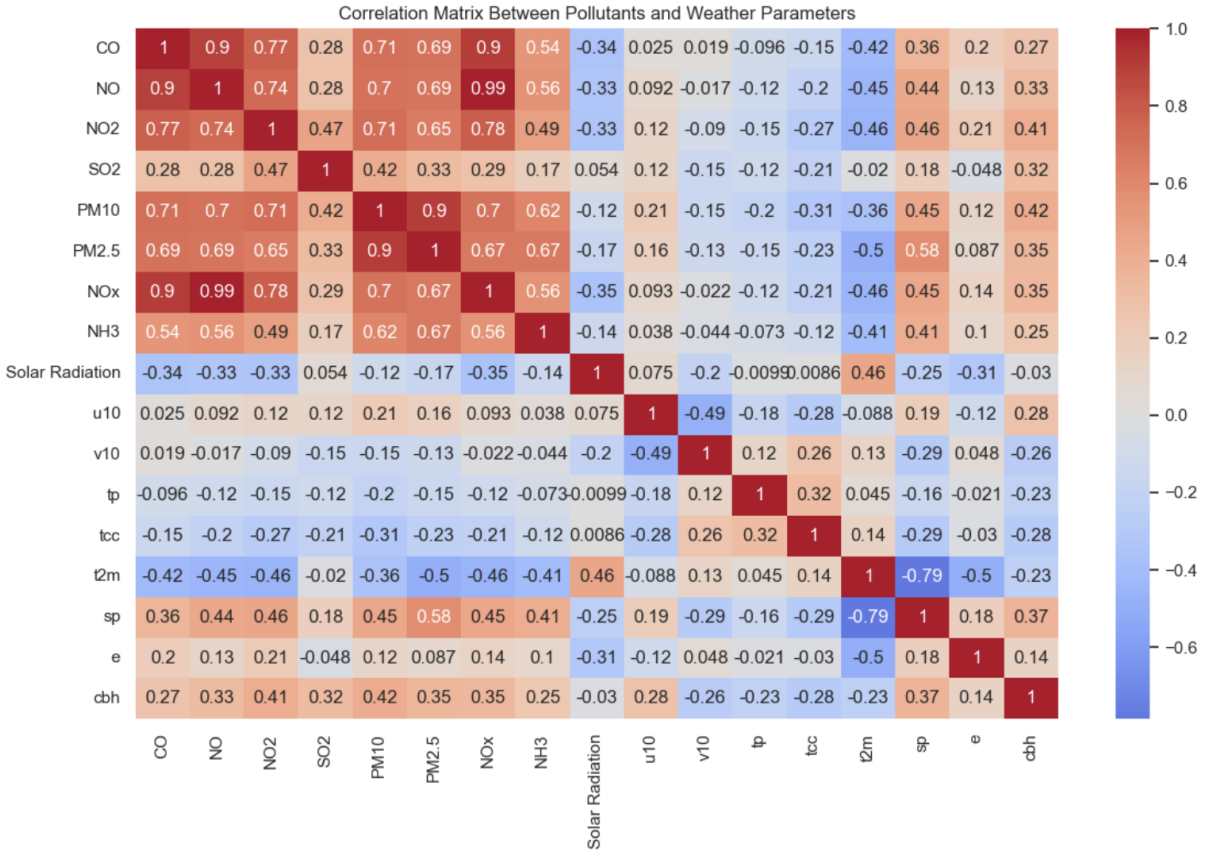



Figure 7: Correlation Matrix Between Pollutants and Weather Parameters

The correlation matrix in Figure 7 highlights the relationships between pollutants and meteorological factors:

#### 4.2.1 Strong Positive Correlations

- **NO and $NO_x$** (r = 0.99): An almost perfect correlation indicating they share common emission sources, primarily vehicular traffic.
- **CO and NO** (r = 0.90): Suggests that these pollutants often originate from similar combustion processes.
- **$PM_{10}$ and $PM_{2.5}$** (r = 0.90): Reflects the similar behavior and sources of particulate matter.

#### 4.2.2 Notable Negative Correlations

- **Temperature** with Pollutants (r = -0.42 to -0.50): Indicates higher pollutant concentrations during colder periods, possibly due to temperature inversions trapping pollutants near the ground.
- **Solar Radiation** with $NO_x$ (r = -0.35): Suggests that increased sunlight may enhance photochemical reactions that reduce $NO_x$ levels.

#### 4.2.3 Weather Parameter Influences

- **Wind Components** (u10, v10): Generally weak correlations with pollutants, indicating limited direct influence on pollution levels.
- **Surface Pressure** (sp): Shows a moderate positive correlation with $NO_2$ (r = 0.46), suggesting that higher pressure conditions may be associated with pollutant accumulation.

### 4.3 Environmental Implications

- The strong correlations between NO, $NO_2$, and $NO_x$ emphasize the impact of traffic emissions on air quality.
- Negative correlations with temperature and solar radiation highlight the influence of meteorological conditions on pollutant dispersion and chemical reactions.
- The distribution patterns of $PM_{10}$ and $PM_{2.5}$ suggest frequent occurrences of high particulate matter levels, raising health concerns.

# Model Wise Analysis:

# XGBoost

# 1 Introduction

The following sections detail our attempts at using a XGBoost regression model for the purpose of AQI prediction. Our dataset consists of 10 stations that track CO, NO, NO2, NOX, Ozone, PM10, PM2.5, and Solar Radiation.
In addition to this, we are also tracking Cloud Base Height, Evaporation, Surface Pressure, 2M Temperature, Total Cloud Cover, Total Precipitation, u10m, and v10m components of wind speed. The model was trained on this dataset for 100 iterations, with a depth of 8, and learning rate of 0.05, . This took around 30 minutes on an Nvidia RTX 3060.
The columns are split into features and targets based on the pollutants.
The `Timestamp` column is removed from the features.

# 2 Feature Engineering

Additional features are created to capture temporal dependencies and trends.

## 2.1 Lagged Features

Lagged features are created to include previous observations, by taking the values of a specific column from 1 day, 7 days, 30 days, and 1 year ago.

## 2.2 Rolling Window Features

Rolling mean and standard deviation are calculated over different window sizes to capture local trends:

```
window_sizes = [7, 14, 30]
for target in targets:
    for window in window_sizes:
        data[f'{target}_rolling_mean_{window}'] = data[target].rolling(window).mean()
        data[f'{target}_rolling_std_{window}'] = data[target].rolling(window).std()
```

## 2.3 Time-based Features

Day of the week and month features are extracted to account for seasonal patterns:

```
data['day_of_week'] = data['Timestamp'].apply(lambda x: pd.to_datetime(x).dayofweek)
data['month'] = data['Timestamp'].apply(lambda x: pd.to_datetime(x).month)
```

## 2.4 Combining Features and Targets

All features are combined into `X`, and targets into `y`:

```
X = data[features + [f'{target}_t-1' for target in targets] + ... ]
y = data[targets]
```

# 3 Data Imputation

Missing values are imputed using the median strategy:

```
from sklearn.impute import SimpleImputer

imputer = SimpleImputer(strategy='median')
X_imputed = imputer.fit_transform(X)
y_imputed = imputer.fit_transform(y)
```

# 4 Outlier Detection

An Isolation Forest is used to detect and remove outliers:

```
from sklearn.ensemble import IsolationForest

outlier_detector = IsolationForest(contamination=0.05, random_state=42)
outliers = outlier_detector.fit_predict(X_imputed)
X_imputed = X_imputed[outliers == 1]
y_imputed = y_imputed[outliers == 1]
```

# 5 Feature Scaling

Features are standardized using `StandardScaler`:

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_imputed)
```

# 6 Data Splitting

A time-based split is performed to respect the temporal order of data:

```
train_size = int(len(X_scaled) * 0.8)
X_train_full = X_scaled[:train_size]
X_test = X_scaled[train_size:]
y_train_full = y_imputed[:train_size]
y_test = y_imputed[train_size:]

val_size = int(len(X_train_full) * 0.2)
X_train = X_train_full[:-val_size]
X_val = X_train_full[-val_size:]
y_train = y_train_full[:-val_size]
y_val = y_train_full[-val_size:]
```

# 7 Evaluation Metrics

Mean Absolute Percentage Error (MAPE) and R-squared ($R^2$) score are used:

# 8 Feature Selection

Features are selected based on the model's importance scores:

```
from sklearn.feature_selection import SelectFromModel

selector = SelectFromModel(model, threshold="mean", max_features=30)
X_train_selected = selector.fit_transform(X_train, y_train)
X_val_selected = selector.transform(X_val)
X_test_selected = selector.transform(X_test)
```

# 9 Retraining with Selected Features

The model is retrained using the selected features:

```
model.fit(
    X_train_selected, y_train,
    eval_set=[(X_val_selected, y_val)],
    verbose=True,
)
```

# 10 Final Evaluation

The model is evaluated on the test set:

```
y_test_pred = model.predict(X_test_selected)

for i, target in enumerate(targets):
    mape = mean_absolute_percentage_error(y_test[:, i], y_test_pred[:, i])
    r2 = r2_score(y_test[:, i], y_test_pred[:, i])
```

# 11 AQI Calculation

Air Quality Index is calculated using CPCB standards:
The AQI is computed for actual and predicted values, followed by the Mean Squared Error (MSE)

# 12 Results

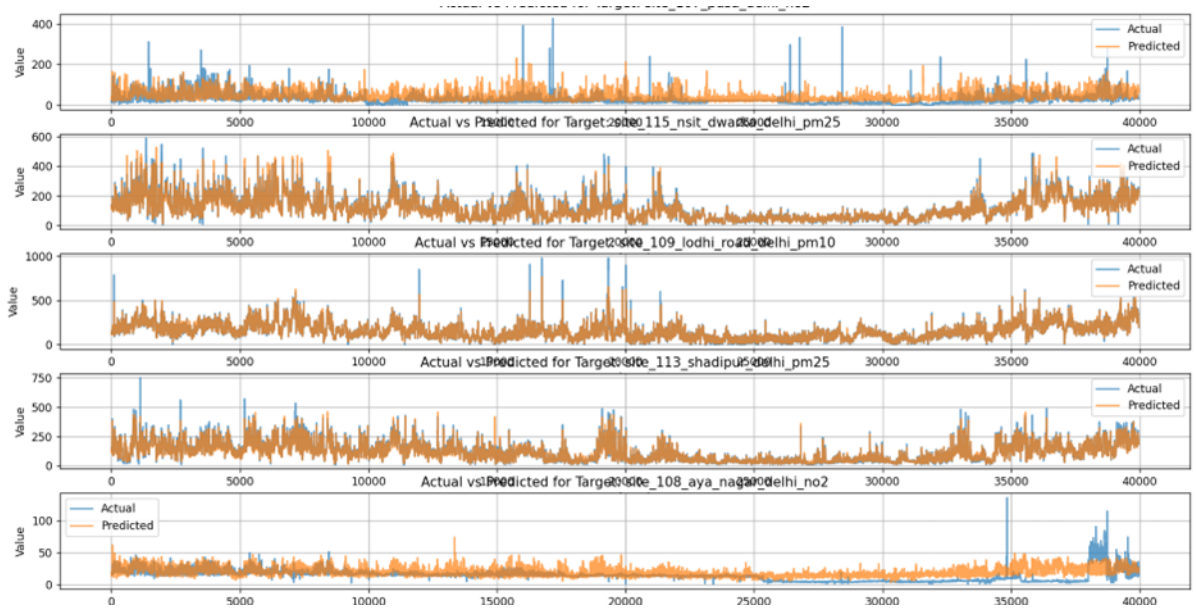



Figure 8: Actual Vs Predicted Features

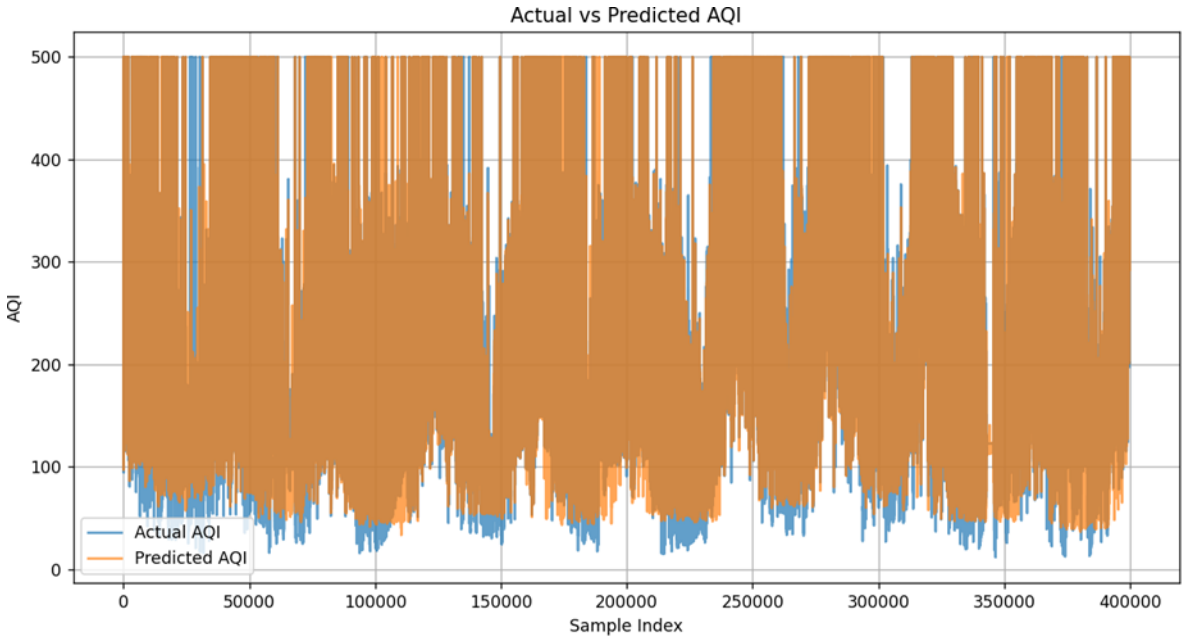



Figure 9: Actual Vs Predicted AQI

MSE for AQI prediction: 1169.9296

| Location | Pollutant | MAPE (%) | $R^2$ Score |
|---|---|---|---|
| CRRI Mathura Road | CO | 9.62e+09 | -0.3195 |
| | NO | 993.03 | -1.1645 |
| | O | 119.14 | 0.0052 |
| | PM | 19.00 | 0.9560 |
| | PM. | 24.30 | 0.9349 |
| Burari Crossing | CO | 1.05e+11 | -0.1857 |
| | NO | 190.08 | -0.2535 |
| | O | 202.46 | -0.2245 |
| | PM | 28.46 | 0.7847 |
| | PM. | 56.27 | 0.9184 |
| North Campus DU | CO | 3.71e+10 | -0.1780 |
| | NO | 254.44 | -0.6648 |
| | O | 209.78 | -0.1198 |
| | PM | 15.19 | 0.9597 |
| | PM. | 21.60 | 0.9697 |
| IGI Airport (T3) | CO | 7.66e+09 | -0.0647 |
| | NO | 313.36 | -5.2892 |
| | O | 214.87 | -0.0099 |
| | PM | 9.97 | 0.9648 |
| | PM. | 20.36 | 0.9720 |
| PUSA | CO | 8.12e+09 | -0.0276 |
| | NO | 137.58 | -0.0414 |
| | O | 221.73 | -0.3936 |
| | PM | 13.46 | 0.9520 |
| | PM. | 32.24 | 0.9306 |
| Aya Nagar | CO | 3.36e+09 | 0.0495 |
| | NO | 96.12 | -0.3306 |
| | O | 135.72 | 0.0067 |
| | PM | 13.56 | 0.9635 |
| | PM. | 33.45 | 0.9339 |
| Lodhi Road | CO | 9.61e+09 | 0.1840 |
| | NO | 88.83 | -0.0922 |
| | O | 70.98 | 0.0885 |
| | PM | 15.97 | 0.9677 |
| | PM. | 34.98 | 0.9724 |

Table 1: Performance metrics for air quality prediction models at key Delhi monitoring stations

# 13 Conclusion

The XGBoost regression model effectively predicts the air quality indices by leveraging extensive feature engineering and proper data preprocessing techniques. Feature selection further enhances the model's performance by reducing overfitting and improving generalization.

# Transformer

# 1 Introduction

The following sections detail our attempts at using a Transformer model for the purpose of AQI prediction. Our dataset consists of 10 stations that track CO, NO, NO2, NOX, Ozone, PM10, PM2.5, and Solar Radiation.
