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.

1. Data Characteristics and Correlation Analysis

1.1 Exploratory Data Analysis (EDA)

Distribution & Outlier Analysis

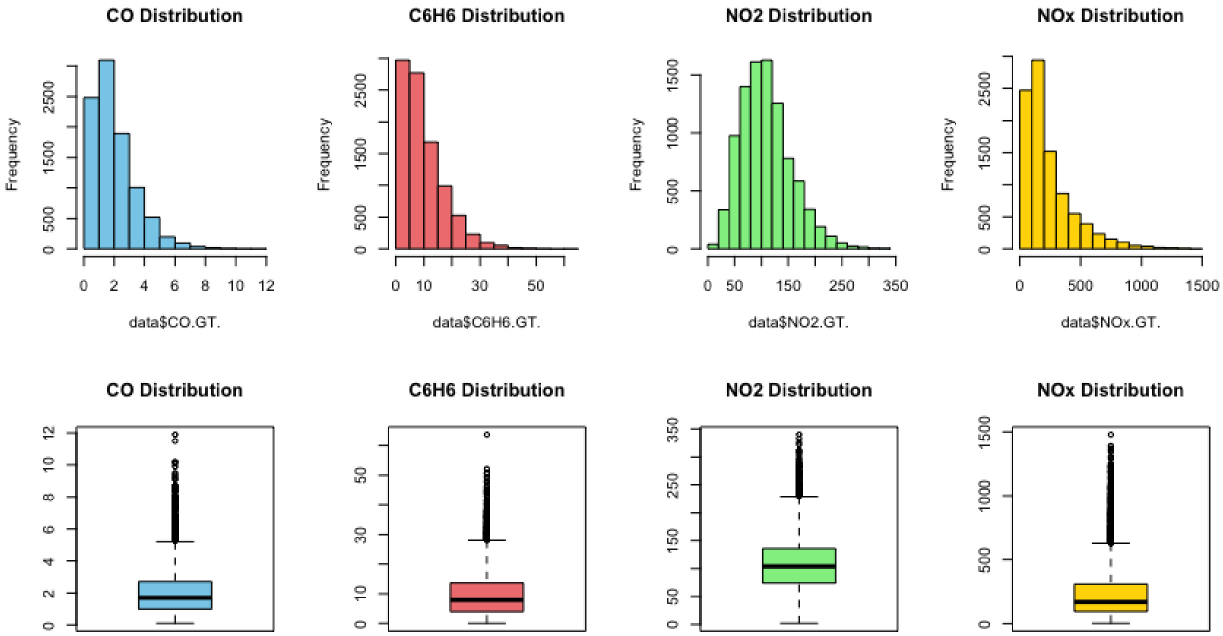


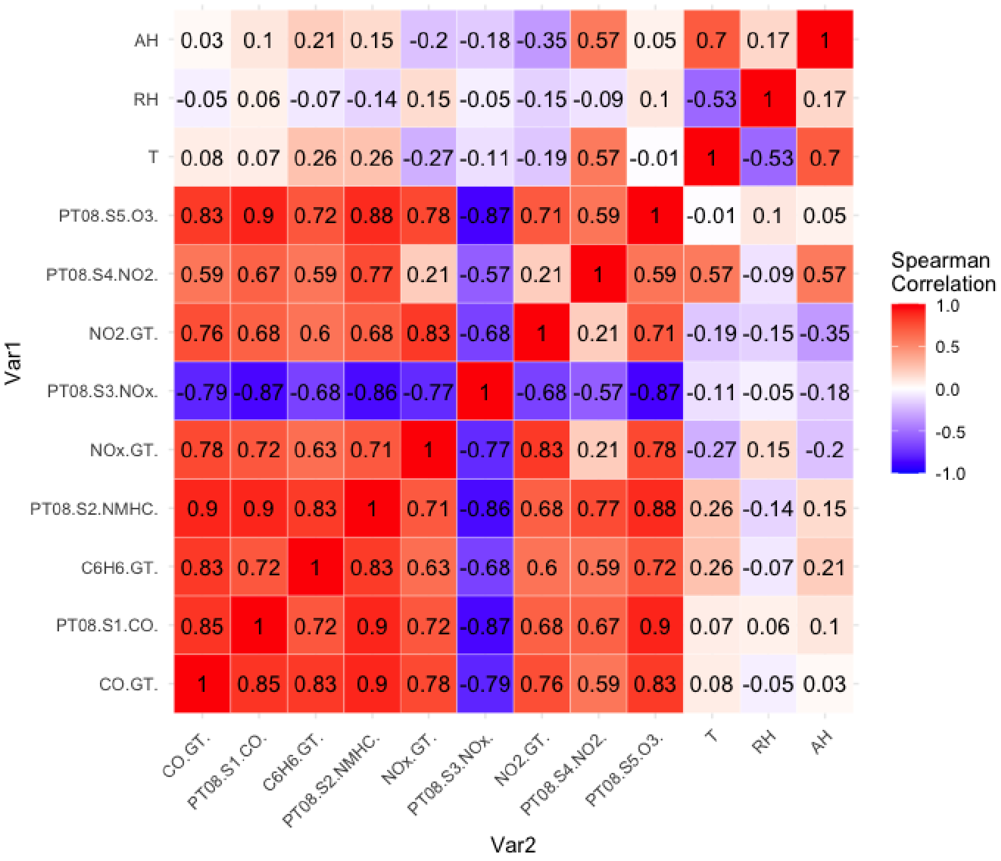
Figure 1: The Histograms reveal right-skewed distributions for all pollutants. This non-normality motivates the use of **non-parametric correlation measures**. Additionally, boxplots highlight the presence of significant outliers across all pollutants. The consistent pattern of **median concentrations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



