

Final Report: Air Quality

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

Number of missing data	n
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
N02.GT.	PT08.S4.N02.	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
N02.GT.	PT08.S4.N02.	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

Correlation and AQI

1. Data Characteristics and Correlation Analysis

1.1 Exploratory Data Analysis (EDA)

Distribution & Outlier Analysis

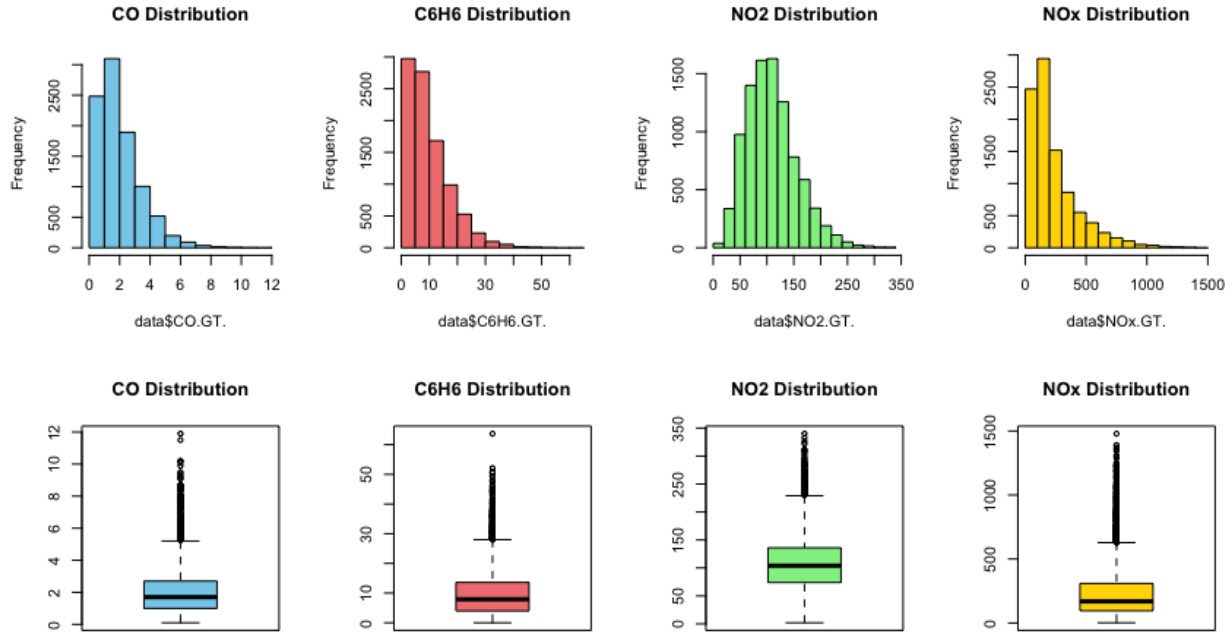


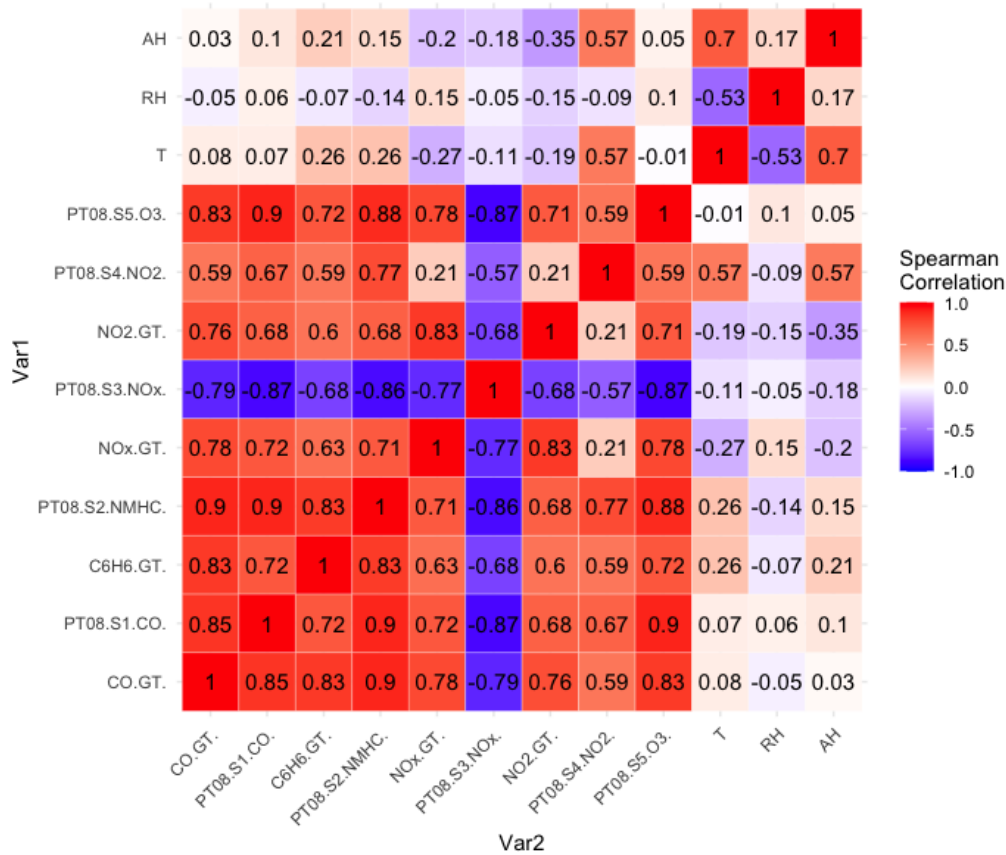
Figure 1: The Histograms reveal right-skewed distributions for all pollutants. This non-normality motivates the use of **non-parametric correlation measures**. Additionally, boxplots highlight the presence of significant