In addition to this, we are also tracking Cloud Base Height, Evaporation, Surface Pressure, 2M Temperature, Total Cloud Cover, Total Precipitation, u10m, and v10m components of wind speed. The model was trained on this dataset with a batch size of 32, for 50 epochs. This took around 4 hours on an Nvidia RTX 3060.

# 2 Data Preprocessing Strategy

Effective data preprocessing is critical for developing a robust air quality prediction model. Our strategy incorporates feature engineering, imputation, normalization, and careful train-test splitting. Below, we detail each step and provide mathematical justification for the choices made while contrasting alternative methods.

## 2.1 Feature Engineering

The preprocessing pipeline constructs features and targets that capture temporal dependencies and integrate relevant data modalities:

- **Lagged Features:** Given a lookback period of 96 time intervals (approximately 1 day for data of 15-minute resolution), lagged pollutant measurements are incorporated to provide historical context for the prediction task. Formally, for a pollutant $P_t$, we construct lagged feature $P_{t-96}$. This approach models the time-series dependency:

  $$\text{Features at time } t = \{P_{t-i}\}.$$

  This method outperforms alternative techniques like rolling averages, which may smooth out critical fluctuations essential for understanding temporal trends.

- **Multiple Pollutant Tracking:** Pollutants such as $PM_{2.5}$, $PM_{10}$, CO, NO, $NO_2$, NOx, Ozone, and $SO_2$ are treated as interrelated. By including all these pollutants as features, we leverage cross-pollutant correlations:

  $$\mathbf{X}_t = [P_t^{(1)}, P_t^{(2)}, \ldots, P_t^{(n)}],$$

  where $P_t^{(i)}$ represents pollutant $i$ at time $t$. Alternative approaches, such as predicting pollutants independently, fail to exploit these interdependencies, leading to reduced prediction accuracy.

- **Weather Integration:** Weather parameters (e.g., temperature, humidity, wind speed) are crucial for predicting pollutant dispersion and reaction rates. Thus, we append weather variables $W_t$ to the feature set:

  $$\text{Feature vector at time } t = [P_t, W_t].$$

  Ignoring weather data, as in simplistic univariate time-series models, results in poor generalization, especially under changing meteorological conditions.

## 2.2 Data Transformation Techniques

1. **Imputation:** Missing data in pollutant and weather measurements are common. We use mean imputation:

   $$\hat{x}_i = \frac{1}{N}\sum_{j=1}^{N} x_j, \quad \text{if } x_i \text{ is missing.}$$

   Alternatives such as median or mode imputation fail to consider the distribution symmetry present in our dataset, and advanced methods like k-nearest neighbors (KNN) are computationally expensive for the size of dataset we are working with.

