Air Quality Analysis

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Introduction

Dataset

Air Quality (UC Irvine) (Vito, S. (2008). Air Quality Dataset. UCI Machine Learning Repository. https://doi.org/10.24432/C59K5F.)

Abstract

Accurate air quality monitoring relies on sensor data to measure pollutants such as ozone, carbon monoxide, and nitrogen oxides. This study examines the correlation between sensor readings and measured pollutant levels to validate monitoring technologies and enhance their predictive capabilities. By leveraging models, I aim to predict carbon monoxide concentrations based on sensor data and other environmental factors.

Goals/Research Question

Descriptive Features: - Continuous - Sensor targeting CO - PT08.S1(CO) - Sensor targeting O3 - PT08.S5(O3) - True averaged sensor response - NOx(GT) - Categorical - Season - Based on Dates

Target Feature: - True Concentration of CO - CO(GT)

Basic Data Cleaning & Preprocessing

Library Loads & Data Imports

```
library(readxl)
library(tidyverse)
```

```
## -- Attaching core tidyverse packages ------------------------ tidyverse 2.0.0 --
## v dplyr     1.1.4     v readr     2.1.5
## v forcats   1.0.0     v stringr   1.5.1
## v ggplot2   3.5.1     v tibble    3.2.1
## v lubridate 1.9.3     v tidyr     1.3.1
## v purrr     1.0.2
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
## i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors
```

```
library(ggplot2)
library(tidymodels)
```

```
## -- Attaching packages --------------------------------------- tidymodels 1.2.0 --
## v broom        1.0.6     v rsample      1.2.1
## v dials        1.3.0     v tune         1.2.1
## v infer        1.0.7     v workflows    1.1.4
## v modeldata    1.4.0     v workflowsets 1.1.0
## v parsnip      1.2.1     v yardstick    1.3.1
## v recipes      1.1.0
## -- Conflicts ------------------------------------------ tidymodels_conflicts() --
## x scales::discard() masks purrr::discard()
## x dplyr::filter()   masks stats::filter()
## x recipes::fixed()  masks stringr::fixed()
## x dplyr::lag()      masks stats::lag()
## x yardstick::spec() masks readr::spec()
## x recipes::step()   masks stats::step()
## * Use tidymodels_prefer() to resolve common conflicts.
```

```
library(patchwork)
library(lubridate)
library(zoo)
```

```
##
## Attaching package: 'zoo'
##
## The following objects are masked from 'package:base':
##
##     as.Date, as.Date.numeric
```

```r
library(reshape2)
```

```
##
## Attaching package: 'reshape2'
##
## The following object is masked from 'package:tidyr':
##
##     smiths
```

```r
library(dplyr)
library(RColorBrewer)
library(ggridges)
library(ggrepel)

air_quality_data <- read_excel("AirQualityUCI.xlsx", sheet = "AirQualityUCI")
```

Creating Categorical Features, Other Preprocessing, & Advanced Data Cleaning

```r
# Data Preprocessing Pipeline
# Steps:
# 1. Create seasonal categories
# 2. Handle missing values and outliers
# 3. Create interaction terms
# 4. Add lagged features

# Define pollutant columns for handling outliers
pollutant_columns <- c("CO(GT)", "NOx(GT)", "NO2(GT)")

# Data Preprocessing Pipeline
air_quality_data <- air_quality_data |>
  mutate(
    Season = case_when(
      format(Date, "%m") %in% c("12", "01", "02") ~ "Winter",
      format(Date, "%m") %in% c("03", "04", "05") ~ "Spring",
      format(Date, "%m") %in% c("06", "07", "08") ~ "Summer",
      format(Date, "%m") %in% c("09", "10", "11") ~ "Autumn"
    )
  ) |>

  # This code drops a bunch of values that were all at -200, likely sensor failures since CO & other le
  drop_na(`CO(GT)`, `NOx(GT)`, `NO2(GT)`) |>
  filter(`CO(GT)` >= 0, `NOx(GT)` >= 0, `NO2(GT)` >= 0) |>
  group_by(Season) |>

  # Winsorize outliers
  mutate(
    across(all_of(pollutant_columns),
           ~ ifelse(. > quantile(., 0.95, na.rm = TRUE), quantile(., 0.95, na.rm = TRUE), .))
  ) |>
  ungroup() |>
```

```r
  # Handle missing values using conditional replacement
  mutate(
    across(c(`NOx(GT)`, `NO2(GT)`), ~ na_if(., -200)),
    `NOx(GT)` = if_else(is.na(`NOx(GT)`), mean(`NOx(GT)`, na.rm = TRUE), `NOx(GT)`),
    `NO2(GT)` = if_else(is.na(`NO2(GT)`), mean(`NO2(GT)`, na.rm = TRUE), `NO2(GT)`)
  ) |>

  # Standardize Continuous Variables
  mutate(
    across(c(T, RH, AH, `PT08.S1(CO)`, `PT08.S5(O3)`), ~ scale(.))
  ) |>

  # Add interaction terms
  mutate(
    NOx_PT08_S1_Interaction = `NOx(GT)` * `PT08.S1(CO)`,
    NOx_Season_Interaction = as.numeric(as.factor(Season)) * `NOx(GT)`
  )

# Create lagged feature for CO(GT) (previous hour)
air_quality_data <- air_quality_data |>
  arrange(Date, Time) |>
  mutate(
    Lagged_CO = lag(`CO(GT)`, n = 1, default = NA)
  )

# Drop rows with missing values introduced by lagged features
air_quality_data <- drop_na(air_quality_data)

# Improved data cleaning for CO(GT)
air_quality_clean <- air_quality_data |>
  # Replace -200 values with NA since they appear to be missing data
  mutate(
    `CO(GT)` = ifelse(`CO(GT)` == -200, NA, `CO(GT)`)
  ) |>
  drop_na(`CO(GT)`) |>
  filter(`CO(GT)` >= 0)

# Add a custom function for data cleaning
clean_sensor_data <- function(data, threshold) {
  data |>
    mutate(sensor_status = case_when(
      `PT08.S1(CO)` > threshold ~ "High",
      `PT08.S1(CO)` < -threshold ~ "Low",
      TRUE ~ "Normal"
    ))
}

# Add pivot operations for sensor readings
sensor_long <- air_quality_data |>
  pivot_longer(
    cols = starts_with("PT08"),
    names_to = "sensor_type",
    values_to = "reading"
```

```
  )

# Final Dataset Split
set.seed(123)
data_split <- initial_split(air_quality_data, prop = 0.6)
train_data <- training(data_split)
temp_data <- testing(data_split)
validation_split <- initial_split(temp_data, prop = 0.5)
validation_data <- training(validation_split)
test_data <- testing(validation_split)
```