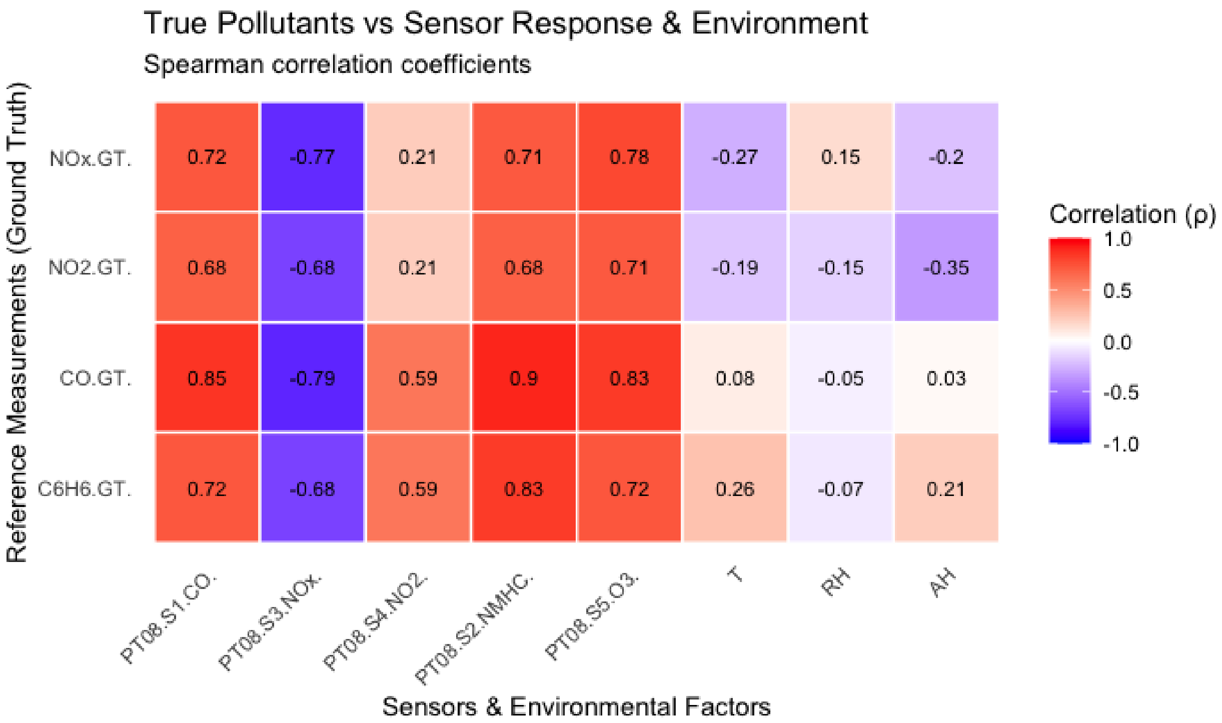


Figure 2: The Correlation Heatmap reveals: The relationships between pollutants and sensors show a strong positive correlation for CO and Sensor CO (ρ = 0.85) and a strong negative correlation for NO_x and Sensor NOx (ρ = -0.77), while NO2 and Sensor NO2 have a weak correlation (ρ = 0.21). Pollutants 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