2. **Normalization:** StandardScaler is applied to transform features and targets to zero mean and unit variance:

   $$\hat{x} = \frac{x - \mu}{\sigma}.$$

   This standardization ensures numerical stability in model training, particularly for the transformer architecture, which can be sensitive to unscaled inputs. Alternatives like Min-Max scaling can compress data, losing the contribution of outliers, which are often critical in air quality data.

3. **Train-Test Split:** An 80%-20% train-test split ensures a sufficient training set for learning patterns while preserving a large enough test set for evaluation. A more imbalanced split (e.g., 90%-10%) risks overfitting, while stratified sampling is unnecessary here as pollutant data is not categorical.

### 2.3 Comparative Analysis

Our methodology is optimized for air quality prediction tasks, balancing computational efficiency and predictive power. By incorporating historical pollutant data, weather conditions, and robust preprocessing techniques, the model is well-positioned to outperform simpler models such as univariate ARIMA or naive baselines that ignore weather data and cross-pollutant relationships.

## 3 Transformer Model Architecture

### 3.1 Model Components

The Transformer model consists of three primary layers:

- **Embedding Layer:** Linear transformation reducing input dimension to 32
- **Transformer Encoder:** Self-attention mechanism with configurable:
  - Number of heads (default: 4)
  - Number of layers (default: 2)
  - Dropout rate (default: 0.2)
- **Output Layer:** Linear layer mapping to pollutant prediction dimensions

### 3.2 Why Transformer?

Advantages over traditional models:

- Captures complex non-linear relationships
- Handles multiple input features simultaneously
- Inherent attention mechanism learns intricate temporal dependencies

## 4 Training Strategy

### 4.1 Loss and Optimization

- **Loss Function:** Mean Absolute Error (MAE)
- **Optimizer:** Adam with weight decay
- **Learning Rate Schedule:** Step learning rate reduction

# 5 Evaluation Metrics

Multiple metrics provide comprehensive model assessment:

- Mean Absolute Percentage Error (MAPE)
- Symmetric Mean Absolute Percentage Error (SMAPE)
- Comprehensive AQI Calculation
- Confusion Matrix for AQI Categories

# 6 Results

| **Site** | **MSE** | **MAPE (%)** | **SMAPE (%)** |
|---|---|---|---|
| site_103_crri_mathura_road_delhi_co | 3.1706 | 27212412.00 | 68.28 |
| site_103_crri_mathura_road_delhi_no | 5520.9951 | 484.99 | 70.01 |
| site_103_crri_mathura_road_delhi_no2 | 734.6662 | 452.25 | 51.30 |
| site_103_crri_mathura_road_delhi_nox | 5129.6509 | 174867792.00 | 57.44 |