Exploratory & Model Plots

Exploratory Plot/Table 1

```
plot1 <- ggplot(air_quality_data, aes(x = `NOx(GT)`, y = `CO(GT)`)) +
  geom_hex(bins = 30) +
  scale_fill_viridis_c() +
  geom_smooth(method = "lm", se = TRUE, color = "darkred", linetype = "dashed", size = 1) +
  scale_y_continuous(limits = c(-10, 10), breaks = seq(-10, 10, by = 5)) +
  scale_x_continuous(limits = c(0, 600), breaks = seq(0, 600, by = 100)) +
  labs(
    title = "Density of NOx and CO Measurements",
    x = "NOx(GT) (Nitrogen Oxides)",
    y = "CO(GT) (Carbon Monoxide)",
    fill = "Count"
  ) +
  theme_minimal(base_size = 12) +
  theme(plot.title = element_text(face = "bold"))
```

```
## Warning: Using ‘size‘ aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use ‘linewidth‘ instead.
## This warning is displayed once every 8 hours.
## Call ‘lifecycle::last_lifecycle_warnings()‘ to see where this warning was
## generated.
```

```
# This plot showcases the relationship betwen NOx(GT) and CO(GT), critical to the research question bec
```

Exploratory Plot/Table 2

```
plot2 <- ggplot(air_quality_data, aes(x = `NOx(GT)` * `PT08.S1(CO)`, y = `CO(GT)`, color = Season)) +
  geom_point(alpha = 0.6, size = 1.5) +
  geom_smooth(method = "lm", se = TRUE, color = "orange", linetype = "dotted", size = 1) +
  scale_y_continuous(limits = c(-10, 10), breaks = seq(-10, 10, by = 5)) +
  scale_x_continuous(limits = c(-2000, 1000), breaks = seq(-2000, 1000, by = 500)) +
  scale_color_brewer(palette = "Set2") +
  labs(
```

```
    title = "Interaction Between NOx(GT) and Sensor Data on CO(GT)",
    x = "NOx(GT) * PT08.S1(CO) (Interaction Term)",
    y = "CO(GT) (Carbon Monoxide)",
    color = "Season"
  ) +
  theme_minimal(base_size = 12) +
  theme(
    plot.title = element_text(face = "bold"),
    legend.position = "bottom"
  )

# This plot examine show the interaction of NOx(GT) and PT08.S1(CO) relates to CO(GT). By categorizing
```

```
# Combine the two plots
final_exploratory_plot <- plot1 | plot2 +
  plot_layout(guides = "collect") &
  theme(legend.position = "bottom")
final_exploratory_plot
```

```
## Warning: Removed 512 rows containing non-finite outside the scale range
## (`stat_binhex()`).
```

```
## `geom_smooth()` using formula = 'y ~ x'
```