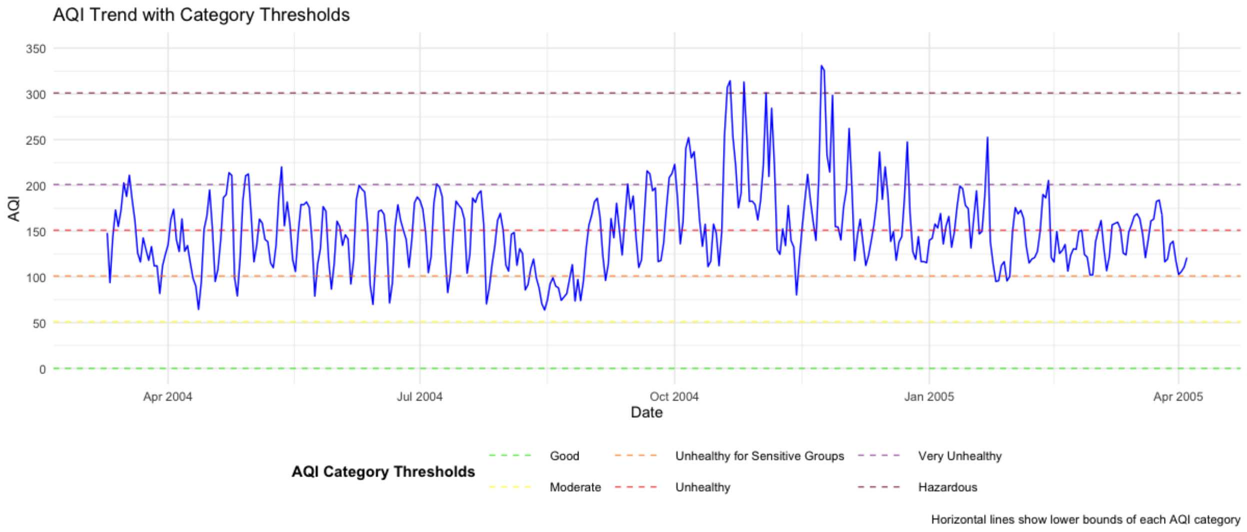
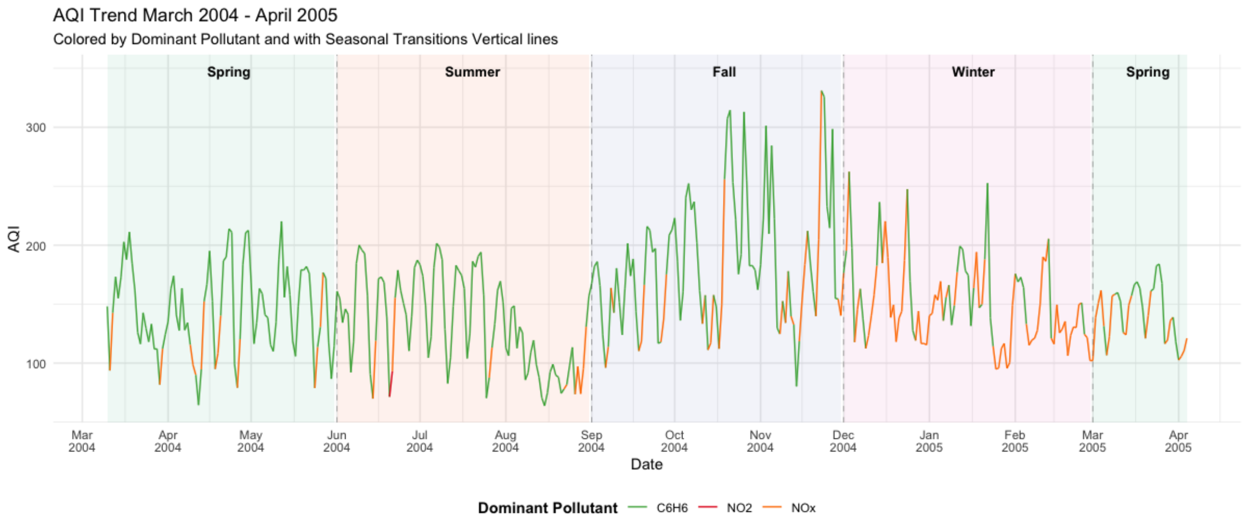