| site_103_crri_mathura_road_delhi_ozone | 524.4279 | 69.61 | 45.55 |
| site_103_crri_mathura_road_delhi_pm10 | 14340.3438 | 117.41 | 44.01 |
| site_103_crri_mathura_road_delhi_pm25 | 4091.4817 | 84.93 | 44.79 |
| site_104_burari_crossing_delhi_co | 0.8770 | 67661792.00 | 44.19 |
| site_104_burari_crossing_delhi_no | 2156.2156 | 60.71 | 44.89 |
| site_104_burari_crossing_delhi_no2 | 730.9974 | 147.60 | 64.90 |
| site_104_burari_crossing_delhi_nox | 2138.7451 | 110942304.00 | 39.09 |
| site_104_burari_crossing_delhi_ozone | 775.6478 | 156.66 | 65.76 |
| site_104_burari_crossing_delhi_pm10 | 17056.8926 | 93.39 | 43.35 |
| site_104_burari_crossing_delhi_pm25 | 5646.0664 | 116.27 | 52.24 |
| site_105_north_campus_du_delhi_co | 4.7776 | 620704704.00 | 73.41 |
| site_105_north_campus_du_delhi_no | 4952.4858 | 288.57 | 96.08 |
| site_105_north_campus_du_delhi_no2 | 305.5740 | 131.49 | 43.07 |
| site_105_north_campus_du_delhi_nox | 5008.7295 | 37507180.00 | 60.33 |
| site_105_north_campus_du_delhi_ozone | 221.2104 | 104.49 | 41.18 |
| site_105_north_campus_du_delhi_pm10 | 10989.6709 | 88.25 | 39.07 |
| site_105_north_campus_du_delhi_pm25 | 6469.1362 | 96.30 | 48.02 |
| site_106_igi_airport_(t3)_delhi_co | 1.9693 | 11630871.00 | 46.17 |
| site_106_igi_airport_(t3)_delhi_no | 8169.2842 | 74.39 | 79.54 |
| site_106_igi_airport_(t3)_delhi_no2 | 168.4816 | 92.61 | 35.42 |
| site_106_igi_airport_(t3)_delhi_nox | 7520.1978 | 4905972.50 | 51.87 |
| site_106_igi_airport_(t3)_delhi_ozone | 150.3093 | 74.31 | 46.70 |
| site_106_igi_airport_(t3)_delhi_pm10 | 14275.5889 | 54.60 | 40.58 |
| site_106_igi_airport_(t3)_delhi_pm25 | 5256.0942 | 88.59 | 48.71 |
| site_107_pusa_delhi_co | 2.3300 | 72739560.00 | 38.41 |
| site_107_pusa_delhi_no | 818.3304 | 78.07 | 62.57 |
| site_107_pusa_delhi_no2 | 461.5032 | 49.56 | 40.94 |
| site_107_pusa_delhi_nox | 1893.2133 | 1684597.88 | 40.78 |
| site_107_pusa_delhi_ozone | 123.3067 | 76.26 | 34.13 |

| Site | MSE | MAPE (%) | SMAPE (%) |
|---|---|---|---|
| site_107_pusa_delhi_pm10 | 9742.3115 | 64.79 | 44.39 |
| site_107_pusa_delhi_pm25 | 4608.8643 | 111.18 | 56.59 |
| site_108_aya_nagar_delhi_co | 1.1014 | 144262736.00 | 33.18 |
| site_108_aya_nagar_delhi_no | 367.7643 | 74.53 | 63.66 |
| site_108_aya_nagar_delhi_no2 | 31.7549 | 33.07 | 25.96 |
| site_108_aya_nagar_delhi_nox | 349.9889 | 3759977.25 | 25.22 |
| site_108_aya_nagar_delhi_ozone | 331.3746 | 91.24 | 32.92 |
| site_108_aya_nagar_delhi_pm10 | 12953.5254 | 66.12 | 43.07 |
| site_108_aya_nagar_delhi_pm25 | 4191.9048 | 109.66 | 52.81 |
| site_109_lodhi_road_delhi_co | 0.7940 | 10424999.00 | 37.89 |
| site_109_lodhi_road_delhi_no | 1843.8599 | 119.16 | 69.52 |
| site_109_lodhi_road_delhi_no2 | 172.0291 | 59.98 | 35.98 |
| site_109_lodhi_road_delhi_nox | 1736.7333 | 93551216.00 | 47.37 |

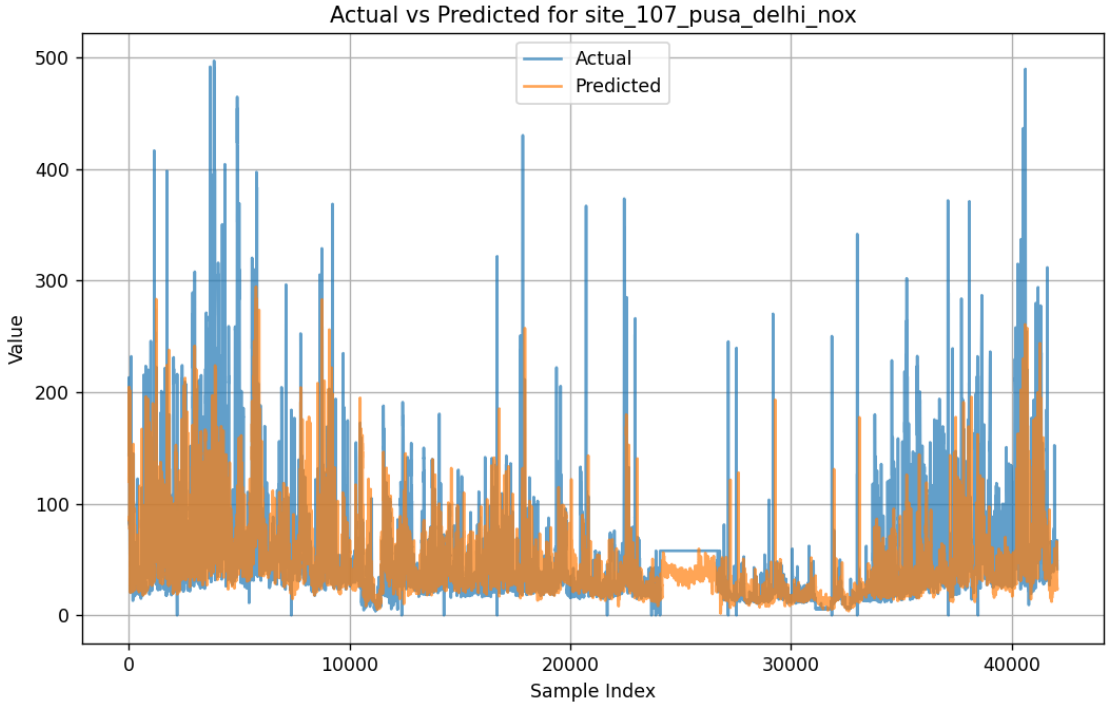