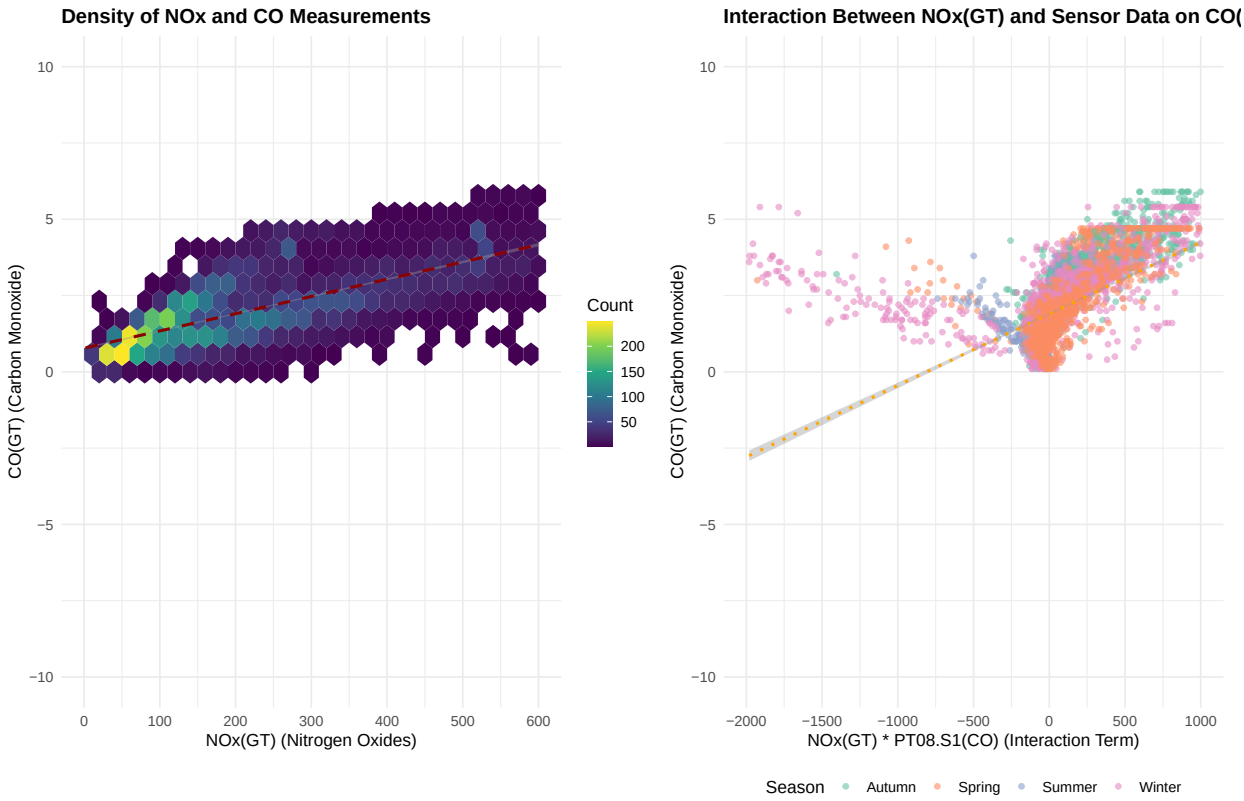
```
## Warning: Removed 512 rows containing non-finite outside the scale range
## (`stat_smooth()`).
```

```
## Warning: Removed 3 rows containing missing values or values outside the scale range
## (`geom_hex()`).
```

```
## `geom_smooth()` using formula = 'y ~ x'
```

```
## Warning: Removed 249 rows containing non-finite outside the scale range
## (`stat_smooth()`).
```

```
## Warning: Removed 249 rows containing missing values or values outside the scale range
## (`geom_point()`).
```




```
# In plot 1, the positive correlation between NOx(GT) and CO(GT) indicates that higher NOx levels are a

# In plot 2, the interaction term highlights the complex relationship between NOx(GT) and PT08.S1(CO),
```

Model Plot 1

```
model_plot1 <- ggplot(train_data, aes(x = `CO(GT)`, y = Season, fill = Season)) +
  geom_density_ridges(alpha = 0.7) +
  facet_wrap(~ cut(`PT08.S1(CO)`, breaks = 3, labels = c("Low", "Medium", "High"))) +
  geom_label(
    data = train_data |>
      group_by(Season) |>
      summarise(mean_co = mean(`CO(GT)`), y = as.numeric(factor(first(Season)))),
    aes(x = mean_co, y = y, label = round(mean_co, 2)),
    inherit.aes = FALSE
  ) +
  labs(
    title = "CO Distribution by Season and Sensor Level",
    subtitle = "Seasonal Variations in CO Levels Across Sensor Categories",
    caption = "Note: Sensor levels determined by tertile splits of PT08.S1(CO) readings",
    x = "CO(GT) Ground Truth",
    y = "Season"
  ) +
  theme_minimal()
```

Model Plot 2

```
model_plot2 <- ggplot(train_data, aes(x = `PT08.S5(O3)`, y = `CO(GT)`, color = `NOx(GT)`)) +
  geom_point(alpha = 0.6) +
  scale_color_viridis_c() +
  geom_smooth(method = "lm", se = TRUE) +
  labs(
    title = "O3 Sensor vs CO with NOx Levels",
    x = "PT08.S5(O3) Sensor Reading (Standardized)",
    y = "CO(GT) Ground Truth"
  ) +
  theme_minimal()
```

```
model_plot1 | model_plot2
```

