UCI Air Quality Analysis in Rome (March 2004 - April 2005)

Final Report

Data 2010: Tools and Techniques for Data Science

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Introduction:

The **UCI Air Quality dataset** provides a comprehensive record of pollution levels in Rome, Italy, capturing hourly measurements of key pollutants—including Carbon Monoxide (CO), Nitrogen Dioxide (NO_2), Total Nitrogen Oxides (NO_x), Benzene (C_6H_6), and Non-Methane Hydrocarbons ($NMHC$)—alongside sensor responses and environmental variables such as temperature and humidity. This dataset offers a unique opportunity to analyze sensor performance, assess air quality trends, and develop predictive models for pollutant concentrations.

This analysis is structured into four key components: **sensor calibration and air quality assessment**, which evaluates the correlation between sensor readings and true pollutant concentrations while detecting cross-sensitivities and analyzing seasonal AQI variations; **regression-based CO prediction**, which aims to develop models for estimating CO levels based on sensor and environmental data; **time series and hybrid modeling**, which explores temporal trends and advanced modeling techniques for pollutant forecasting; and **machine learning comparison**, which assesses different algorithms to determine the most effective approaches for air quality prediction and monitoring.

Preprocessing

Formating

The air quality data was initially cleaned by removing empty rows and columns, and by converting character columns—where commas were used as decimal points—into proper numeric format. The Date column was also converted from string format to a proper date type.

CO.GT.	NMHC.GT.	C6H6.GT.	NOx.GT.	NO2.GT.	T	RH	AH
1683	8443	366	1639	1642	366	366	366

PT08.S1.CO.	PT08.S2.NMHC.	PT08.S3.NOx.	PT08.S4.NO2.	PT08.S5.O3.
366	366	366	366	366

Number of missing data	n
0	827
1	6138
2	467
3	364
4	1195
9	26
10	291
11	6
12	12
13	31

To handle missing data, we first identified gaps using the is.na() and summary() functions. Since -200 was used as a placeholder for missing values, it was temporarily replaced with 0 to allow for five-number summary analysis and help determine which variables were most affected. During this process, we observed that the median value of NMHC_GT is 0, indicating that this variable may contain a large number of zero values, which could impact interpretation and imputation strategies.

```
     CO.GT.          PT08.S1.CO.      NMHC.GT.         C6H6.GT.          PT08.S2.NMHC.       NOx.GT.          PT08.S3.NOx.
 Min.   :-200.00   Min.   :-200   Min.   :-200.0   Min.   :-200.000   Min.   :-200.0   Min.   :-200.0   Min.   :-200
 1st Qu.:   0.60   1st Qu.: 921   1st Qu.:-200.0   1st Qu.:   4.000   1st Qu.: 711.0   1st Qu.:  50.0   1st Qu.: 637
 Median :   1.50   Median :1053   Median :-200.0   Median :   7.900   Median : 895.0   Median : 141.0   Median : 794
 Mean   : -34.21   Mean   :1049   Mean   :-159.1   Mean   :   1.866   Mean   : 894.6   Mean   : 168.6   Mean   : 795
 3rd Qu.:   2.60   3rd Qu.:1221   3rd Qu.:-200.0   3rd Qu.:  13.600   3rd Qu.:1105.0   3rd Qu.: 284.0   3rd Qu.: 960
 Max.   :  11.90   Max.   :2040   Max.   :1189.0   Max.   :  63.700   Max.   :2214.0   Max.   :1479.0   Max.   :2683
    NO2.GT.          PT08.S4.NO2.    PT08.S5.O3.            T                   RH                  AH
 Min.   :-200.00   Min.   :-200   Min.   :-200.0   Min.   :-200.000   Min.   :-200.00   Min.   :-200.0000
 1st Qu.:  53.00   1st Qu.:1185   1st Qu.: 700.0   1st Qu.:  10.900   1st Qu.:  34.10   1st Qu.:   0.6923
 Median :  96.00   Median :1446   Median : 942.0   Median :  17.200   Median :  48.60   Median :   0.9768
 Mean   :  58.15   Mean   :1391   Mean   : 975.1   Mean   :   9.778   Mean   :  39.49   Mean   :  -6.8376
 3rd Qu.: 133.00   3rd Qu.:1662   3rd Qu.:1255.0   3rd Qu.:  24.100   3rd Qu.:  61.90   3rd Qu.:   1.2962
 Max.   : 340.00   Max.   :2775   Max.   :2523.0   Max.   :  44.600   Max.   :  88.70   Max.   :   2.2310
```