Figure 10: Feature Data Comparison 1

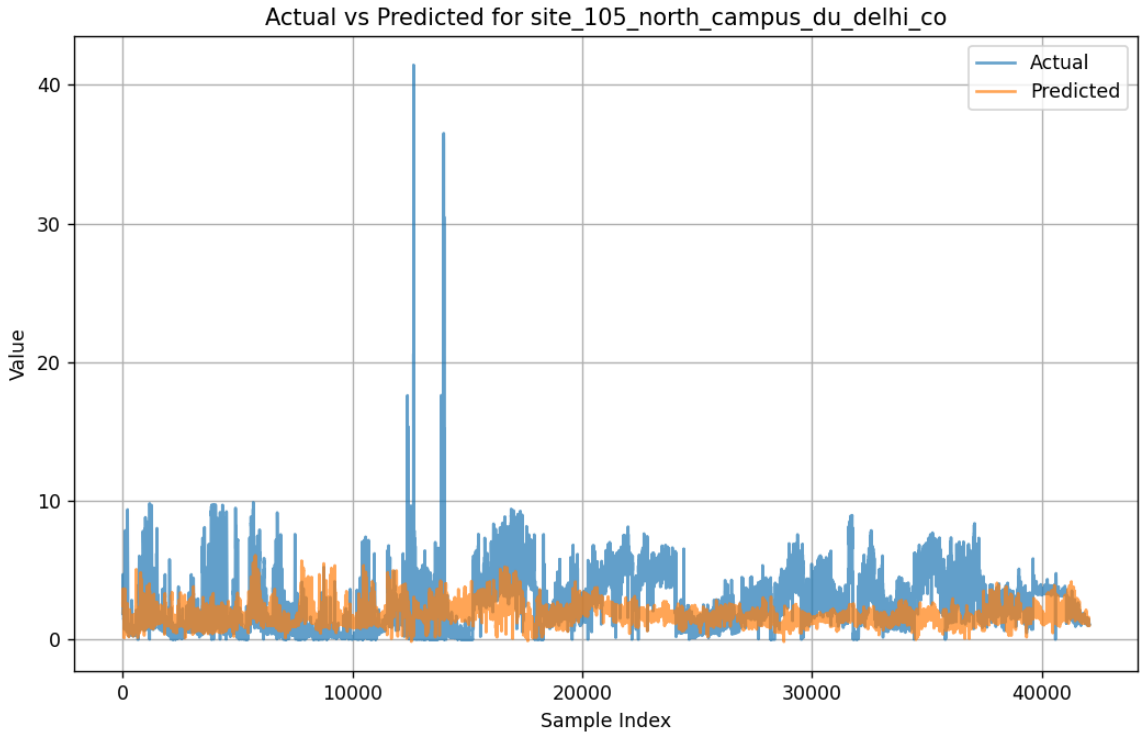



Figure 11: Feature Data Comparison 2

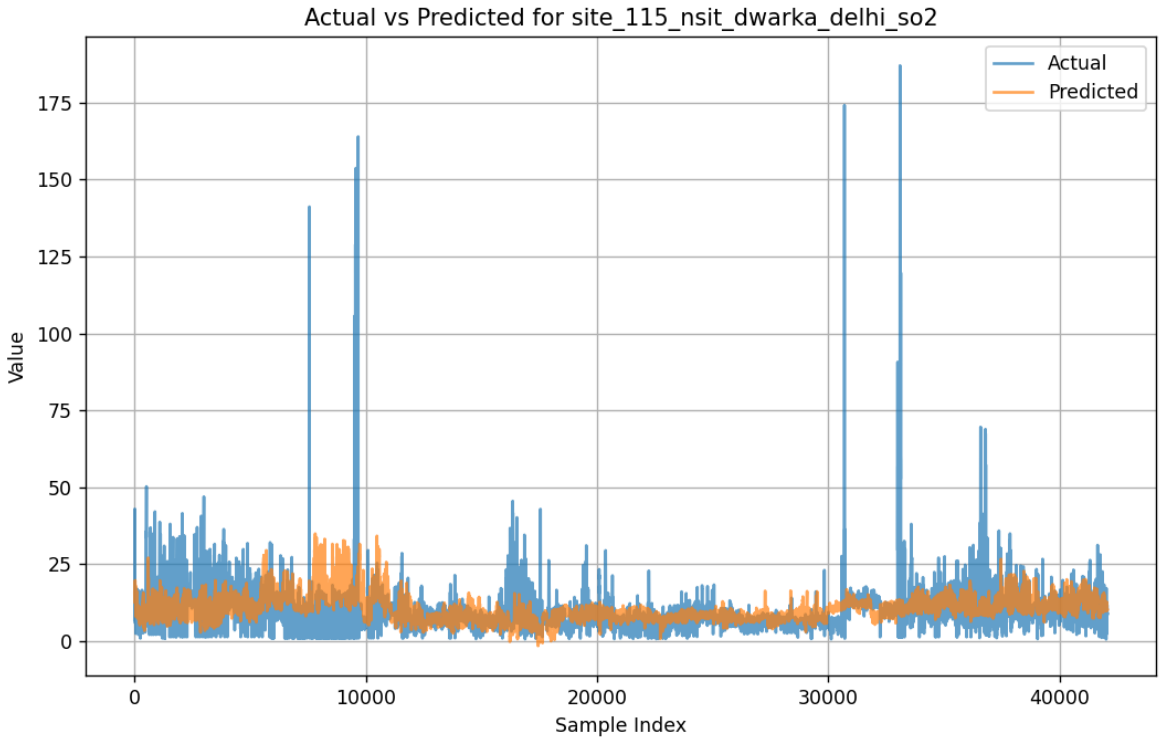



Figure 12: Feature Data Comparison 3

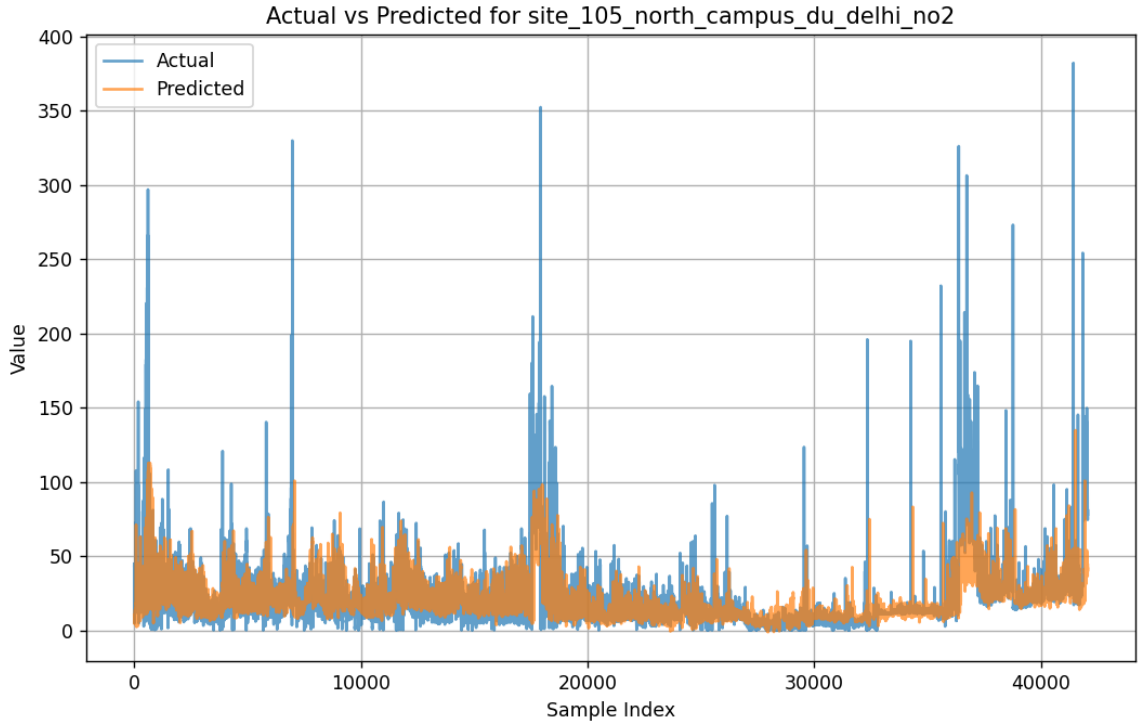



Figure 13: Feature Data Comparison 4

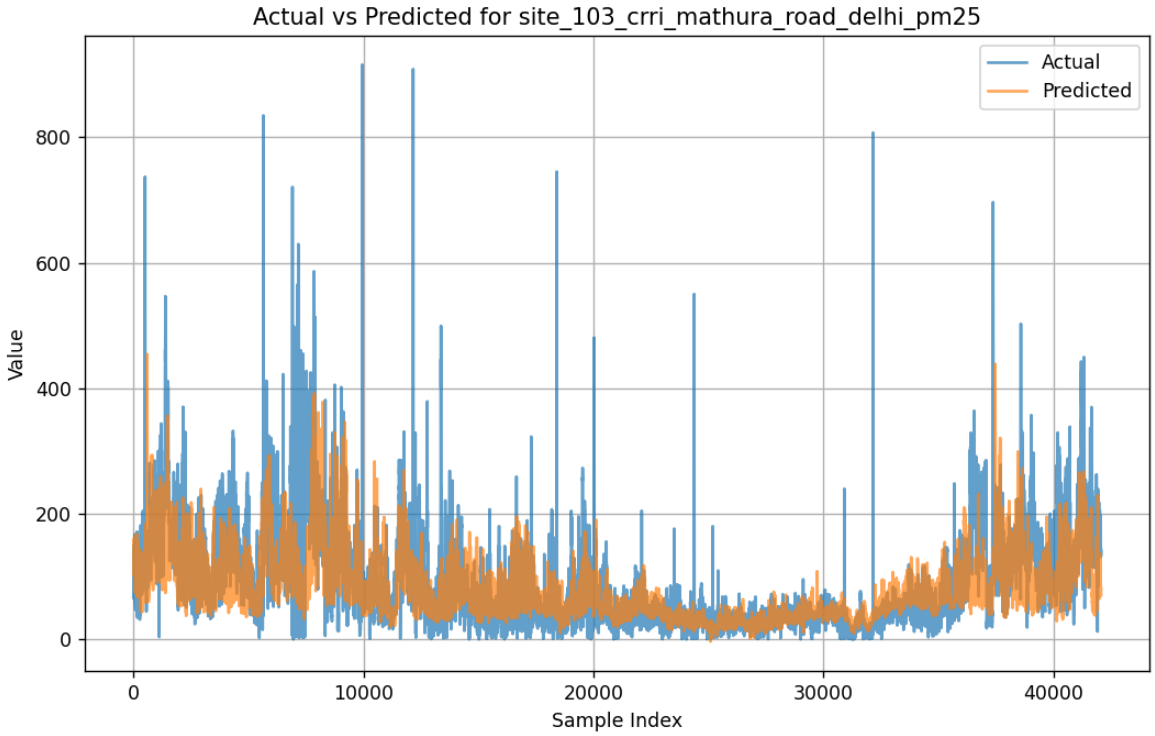



Figure 14: Feature Data Comparison 5

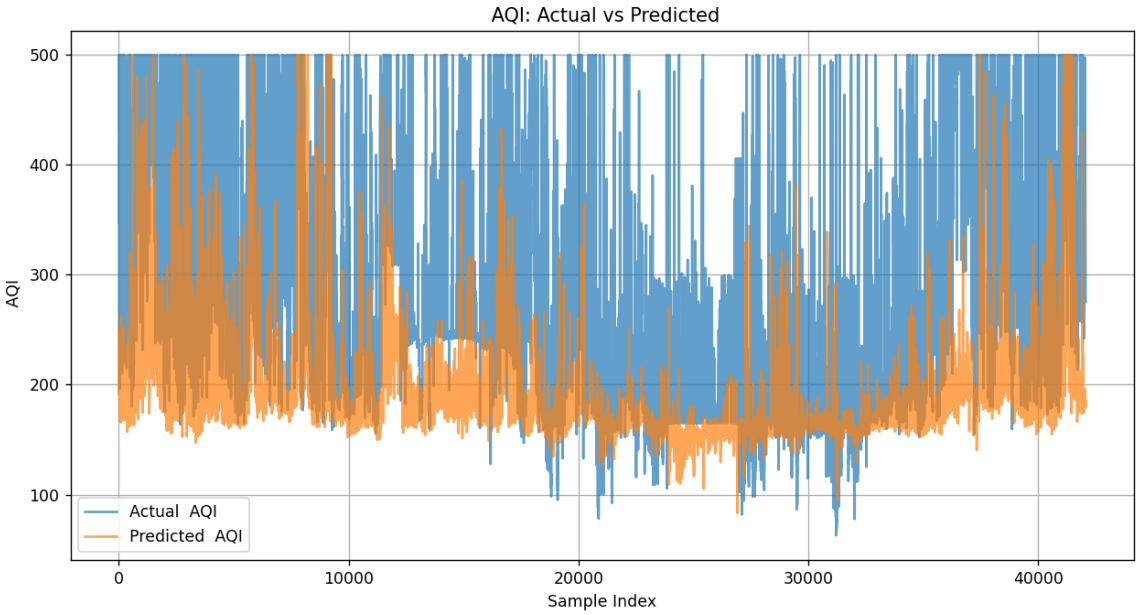



Figure 15: Calculated AQI Actual vs Predicted Values

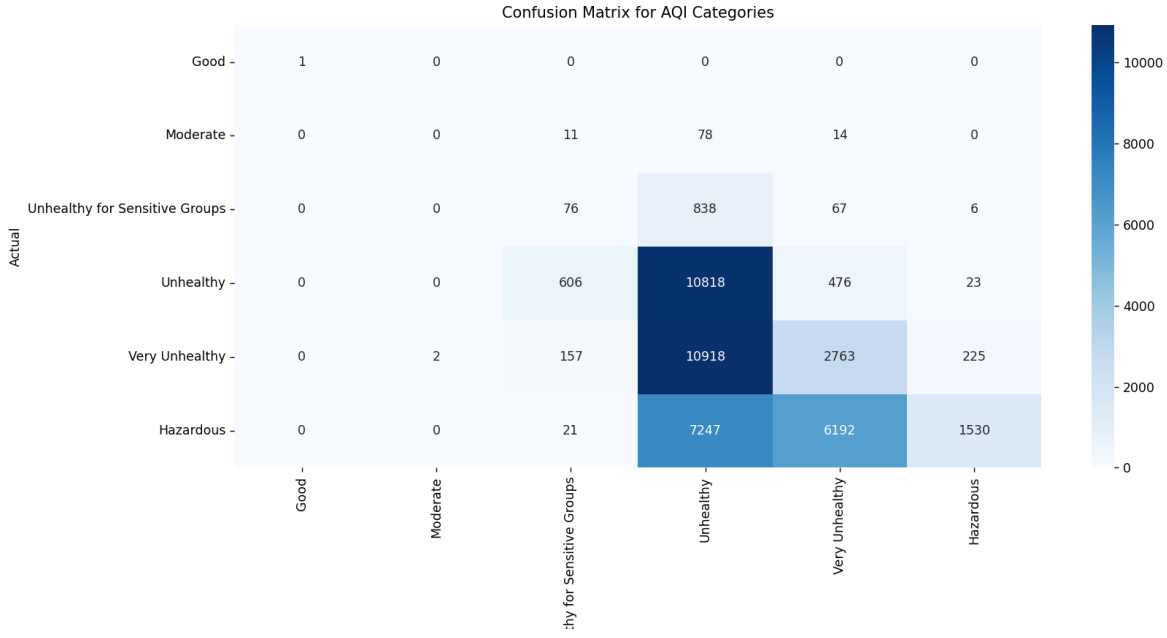



Figure 16: Confusion Matrix

# 7 Conclusion

This Transformer-based approach represents a sophisticated method for multivariate air quality prediction, demonstrating the power of deep learning in environmental monitoring.

| Class | Precision | Recall | F1-Score | Support |
|---|---|---|---|---|
| Good | 1.00 | 1.00 | 1.00 | 1 |
| Moderate | 0.86 | 0.10 | 0.18 | 14,990 |
| Unhealthy for Sensitive Groups | 0.00 | 0.00 | 0.00 | 103 |
| Unhealthy | 0.36 | 0.91 | 0.52 | 11,923 |
| Very Unhealthy | 0.09 | 0.08 | 0.08 | 987 |
| Hazardous | 0.29 | 0.20 | 0.23 | 14,065 |
| **Accuracy** | 0.36 (on 42,069 instances) | | | |
| **Macro Avg** | 0.43 | 0.38 | 0.34 | 42,069 |
| **Weighted Avg** | 0.51 | 0.36 | 0.29 | 42,069 |

Table 3: Classification Report

| Station | Pollutant | MSE | MAPE | RMSE |
|---|---|---|---|---|
| site_1431 | co | 476.2848511 | 0.818838239 | 21.82395172 |
| site_1431 | nh3 | 468.022644 | 1.322046399 | 21.63383102 |
| site_1431 | no | 533.4741211 | 0.300118834 | 23.09705925 |
| site_1431 | no2 | 387.1081848 | 0.347151875 | 19.67506599 |
| site_1431 | nox | 188.6734467 | 1.895005822 | 13.73584557 |
| site_1431 | ozone | 1946.36731 | 0.219041005 | 44.11765289 |
| site_1431 | pm10 | 797.6629028 | 0.819417179 | 28.24292755 |
| site_1431 | pm25 | 27.60520935 | 1.101059794 | 5.25406599 |
| site_1431 | so2 | 11659.03906 | 3.528970242 | 107.9770279 |
| site_1431 | avg | 1831.58197 | 1.150183265 | 42.79698553 |
| site_105 | co | 3.786857367 | 7.49151E+13 | 1.94598496 |
| site_105 | no | 513.8780518 | 1.333410144 | 22.66887856 |
| site_105 | no2 | 197.2561188 | 1.970907211 | 14.04478931 |
| site_105 | nox | 505.6847229 | 2.303E+15 | 22.48743439 |
| site_105 | ozone | 66.20107269 | 0.664623857 | 8.136404037 |
| site_105 | pm10 | 1093.631348 | 0.26621747 | 33.07009888 |
| site_105 | pm25 | 857.1174316 | 0.360151201 | 29.27656746 |
| site_105 | avg | 462.5079433 | 3.39702E+14 | 21.50599784 |

Table 4: Pollutant Data Analysis

# Alternate Transformer

## 1 Introduction

We have included this primarily as a way to showcase the difference hyperparameter tuning can make.