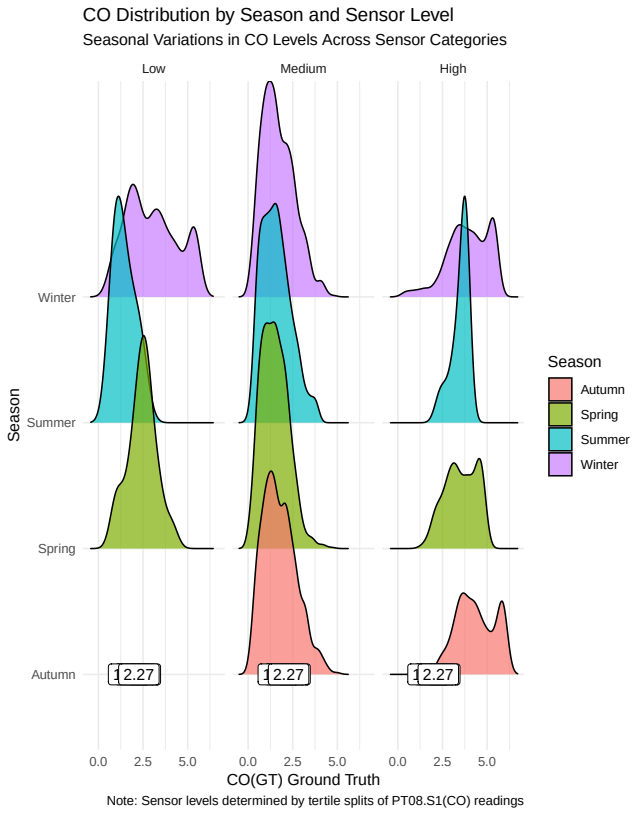
```
## Picking joint bandwidth of 0.343
```

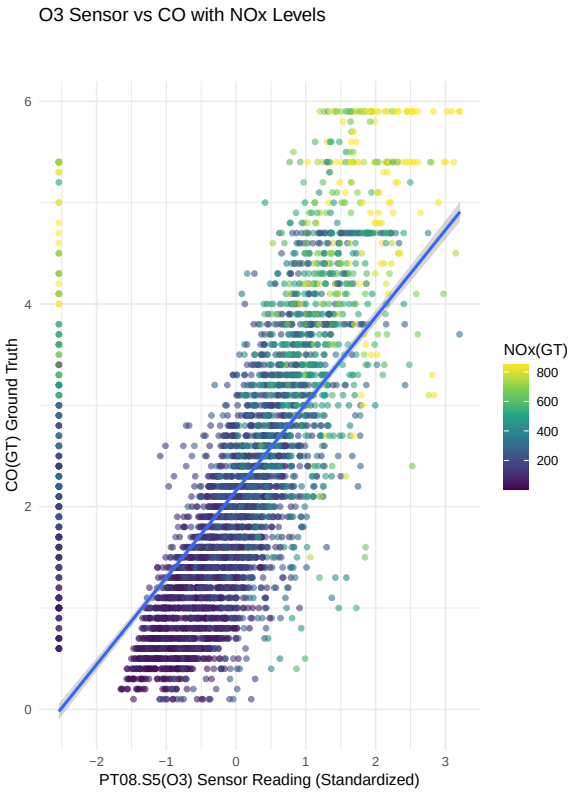
```
## Picking joint bandwidth of 0.201
```

```
## Picking joint bandwidth of 0.271
```

```
## `geom_smooth()` using formula = 'y ~ x'
```

```
## Warning: The following aesthetics were dropped during statistical transformation:
## colour.
## i This can happen when ggplot fails to infer the correct grouping structure in
##   the data.
## i Did you forget to specify a `group` aesthetic or to convert a numerical
##   variable into a factor?
```






```
# The ridgeline plot in Model Plot 1 demonstrates the relationship between multiple features (Seasons,

# The scatter plot in Model Plto 2 examines the relationship between the O3 sensor and CO ground truthm
```

Linear Models

Exploratory Linear Model 1

```
# First model focusing on main effects and seasonal interaction
model_with_feature <- linear_reg() |>
  set_engine("lm") |>
  fit(`CO(GT)` ~ `PT08.S1(CO)` + `NOx(GT)` + Season, data = train_data)

model_without_feature <- linear_reg() |>
  set_engine("lm") |>
  fit(`CO(GT)` ~ `PT08.S1(CO)` + Season, data = train_data)

# Calculate RMSE comparison using validation data
val_metrics_with <- augment(model_with_feature, new_data = validation_data) |>
  summarize(rmse = sqrt(mean((`CO(GT)` - .pred)^2)))

val_metrics_without <- augment(model_without_feature, new_data = validation_data) |>
  summarize(rmse = sqrt(mean((`CO(GT)` - .pred)^2)))
```

```r
# Print results
print("RMSE with NOx(GT):")
```

```
## [1] "RMSE with NOx(GT):"
```

```r
print(val_metrics_with)
```

```
## # A tibble: 1 x 1
##    rmse
##   <dbl>
## 1 0.702
```

```r
print("RMSE without NOx(GT):")
```

```
## [1] "RMSE without NOx(GT):"
```

```r
print(val_metrics_without)
```

```
## # A tibble: 1 x 1
##    rmse
##   <dbl>
## 1  1.15
```