After examining the data's summary statistics and missingness patterns, we found that some variables exhibit Missing Not At Random (MNAR) behavior, while others are Missing At Random (MAR). Imputation was then applied based on variable type: for time-series columns such as T, RH, and AH, we used multiple imputation methods including forward fill, backward fill, and interpolation. For correlated sensor variables, we applied KNN imputation, as these features included both continuous and categorical data. The improvements from cleaning and imputing were evident upon reviewing the updated five-number summaries.

```
     CO.GT.         PT08.S1.CO.       C6H6.GT.        PT08.S2.NMHC.       NOx.GT.          PT08.S3.NOx.
 Min.   : 0.10   Min.   : 647   Min.   : 0.000   Min.   : 383.0   Min.   :   2.0   Min.   : 322.0
 1st Qu.: 1.00   1st Qu.: 941   1st Qu.: 4.000   1st Qu.: 741.0   1st Qu.:  96.0   1st Qu.: 642.0
 Median : 1.70   Median :1072   Median : 7.900   Median : 920.0   Median : 169.0   Median : 796.0
 Mean   : 2.06   Mean   :1116   Mean   : 9.689   Mean   : 956.8   Mean   : 235.7   Mean   : 822.8
 3rd Qu.: 2.70   3rd Qu.:1253   3rd Qu.:13.600   3rd Qu.:1136.0   3rd Qu.: 309.0   3rd Qu.: 960.0
 Max.   :11.90   Max.   :2040   Max.   :63.700   Max.   :2214.0   Max.   :1479.0   Max.   :2683.0
    NO2.GT.        PT08.S4.NO2.    PT08.S5.O3.          T                RH                AH
 Min.   :  2.0   Min.   : 551   Min.   : 221   Min.   :-1.90   Min.   : 9.20   Min.   :0.1847
 1st Qu.: 74.0   1st Qu.:1242   1st Qu.: 742   1st Qu.:11.90   1st Qu.:35.40   1st Qu.:0.7262
 Median :104.0   Median :1479   Median : 979   Median :17.60   Median :48.90   Median :0.9875
 Mean   :109.2   Mean   :1480   Mean   :1044   Mean   :18.32   Mean   :48.82   Mean   :1.0174
 3rd Qu.:136.0   3rd Qu.:1702   3rd Qu.:1307   3rd Qu.:24.30   3rd Qu.:61.90   3rd Qu.:1.3067
 Max.   :340.0   Max.   :2775   Max.   :2523   Max.   :44.60   Max.   :88.70   Max.   :2.2310
```

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1. Data Characteristics and Correlation Analysis