outliers across all pollutants. The consistent pattern of **median concentrations 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:



True Pollutants vs Sensor Response & Environment
Spearman correlation coefficients

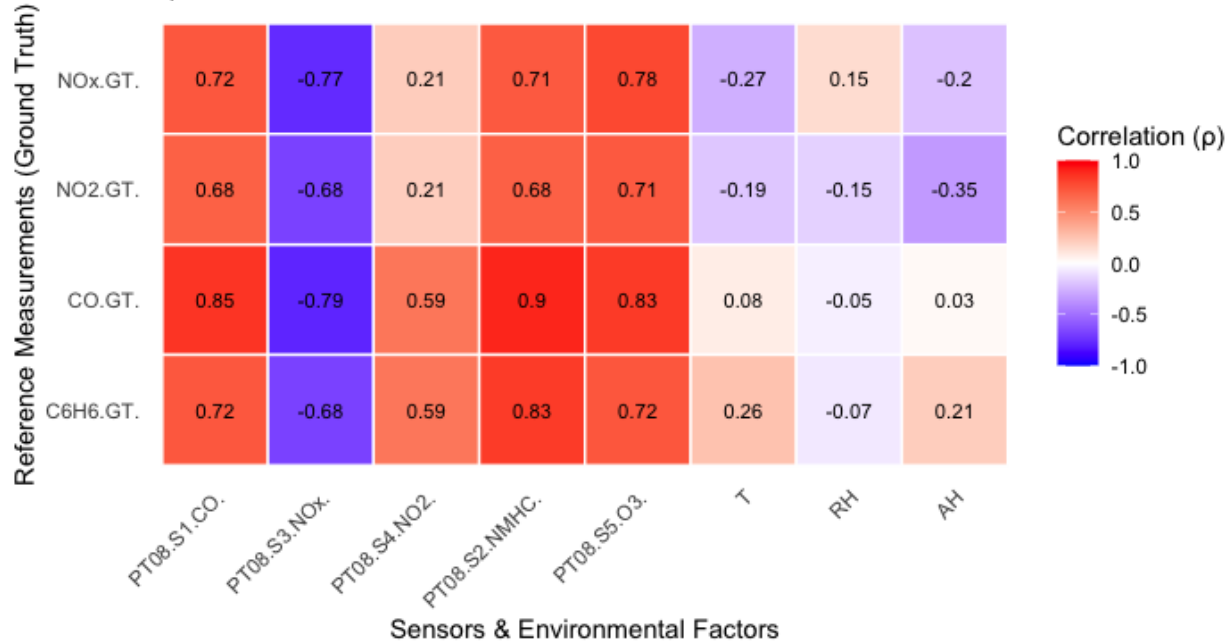


Figure 2: The Correlation Heatmap reveals: The relationships between pollutants and sensors show a strong positive correlation for CO and Sensor CO ($\rho = 0.85$) and a strong negative correlation for NO_x and Sensor NOx ($\rho = -0.77$), while NO2 and Sensor NO2 have a weak correlation ($\rho = 0.21$). 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 higher 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	AQI_{Range}	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