Exploratory linear model 2

```r
# Second model incorporating O3 sensor and interaction terms
model_with_o3 <- linear_reg() |>
  set_engine("lm") |>
  fit(`CO(GT)` ~ `PT08.S1(CO)` + `PT08.S5(O3)` + `NOx(GT)` + Season, data = train_data)

# Add a categorical feature interaction model
model_with_interaction <- linear_reg() |>
  set_engine("lm") |>
  fit(`CO(GT)` ~ `PT08.S1(CO)` * Season + `NOx(GT)`, data = train_data)

# Calculate RMSE for models
val_metrics_interaction <- augment(model_with_interaction, new_data = validation_data) |>
  summarize(rmse = sqrt(mean((`CO(GT)` - .pred)^2)))

val_metrics_o3 <- augment(model_with_o3, new_data = validation_data) |>
  summarize(rmse = sqrt(mean((`CO(GT)` - .pred)^2)))

# Compare all models
model_comparison <- tibble(
  Model = c("With NOx", "Without NOx", "With Interaction", "With O3"),
  RMSE = c(
    val_metrics_with$rmse,
    val_metrics_without$rmse,
    val_metrics_interaction$rmse,
```

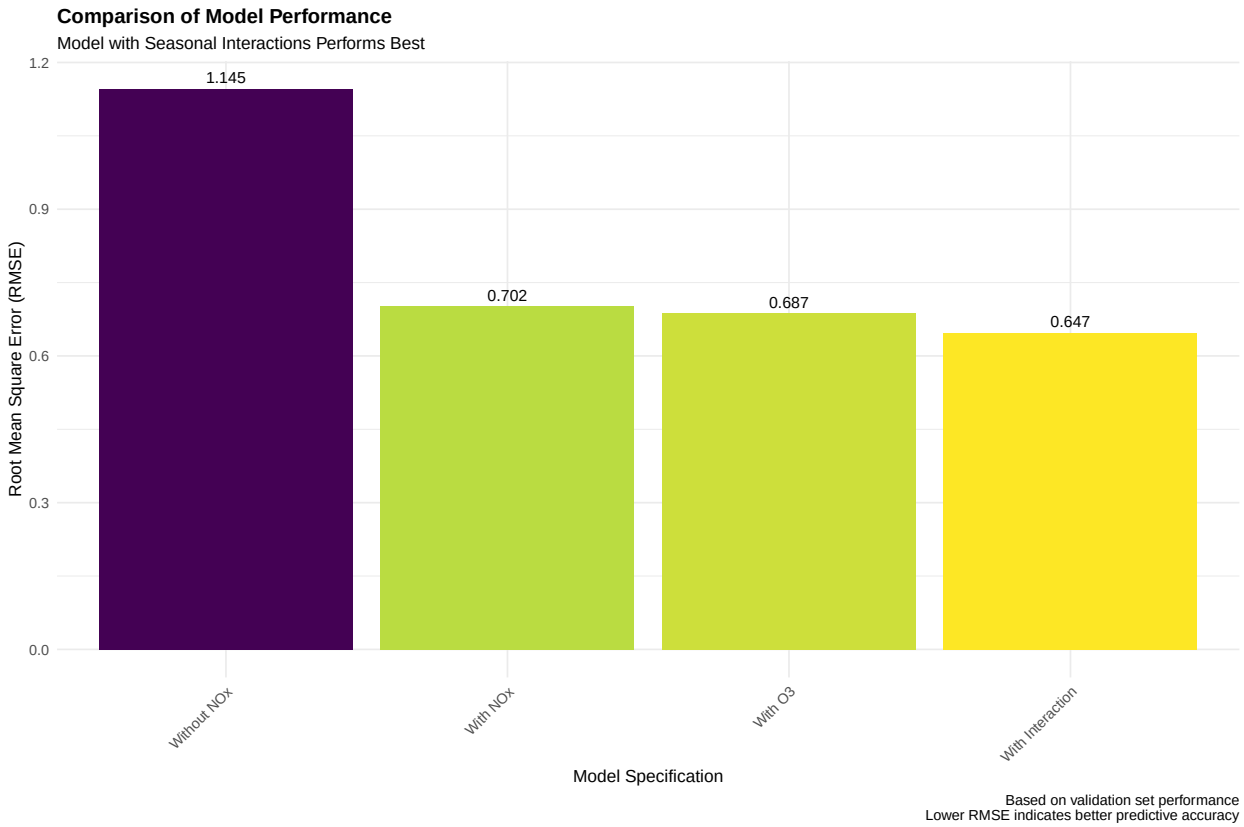
```
    val_metrics_o3$rmse
  )
) |>
  arrange(RMSE)
```

```
# Create comparison plot
model_comparison_plot <- ggplot(model_comparison, aes(x = reorder(Model, -RMSE), y = RMSE)) +
  geom_col(aes(fill = RMSE)) +
  scale_fill_viridis_c(direction = -1) +
  geom_text(aes(label = sprintf("%.3f", RMSE)), vjust = -0.5) +
  labs(
    title = "Comparison of Model Performance",
    subtitle = "Model with Seasonal Interactions Performs Best",
    x = "Model Specification",
    y = "Root Mean Square Error (RMSE)",
    caption = "Based on validation set performance\nLower RMSE indicates better predictive accuracy"
  ) +
  theme_minimal(base_size = 12) +
  theme(
    axis.text.x = element_text(angle = 45, hjust = 1),
    plot.title = element_text(face = "bold"),
    legend.position = "none"
  )

# Display the comparison
print(model_comparison)
```

```
## # A tibble: 4 x 2
##   Model             RMSE
##   <chr>            <dbl>
## 1 With Interaction 0.647
## 2 With O3          0.687
## 3 With NOx         0.702
## 4 Without NOx      1.15
```