1.1 Exploratory Data Analysis (EDA)

Distribution & Outlier Analysis

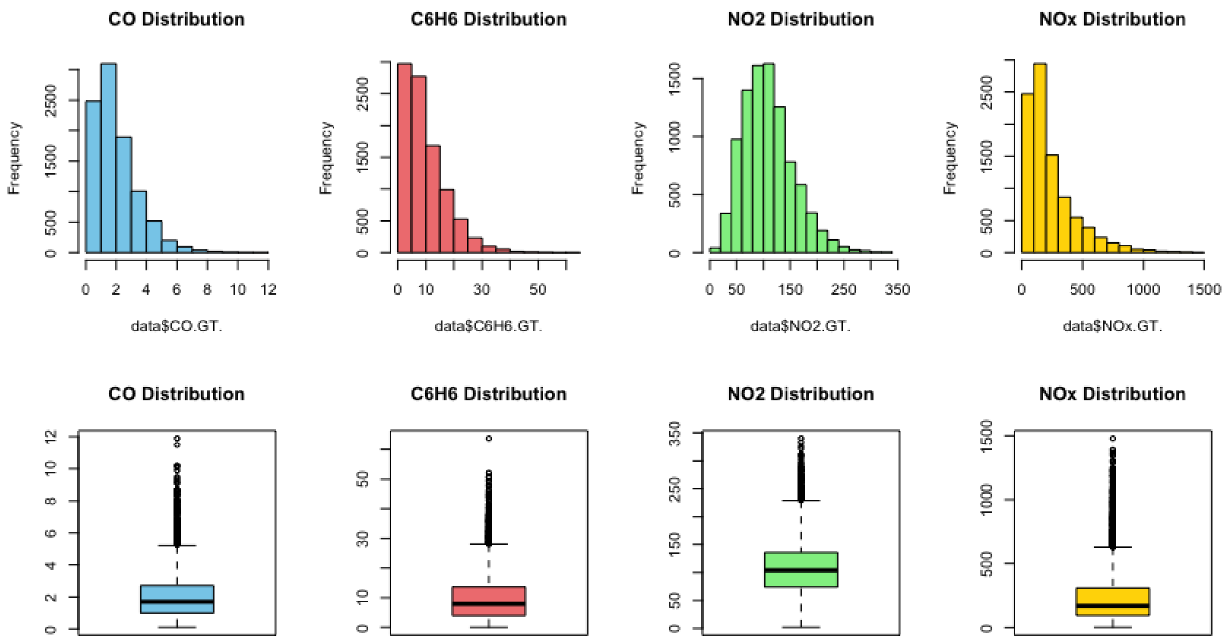


Figure 1: The Histograms reveal right-skewed distributions for all pollutants. This non-normality motivates the use of **non-parametric correlation measures**. Additionally, boximages highlight the presence of significant outliers across all pollutants. The consistent pattern of **median concentrations being lower than the means** confirms the positive skewness of the data.

1.2 Correlation Matrix Interpretation

Methodology

Given the non-normal distributions and the presence of extreme values, we utilize Spearman's rank correlation (ρ), a non-parametric measure that captures monotonic relationships without assuming linearity.

Sensor-Pollutant Relationships:

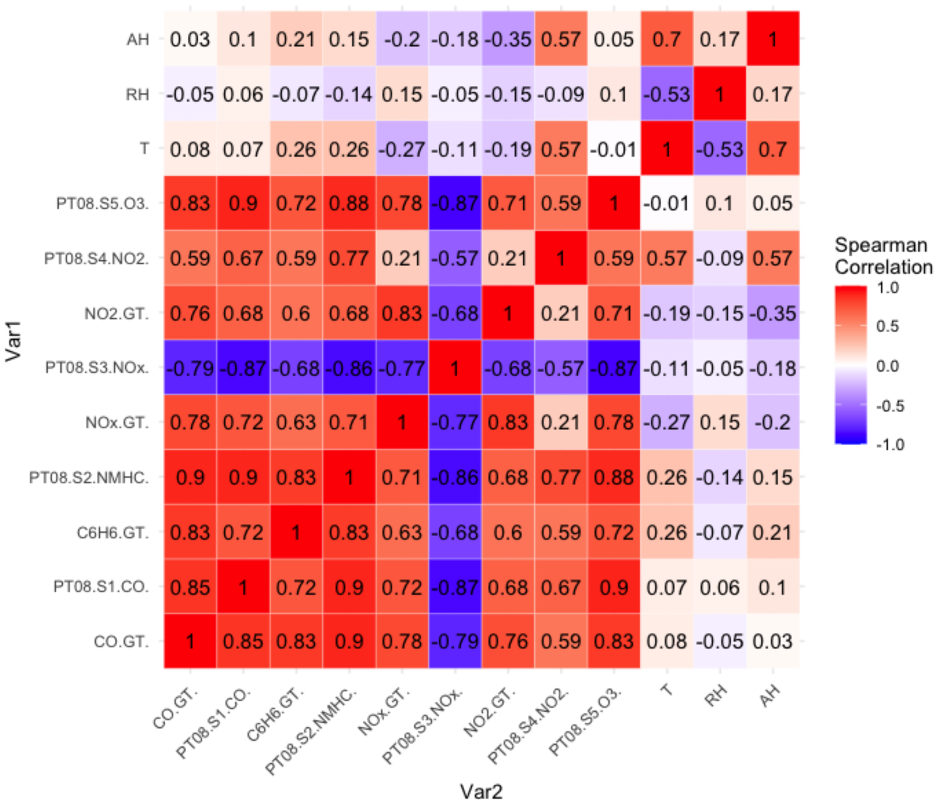


Figure 2: The Correlation Heatmap reveals: The relationships between pollutants and sensors show a strong positive correlation for `CO` and `Sensor CO` ($\rho = 0.85$) and a strong negative correlation for NO_x and `Sensor`