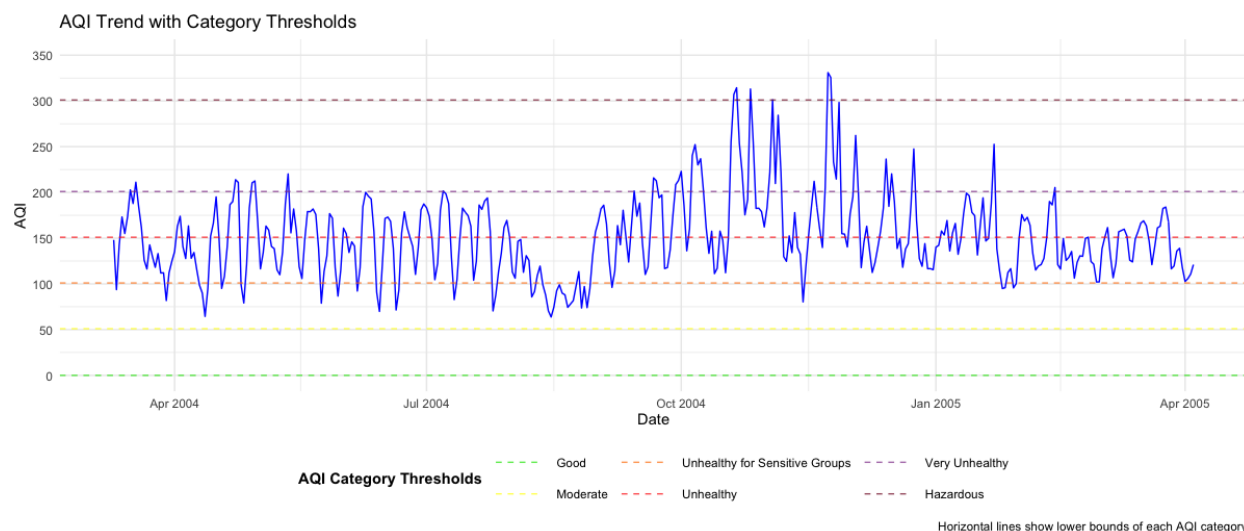
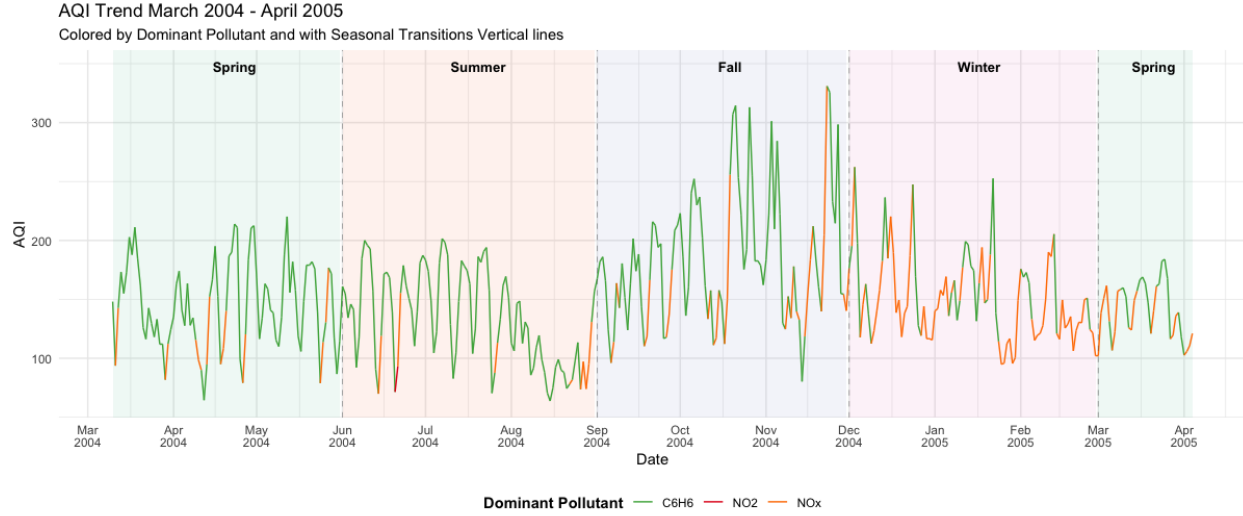