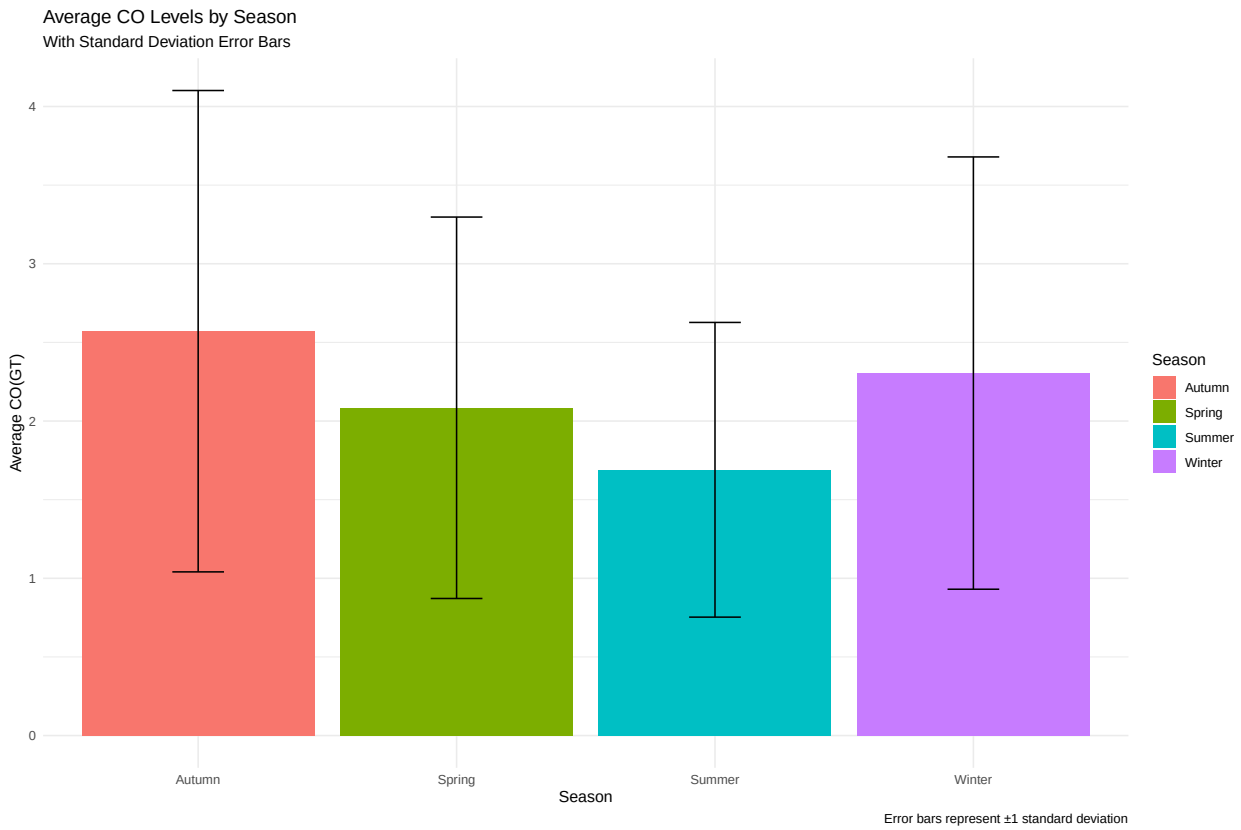
```
model_comparison_plot
```



Bar Plot

```
# Create seasonal average bar plot
seasonal_plot <- ggplot(air_quality_data |>
                        group_by(Season) |>
                        summarise(avg_co = mean(`CO(GT)`),
                                  sd_co = sd(`CO(GT)`)),
                      aes(x = Season, y = avg_co)) +
  geom_col(aes(fill = Season)) +
  geom_errorbar(aes(ymin = avg_co - sd_co,
                    ymax = avg_co + sd_co),
                width = 0.2) +
  labs(
    title = "Average CO Levels by Season",
    subtitle = "With Standard Deviation Error Bars",
    x = "Season",
    y = "Average CO(GT)",
    caption = "Error bars represent ±1 standard deviation"
  ) +
  theme_minimal()

# Add this to your plot display section
seasonal_plot
```