`NOx` (ρ = -0.77), while `NO2` and `Sensor NO2` have a weak correlation (ρ = 0.21). Pollutants exhibit weak or no correlation with environmental factors ($\rho \in$ (-0.35, 0.28)). However, cross-sensitivity detection suggests potential sensor interference, as `CO` correlates highly with `Sensor NOx, NMHC, and O3`, NO_x and `NO2` show moderate correlation with `Sensor CO, NMHC, and O3`, and C_6H_6 has high correlation with `Sensor NMHC` and moderate correlation with other sensors.

1.3 Robust Correlation Validation

Methodology

To verify sensor-reference pollutant correlations beyond traditional correlation metrics, we conducted permutation tests (n = 1000 iterations). This non-parametric approach: First we compute the observed Spearman's ρ, then generating a null distribution by shuffling reference values, using those to calculate empirical p-values

Result

The permutation test for CO, NO_2 and NO_x against their respective sensors yielded empirical **p-value < 0.001**, we have sufficient evidence to conclude that there are strong and statistically significant correlation between sensor and corresponding concentration. As a **non-parametric test**, this validation method strengthens the confidence in our findings **without relying on normality assumptions**.

2. Air Quality Index (AQI) Analysis

2.1 Understanding AQI

What is AQI?

The Air Quality Index (AQI) is a standardized metric used to communicate the health risks of air pollution. It translates complex pollutant concentration data into a single, easy-to-understand value on a 0 - 500 scale, with higer values indicating worse air quality.

Custom AQI Methodology

In this study, we employ a **Custom AQI** methodology where CO and NO_2 follow standard **EPA AQI** breakpoints, benzene (C_6H_6) is assessed using **WHO exposure limits**, and NO_x is evaluated using the same breakpoints ranges as NO_2. This approach ensures alignment with established regulatory standards while incorporating WHO-recommended guidelines for benzene exposure.

2.2 AQI Calculation Methodology

The AQI is computed as:

$$AQI = \max\left(\frac{I_{HI} - I_{LO}}{BP_{HI} - BP_{LO}}(C - BP_{LO}) + I_{LO}\right) \text{ across all pollutants}$$

where:

- $I_{HI/LO}$ = AQI category thresholds
- $BP_{HI/LO}$ = Breakpoints concentrations
- C = Observed pollutant concentration

Breakpoints reference table:

Category	*AQIRange*	*CO*	NO_2	NO_x	C_6H_6
Good	0-50	0-4.4	0-53	0-53	0-3
Moderate	51-100	4.4-9.4	53-100	53-100	3-7
Unhealthy for Sensitive Groups	101-150	9.4-12.4	100-360	100-360	7-10
Unhealthy	151-200	12.4-15.4	360-649	360-649	10-15
Very Unhealthy	201-300	15.4-30.4	649-1249	649-1249	15-20
Hazardous	301-500	30.4-50.4	1249-2049	1249-2049	20-30