**Differences from previous approach:** This one primarily focuses on data preprocessing, utilizing forward and backward filling for imputation and applying a MinMaxScaler for feature scaling while excluding timestamp columns from processing. In contrast, the old one presents a comprehensive machine learning pipeline that includes mean imputation, standard scaling, feature engineering with lagged variables, model training, evaluation, and detailed AQI calculations.

Most importantly, however this new model is much more complex. The model has an 8 times larger dimension, twice the number of heads, 8 times the encoder layers, and 4 times the number of feedforward layers. This model was already trained for a much longer time, on the entire dataset, and on a more powerful GPU.
The data processing stays largely the same.

# 2 Training Results

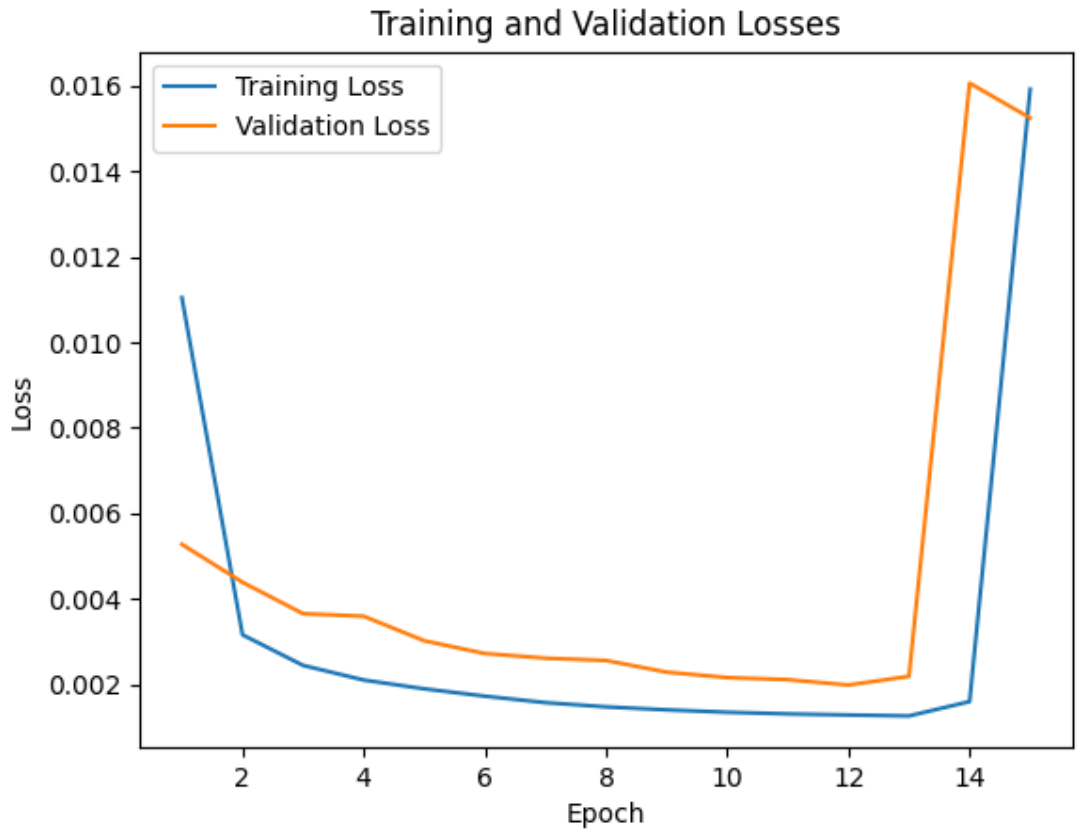



Figure 17: Training vs Validation Loss. We are using epoch 12 for all further evaluation

# 3 Evaluation Results

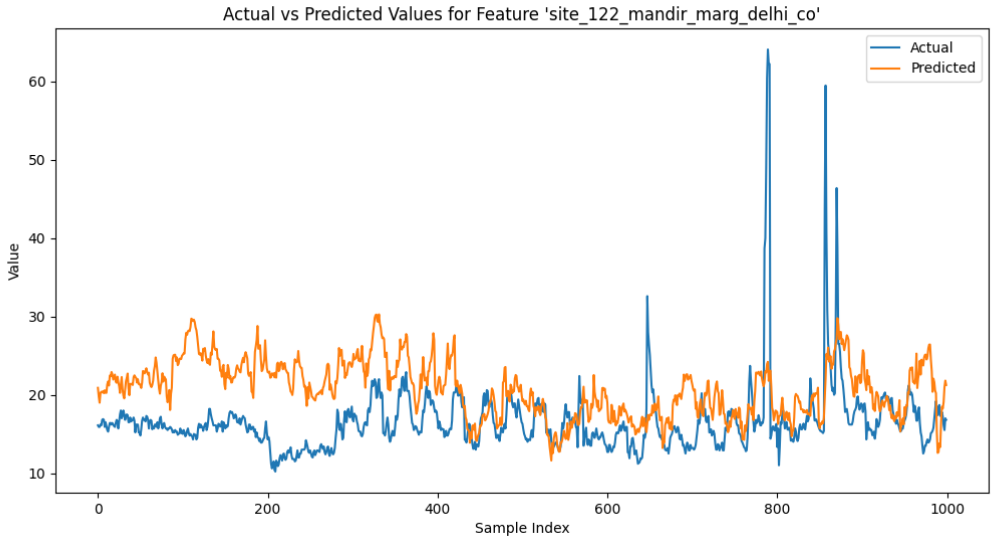



Figure 18: 1

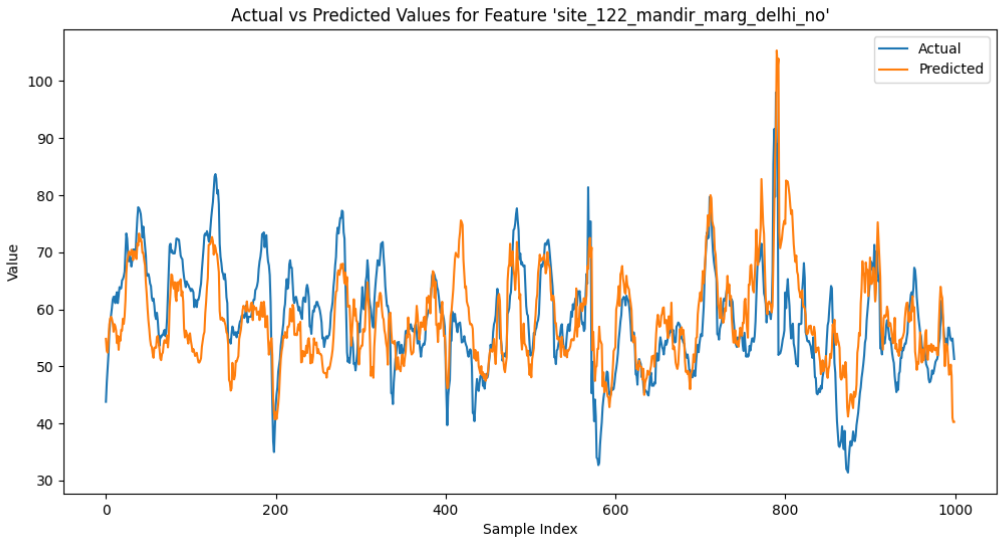



Figure 19: 2

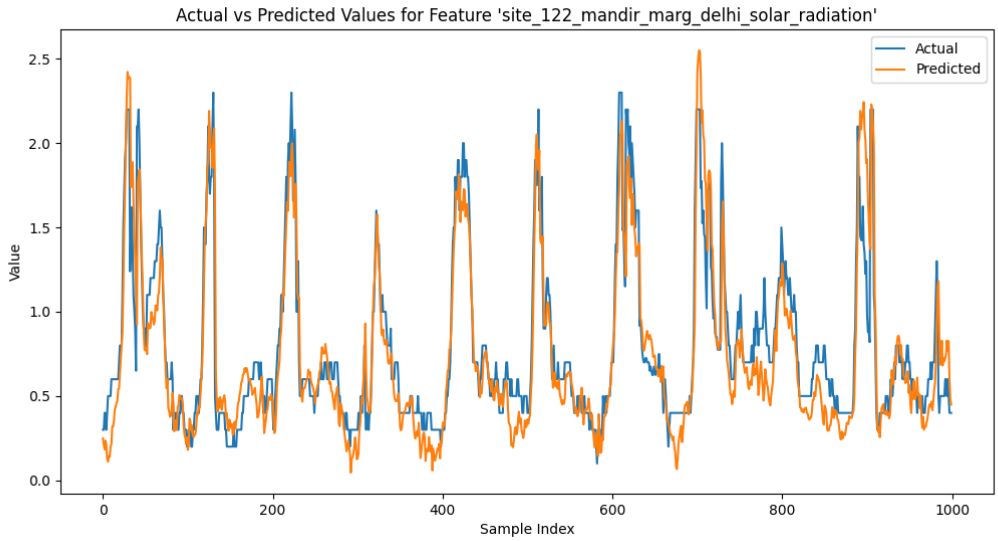



Figure 20: 3

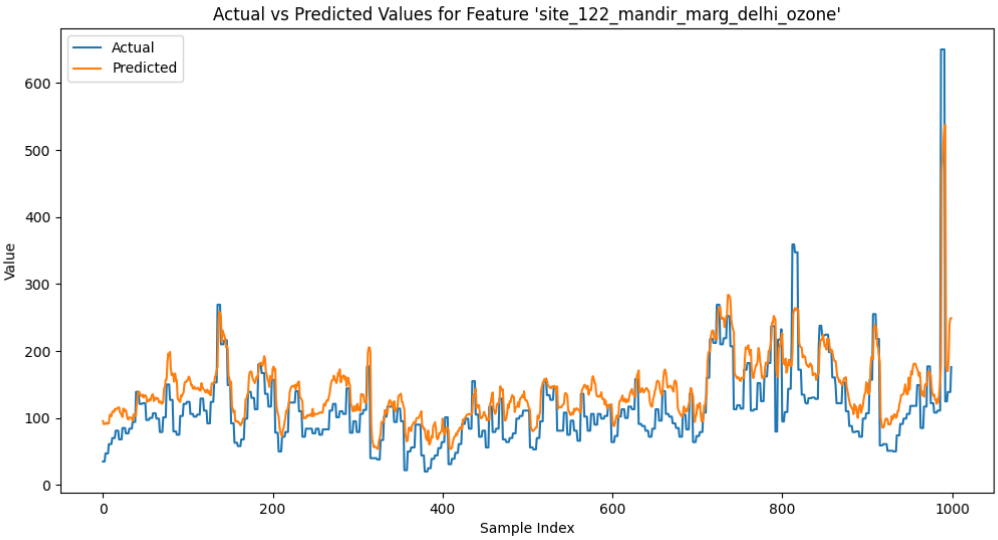



Figure 21: 4

# LSTM

We are testing the ability of LSTM's to excel at capturing long-term dependencies in sequential data. Unlike traditional models, LSTMs can retain and learn patterns over extended periods, making them ideal for time series data where past observations significantly influence future outcomes. Again, we have trained this on the full dataset, for around 4 hours.

# Model Overview

In this project, we developed a Long Short-Term Memory (LSTM) model using PyTorch to handle sequential data effectively. The model architecture and data preprocessing steps are outlined below.

## Model Architecture

**Parameters**:

- `num_features`: Number of input features per timestep.
- `hidden_size`: Number of features in the LSTM's hidden state.
- `num_layers`: Number of stacked LSTM layers.
- `output_size`: Dimension of the model's output.

**Layers**:

- **LSTM Layer**: Captures temporal dependencies in the input sequence.
- **Fully Connected (FC) Layer**: Transforms the LSTM output to the desired output size.

**Initialization** involves setting up the LSTM and FC layers using PyTorch's `nn.LSTM` and `nn.Linear` modules.

## Data Flow

1. **Input**: Sequence data with shape `(batch_size, seq_length, num_features)`.
2. **LSTM Processing**: The input passes through the LSTM layer, producing hidden states for each timestep.
3. **Sequence Summarization**: The hidden state from the last timestep is extracted to represent the entire sequence.
4. **Output Generation**: The summarized representation is fed into the FC layer to produce the final output with shape `(batch_size, output_size)`.

## Training Strategy

- **Loss Function**: Mean Squared Error (MSE) for regression tasks or Cross-Entropy Loss for classification.