Final Linear Model, Diagnostics & Interpretations

```
# Train final model on combined train + validation data
final_training_data <- bind_rows(train_data, validation_data)

# Final model with interactions
final_model <- linear_reg() |>
  set_engine("lm") |>
  fit(`CO(GT)` ~ `PT08.S1(CO)` * Season + `NOx(GT)` + `PT08.S5(O3)`,
      data = final_training_data)

# Evaluate on test set
final_metrics <- augment(final_model, new_data = test_data) |>
  summarize(
    rmse = sqrt(mean((`CO(GT)` - .pred)^2)),
    r2 = cor(`CO(GT)`, .pred)^2
  )

# Scatter for predicted vs actual
diagnostics_plot1 <- augment(final_model, new_data = test_data) |>
  ggplot(aes(x = .pred, y = `CO(GT)`)) +
  geom_point(alpha = 0.5) +
  geom_abline(color = "red", linetype = "dashed") +
  geom_label_repel(
```

```
    data = function(x) {
      x |>
        filter(abs(.resid) > quantile(abs(.resid), 0.99)) |>
        slice_max(order_by = abs(.resid), n = 3)
    },
    aes(label = round(.resid, 2)),
    box.padding = 0.5,
    max.overlaps = 3
  ) +
  labs(
    title = "Predicted vs Actual CO(GT) Values",
    subtitle = "Test Set Performance",
    x = "Predicted Values",
    y = "Actual Values",
    caption = "Red line indicates perfect prediction. Labels show largest residuals."
  ) +
  theme_minimal()

# Q-Q plot with enhancements
diagnostics_plot2 <- augment(final_model, new_data = test_data) |>
  ggplot(aes(sample = .resid)) +
  stat_qq() +
  stat_qq_line(color = "red") +
  labs(
    title = "Normal Q-Q Plot of Residuals",
    subtitle = "Assessing Normality of Residuals",
    x = "Theoretical Quantiles",
    y = "Sample Quantiles",
    caption = "Labels show extreme residuals"
  ) +
  theme_minimal()

# Residuals vs Fitted plot
diagnostics_plot3 <- augment(final_model, new_data = test_data) |>
  ggplot(aes(x = .pred, y = .resid)) +
  geom_point(alpha = 0.5, aes(color = abs(.resid))) +
  scale_color_viridis_c() +
  geom_hline(yintercept = 0, color = "red", linetype = "dashed") +
  geom_smooth(se = TRUE, color = "blue") +
  labs(
    title = "Residuals vs Fitted Values",
    subtitle = "Checking Homoscedasticity & Linearity",
    x = "Fitted Values",
    y = "Residuals",
    color = "Absolute\nResidual"
  ) +
  theme_minimal() +
  theme(legend.position = "right")

# Updated plot combination
final_diagnostics <- (diagnostics_plot1 | diagnostics_plot2) / diagnostics_plot3 +
  plot_layout(heights = c(2, 1.2)) +
  plot_annotation(
```

```
    title = "Model Diagnostic Plots",
    subtitle = sprintf("Final Model RMSE: %.3f | R²: %.3f | Performance on Test Set",
                       final_metrics$rmse, final_metrics$r2)
  ) &
  theme(plot.title = element_text(face = "bold"))

# Print model summary and diagnostics
print("Final Model Summary:")
```

```
## [1] "Final Model Summary:"
```

```
tidy(final_model) |>
  mutate(across(where(is.numeric), round, 4))
```

```
## Warning: There was 1 warning in `mutate()`.
## i In argument: `across(where(is.numeric), round, 4)`.
## Caused by warning:
## ! The `...` argument of `across()` is deprecated as of dplyr 1.1.0.
## Supply arguments directly to `.fns` through an anonymous function instead.
##
##   # Previously
##   across(a:b, mean, na.rm = TRUE)
##
##   # Now
##   across(a:b, \(x) mean(x, na.rm = TRUE))
```

```
## # A tibble: 10 x 5
##    term                        estimate std.error statistic p.value
##    <chr>                          <dbl>     <dbl>     <dbl>   <dbl>
##  1 (Intercept)                   0.737     0.0282    26.2     0
##  2 `PT08.S1(CO)`                 0.303     0.0333     9.11    0
##  3 SeasonSpring                  0.437     0.0257    17.0     0
##  4 SeasonSummer                  0.565     0.0288    19.6     0
##  5 SeasonWinter                 -0.114     0.0259    -4.42    0
##  6 `NOx(GT)`                     0.0045    0.0001    61.0     0
##  7 `PT08.S5(O3)`                 0.418     0.0251    16.6     0
##  8 `PT08.S1(CO)`:SeasonSpring   -0.0131    0.0327    -0.401   0.689
##  9 `PT08.S1(CO)`:SeasonSummer   -0.347     0.0338   -10.3     0
## 10 `PT08.S1(CO)`:SeasonWinter   -0.636     0.0301   -21.1     0
```

```
print("\nModel Performance Metrics:")
```