2.3 Temporal AQI Patterns

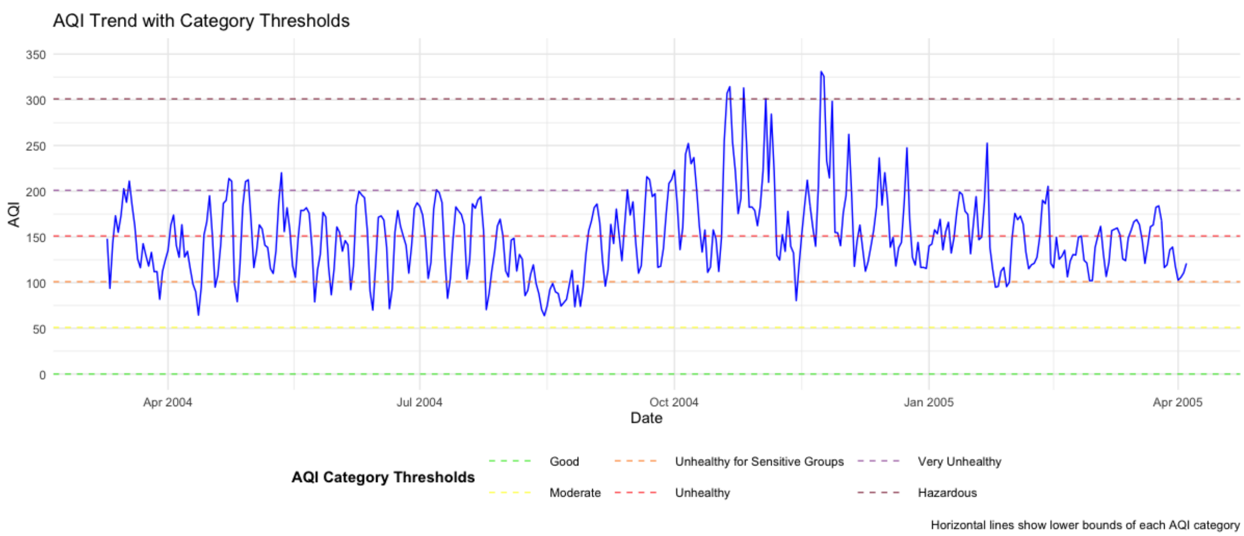
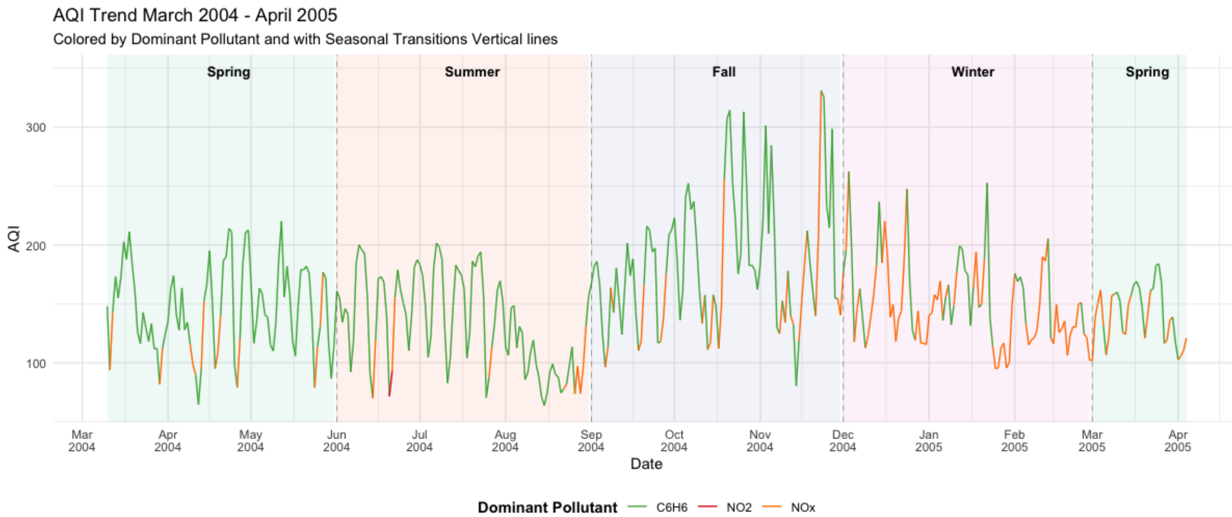


Figure 3: The AQI trend shows significant fluctuations, frequently exceeding the `Unhealthy for Sensitive Groups` and `Unhealthy` thresholds, with occasional peaks reaching `Very Unhealthy` levels. The highest peaks, reaching `Hazardous` range, are observed during late 2004. A sharp rise in AQI during Winter suggests increased pollution, likely due to heightened combustion activities, while Summer peaks align with high benzene (C_6H_6) contributions. Early 2005 shows a slight decline in AQI, though persistent fluctuations suggest evolving emission patterns and seasonal influences on air quality.

2.4 Pollutant-Specific Contributions



Season	Primary Pollutant	Contribution
Spring(2004)	C_6H_6	87.95%
Summer	C_6H_6	90.22%
Fall	C_6H_6	76.92%
Winter	NO_x	67.78%
Spring(2005)	NO_x	54.29%

Figure 4: Table 2 summarizes the seasonal contributions of individual pollutans to AQI, revealing that benzene (C_6H_6) is the dominant pollutant in Spring, Summer and Fall, accounting for over 75% of AQI excrescences, with a peak contributes of 90.22% during Summer. In contrast, Winter AQI is primarily influenced by NO_x , which contributes 67.78%, likely due to increased combustion activities. The transition period in early Spring 2005 marks a shift, where NO_x and C_6H_6 exhibit nearly equal contributions, indicating a changing pollution patterns over time.