Figure 3: The AQI trend shows significant fluctuations, frequently exceeding the `Unhealthy for Sensitive Groups` and `Unhealthy` thresholds, with occasional peaks reaching `Very Unhealthy` levels. The highest peaks, reaching `Hazardous` range, are observed during late 2004. A sharp rise in AQI during 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

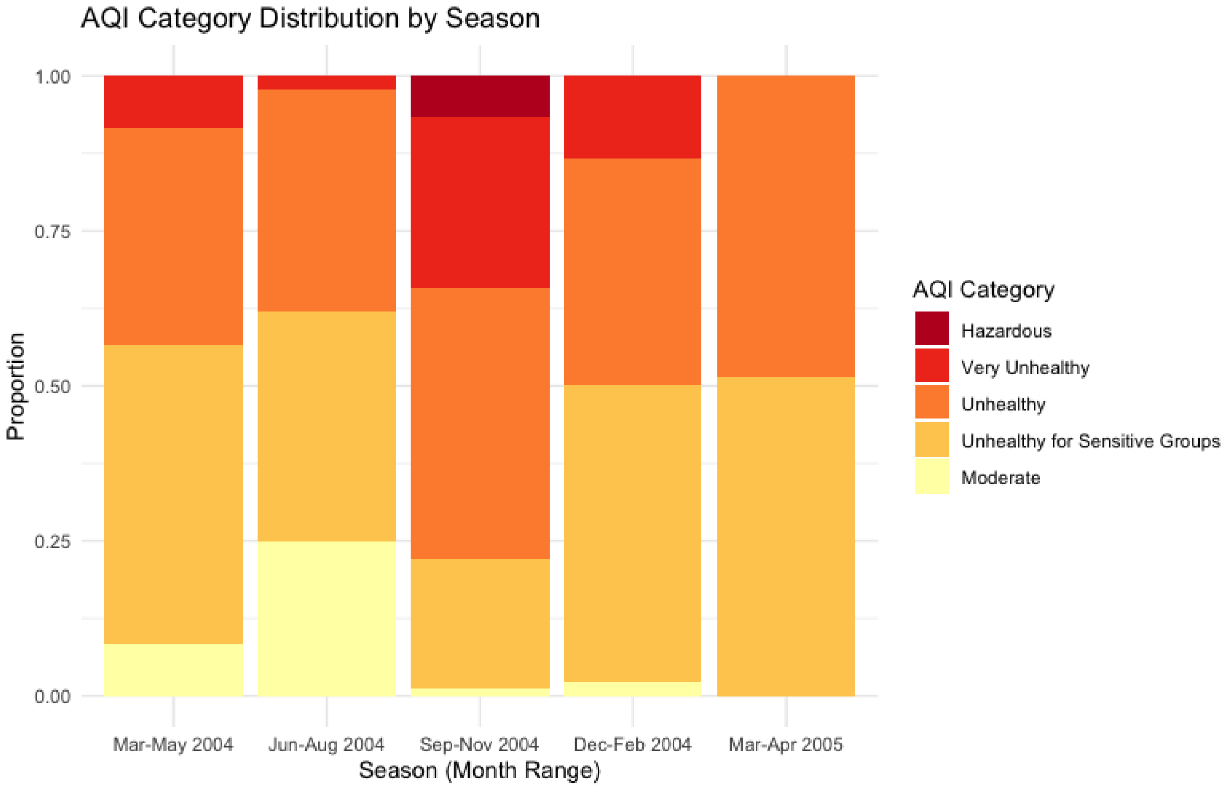


Figure 5: The AQI category distribution varies by season, showing a shift from moderate air quality in Spring (Mar–May 2004) to worsening conditions in Summer (Jun–Aug 2004) and Fall (Sep–Nov 2004), where "Unhealthy" and "Very Unhealthy" categories dominate, with a small proportion reaching "Hazardous"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