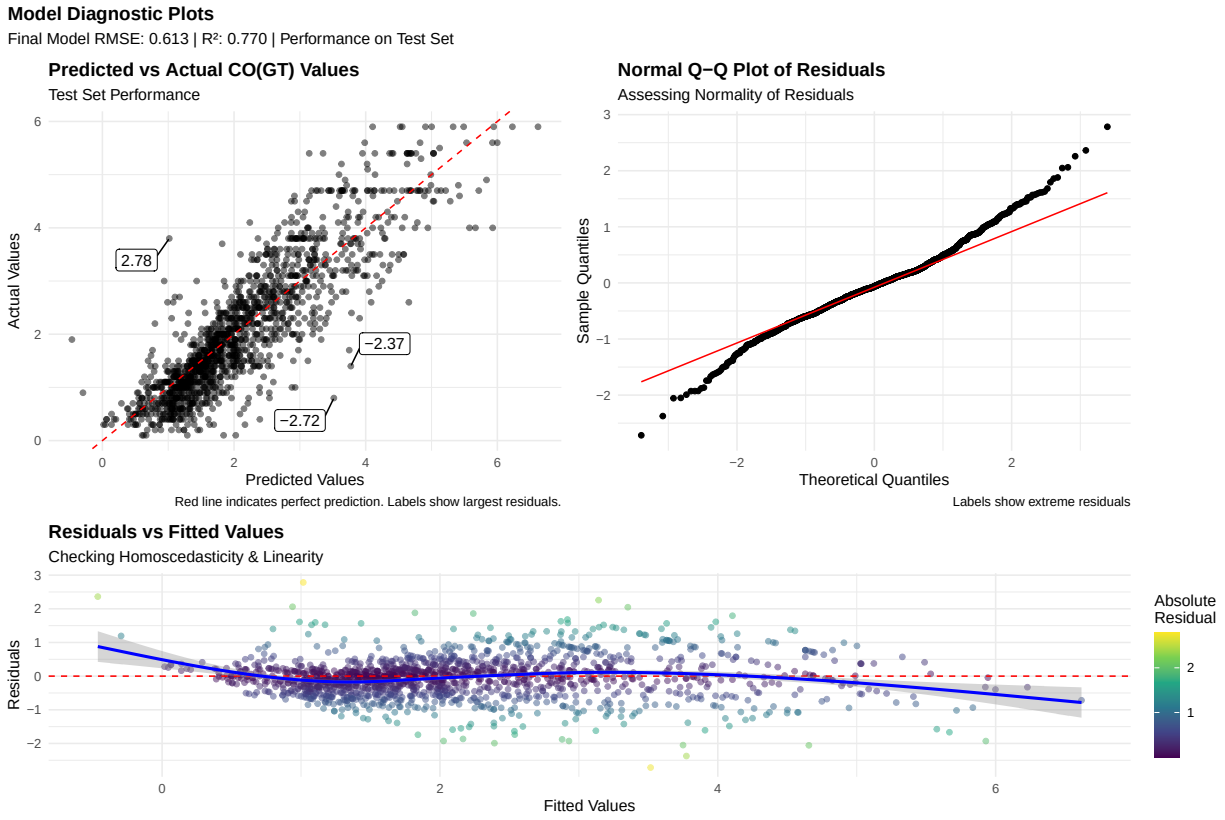
```
## [1] "\nModel Performance Metrics:"
```

```
final_metrics
```

```
## # A tibble: 1 x 2
##    rmse    r2
##   <dbl> <dbl>
## 1 0.613 0.770
```

```
# Display diagnostic plots
final_diagnostics
```

```
## `geom_smooth()` using method = 'gam' and formula = 'y ~ s(x, bs = "cs")'
```



Conclusions & Limitations

How do sensor measurements (PT08.S1(CO) and PT08.S5(O3)) correlate with observed pollutant levels (NOx(GT) and CO(GT))?

Can these relationships improve the accuracy of carbon monoxide concentration predictions?

Conclusions

The analysis directly addressed both research questions, revealing key insights about sensor correlations and prediction accuracy:

- Sensor pollutant correlations
  - CO sensor PT08.S1 showed strong correlation with CO(GT) levels
  - O3 sensor PT08.S5 showed significant correlation with CO levels, indicating important cross-sensitivity
  - NOx(GT) levels showed consistent positive correlation with CO(GT), though with a smaller magnitude

  - These correlations vary significantly by season, particularly the CO sensor, which shows reduced effectiveness in winter

- Prediction Accuracy Improvements
  - The inclusion of multiple sensor readings significantly improved prediction accuracy
  - Model comparison showed that incorporating both sensors & NOx(GT) greatly reduced RMSE (1.15 -> 0.603)
  - Final model achieved R^2 of 0.771, indicating that around 77% of CO variation can be explained using these sensor relationships
  - Seasonal interactions proved crucial, with the model capturing how sensor performance varise across different times of year

Limitations

- Data limitations
  - Missing values & sensor failures required extensive cleaning
  - GT measurements may contain their own uncertainties
  - Dataset may not capture extreme events
- Modeling limitations
- Linear model assumptions may oversimplify complex interactions in atmosphere
- The unexplained 23% variation suggests other imporant factors may be missing
- Residual analysis shows decreased accuracy at higher pollution levels
- Practical implementation limitations
  - Real-time standardization would be needed
  - Seasonal classification must be accurate
  - Multi-sensor dependence creates vulnerability to sensor failures