- **Optimizer**: Adam optimizer is utilized for its adaptive learning rate capabilities.
- **Backpropagation Through Time (BPTT)**: This technique is employed to compute gradients across the unrolled network for training.

### Data Preprocessing

- **Scaling**: Features are normalized using `MinMaxScaler` to fit within the range [0, 1].
- **Handling Missing Values**: Columns with all missing values are removed. Remaining missing entries are filled using forward and backward filling methods.
- **Verification**: A sample plot compares original and scaled feature values to ensure proper scaling.
- **Saving Processed Data**: The cleaned and scaled data is saved for subsequent model training.

### Conclusion

The integration of the LSTM model with robust data preprocessing techniques ensures effective training and reliable predictions. This setup is well-suited for tasks involving sequential data, leveraging the strengths of LSTM in capturing temporal patterns.

# 1 Results

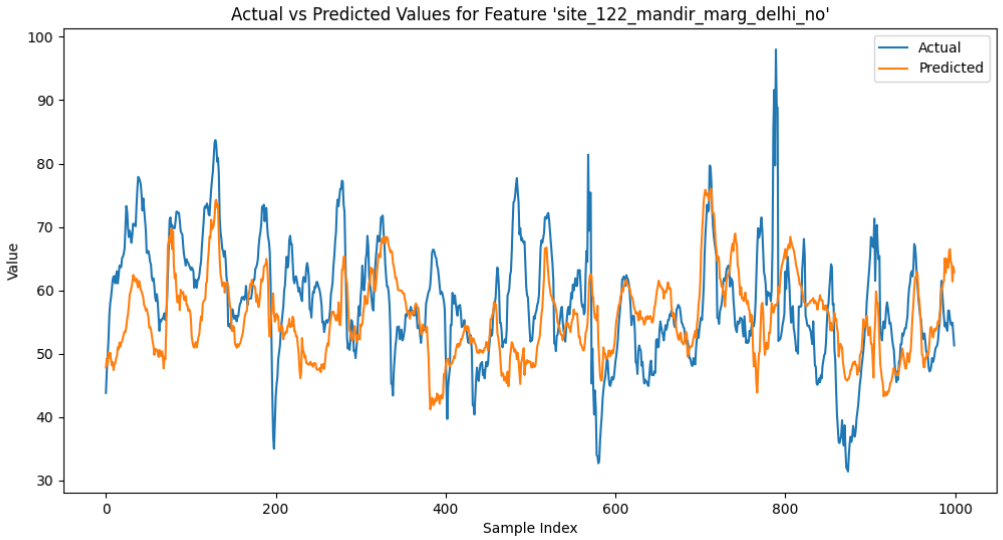



Figure 22: 1

# Limitations

1. Our model only works for data from Delhi. It will not generalize to AQI prediction for all of India.
2. Our data had 40% values `NaN`, which reduced our accuracy.

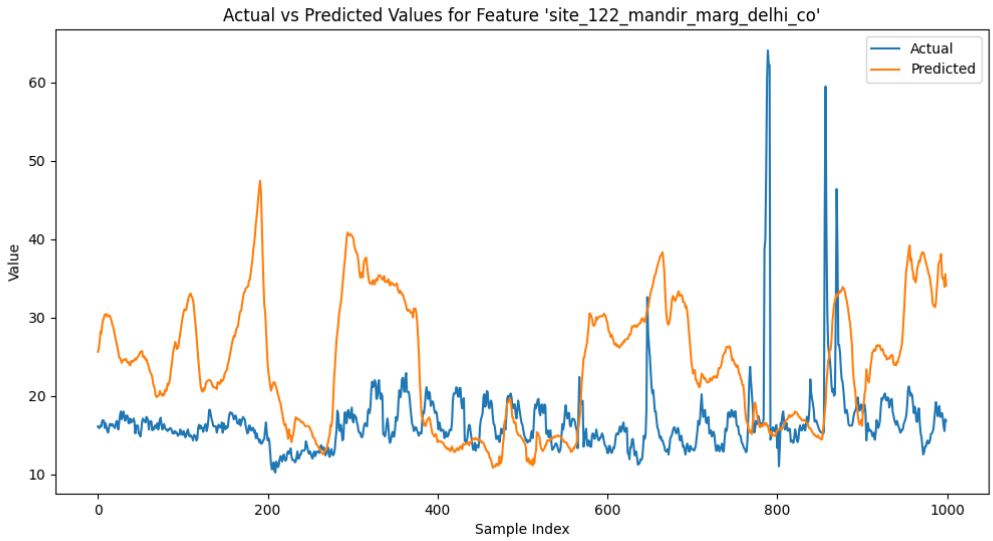



Figure 23: 2

Table 5: Pollutant Statistics for Stations

| Station | Pollutant | MSE | MAPE | RMSE |
|---|---|---|---|---|
| site_1420 | co | 579.196 | 0.4272 | 24.0665 |
| site_1420 | nh3 | 473.704 | 1.1684 | 21.7647 |
| site_1420 | no | 423.844 | 0.8168 | 20.5875 |
| site_1420 | no2 | 542.849 | 0.3168 | 23.2991 |
| site_1420 | nox | 1192.172 | 3.6870 | 34.5278 |
| site_1420 | ozone | 3925.371 | 0.7698 | 62.6528 |
| site_1420 | pm10 | 3338.504 | 0.7276 | 57.7798 |
| site_1420 | pm25 | 240.632 | 3.1522 | 15.5123 |
| site_1420 | so2 | 4229.040 | 1.0416 | 65.0311 |
| site_1420 | avg | 1660.590 | 1.3453 | 40.7503 |
| site_1432 | co | 386.570 | 0.8341 | 19.6614 |
| site_1432 | nh3 | 1449.205 | 2.0503 | 38.0684 |
| site_1432 | no | 707.982 | 2.5677 | 26.6079 |
| site_1432 | no2 | 1020.669 | 0.5903 | 31.9479 |
| site_1432 | nox | 352.389 | 2.4910 | 18.7720 |
| site_1432 | ozone | 4150.792 | 0.2367 | 64.4266 |
| site_1432 | pm10 | 1677.495 | 0.3764 | 40.9572 |
| site_1432 | pm25 | 86.152 | 3.0566 | 9.2818 |
| site_1432 | so2 | 4153.913 | 1.6184 | 64.4509 |
| site_1432 | avg | 1553.908 | 1.5357 | 39.4196 |

3. We would have been able to create a model to better approximate the complex dataset if we had more computational power.

# Next Steps

1. **Incorporate Traffic Data:** Use real-time and historical traffic data to capture vehicular emission patterns, which are a significant contributor to air pollution.

2. **Utilize Satellite Imagery:** Analyze satellite data to track large-scale pollution sources and monitor changes in AQI over time.