4. Seasonal Variation Analysis

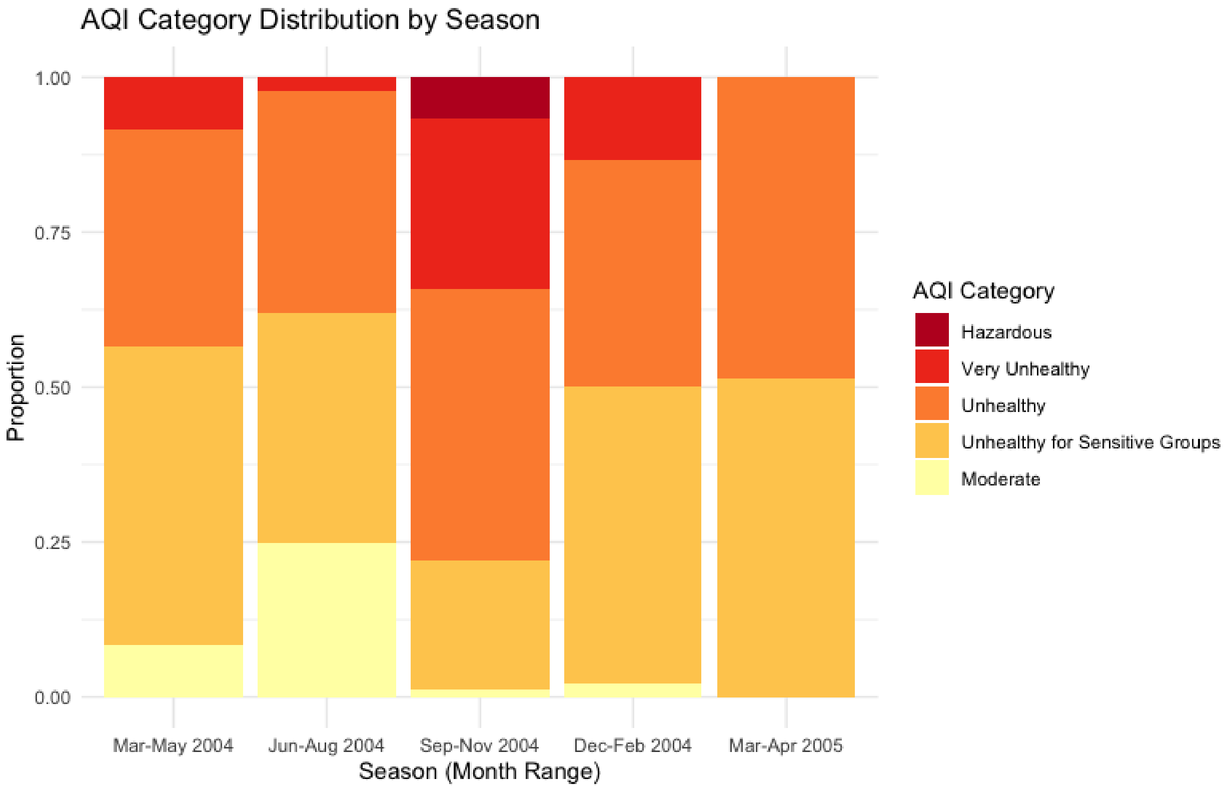


Figure 5: The AQI category distribution varies by season, showing a shift from moderate air quality in Spring (Mar–May 2004) to worsening conditions in Summer (Jun–Aug 2004) and Fall (Sep–Nov 2004), where "Unhealthy" and "Very Unhealthy" categories dominate, with a small proportion reaching "Hazardous" levels. Winter (Dec–Feb 2004) continues to have high pollution, with a majority in the "Unhealthy for Sensitive Groups" and "Unhealthy" categories, while early Spring (Mar–Apr 2005) shows slight improvement with a higher proportion of moderate air quality. This seasonal pattern suggests increased pollution in Fall and Winter, likely due to combustion-related emissions, while air quality improves slightly in transitional periods.