Figure 3: The AQI trend shows significant fluctuations, frequently exceeding the **Unhealthy for Sensitive Groups** and **Unhealthy** thresholds, with occasional peaks reaching **Very Unhealthy** levels. The highest peaks, reaching **Hazardous** range, are observed during late 2004. A sharp rise in AQI 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 pollutants to AQI, revealing that benzene (C_6H_6) is the dominant pollutant in Spring, Summer and Fall, accounting for over 75% of AQI excursions, with a peak contribution 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 pattern over time.

4. Seasonal Variation Analysis

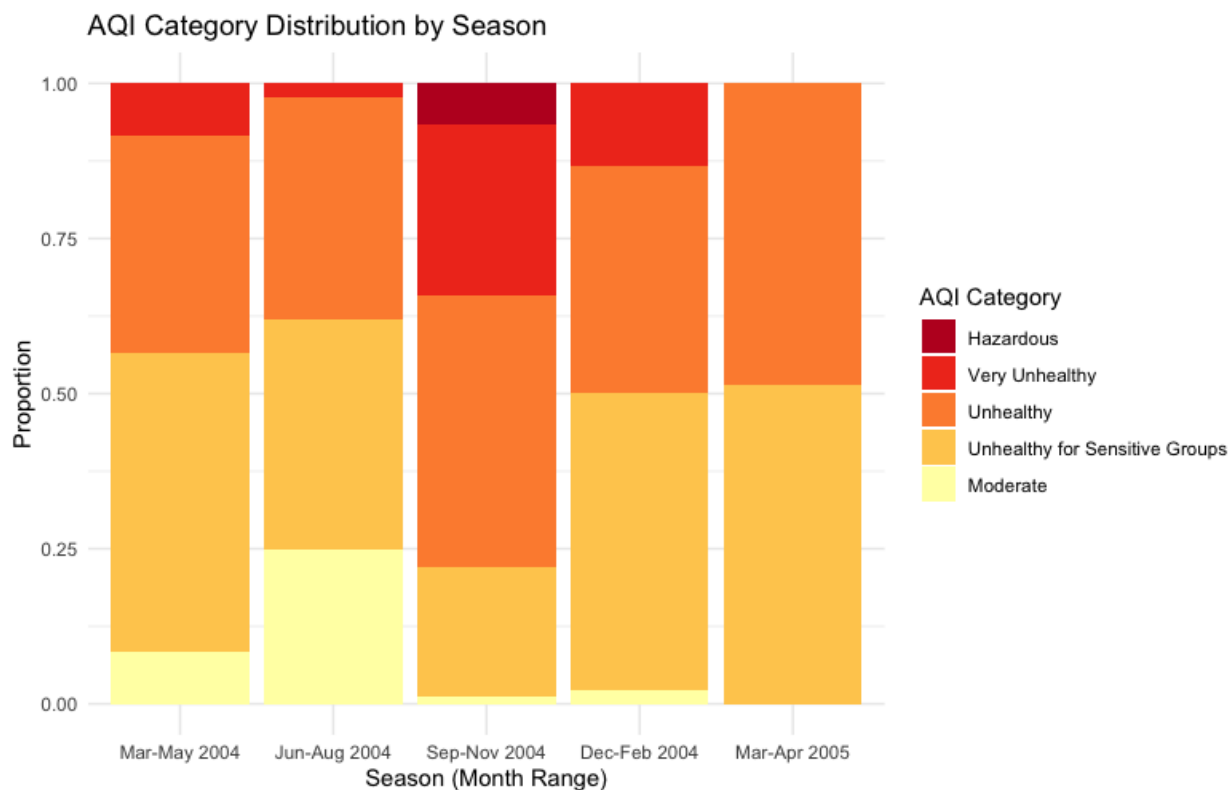


Figure 5: The AQI category distribution varies by season, showing a shift from moderate air quality in Spring (Mar–May 2004) to worsening conditions in Summer (Jun–Aug 2004) and Fall (Sep–Nov 2004), where “Unhealthy” and “Very Unhealthy” categories dominate, with a small proportion reaching “Hazardous” 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.