

Investigation of NO_x (in ppb), O₃ (in ppb), and PM_{2.5} (in µg/m³) trends in Ontario from 2003 to 2022

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1. Description of Datasets

The datasets analyzed in this report are three, one for each of NO_x (in ppb), PM_{2.5} (in µg/m³), and O₃ (in ppb), all containing the same variables. These datasets contain records of the pollutant levels from 2003 (considered the earliest of all three) to 2022. Each dataset contains detailed information of pollutant levels in the form of the following variables:

##	[1]	"Year"	"Station Number"	"City"	"Location"
##	[5]	"Type"	"Valid Hour"	"10th Percentile"	"30th Percentile"
##	[9]	"50th Percentile"	"70th Percentile"	"90th Percentile"	"99 Percentile"
##	[13]	"Mean"	"1-Hour Maximum"	"24-Hour Maximum"	

1. Year: The calendar year when the pollutant data was recorded.
2. Station Number: A unique numerical identifier for the monitoring station.
3. City: The name of the city where the pollutant was measured.
4. Location: A more specific description of the monitoring location (street, area).
5. Type: The type of monitoring station or measurement protocol used.
6. Valid Hour: The number of valid hourly measurements recorded for that pollutant in the given year.
7. Percentiles: Percentile statistics showing the distribution of pollutant levels (in ppb, µg/m³, ppb) throughout the year.
8. Mean: The annual average concentration of the pollutant (in ppb, µg/m³, ppb).
9. 1-Hour Maximum: The highest recorded concentration within a one-hour period during the year.
10. 24-Hour Maximum: The highest average concentration recorded over a 24-hour period in that year.

2. Background of the Data

The data used in this analysis was collected across various cities in Ontario, throughout the period from 2003 to 2022. These measurements were compiled and made available by the Ontario Ministry of the Environment, Conservation and Parks.

The information is publically available and is helpful in assisting researchers, policymakers, and public health officials to investigate air quality trends, evaluate the impact of environmental regulations, and inform policy decisions. It provides a long-term view of pollutant levels in various cities in Ontario, allowing for improving environmental and public health outcomes in Ontario.

3. Overall Research Question

The aim of this paper is to investigate the spatial and temporal trends of air pollutants (NO_x , O_3 , and $\text{PM}_{2.5}$) across various Ontario cities from 2003 to 2022.

1. How have annual mean concentrations (in ppb, $\mu\text{g}/\text{m}^3$, ppb) for each pollutant changed from 2003 to 2022, and which years show the most significant shifts?
2. Which cities consistently rank among the highest (or lowest) in terms of average pollutant levels, and do these rankings shift over time?
3. How do the four pollutants correlate with each other across different cities and years, and what might this indicate about broader air quality patterns?
4. How do the four pollutants project into future years based on current trends?

4. Tables

4.1 The Top 10 Cities With the Highest Pollutant Concentration

NO _x Table (in ppb)		O ₃ Table (in ppb)		PM _{2.5} Table (in $\mu\text{g}/\text{m}_3$)	
City	Conc.	City	Conc.	City	Conc.
Toronto West	31.32	Port Stanley	32.84	Sarnia	9.57
Toronto East	21.82	Tiverton	31.93	Windsor West	9.03
Toronto Downtown	20.41	Grand Bend	31.28	Hamilton Downtown	8.91
Toronto North	19.67	Parry Sound	30.56	Etobicoke West	8.44
Hamilton Downtown	19.36	Chatham	29.88	Windsor Downtown	8.36
Windsor Downtown	18.00	Belleville	29.63	Hamilton West	8.06
Burlington	17.74	Kingston	29.61	Hamilton Mountain	7.91
Hamilton West	17.63	Newmarket	29.13	Toronto West	7.86
Windsor West	16.89	Hamilton Mountain	28.61	Toronto North	7.59
Brampton	15.95	Peterborough	28.55	Kitchener	7.52

Table 1: Top 10 Cities with Highest Concentration of Each Pollutant

The table above is three separate tables each one for a respective pollutant, they are sorted in descending Mean and only the top 10 are being shown based on the overall Mean of the City, over all years from 2003 to 2022; as such, the cities with the high concentration will be listed first. Therefore, we can draw a few key observations about pollutant concentrations across these Ontario cities:

- The highest mean NO_x readings (31.32 ppb) appear at Toronto West, followed closely by other Toronto stations (Toronto East, Toronto Downtown) and industrial/urban areas like Hamilton and Windsor.
- Port Stanley shows the highest O_3 levels (32.84 ppb), with other high concentrations at Tiverton, Grand Bend, and Parry Sound—generally smaller or semi-rural communities.
- Sarnia tops the $\text{PM}_{2.5}$ list (9.57 $\mu\text{g}/\text{m}_3$), followed by Windsor (West and Downtown) and Hamilton stations, reflecting the influence of industrial facilities and cross-border pollution.

4.2 The Top 10 Regions and Years with Highest Concentration of Each Pollutant

In order to view the pollutant concentration changes by region, we grouped the cities by region based on the map of Ontario from the Ministry of Natural Resources and Forestry, and calculated the mean of the cities in each region grouped by year.

NO _x Table (in ppb)			O ₃ Table (in ppb)			PM _{2.5} Table (in µg/m ₃)		
Year	Region	Conc.	Year	Region	Conc.	Year	Region	Conc.
2003	Central Ontario	31.45	2010	Western Ontario	29.54	2005	Western Ontario	9.48
2005	Central Ontario	28.17	2022	Western Ontario	29.49	2014	Western Ontario	9.27
2003	Western Ontario	26.98	2007	Eastern Ontario	29.46	2003	Western Ontario	8.93
2004	Central Ontario	26.94	2010	Eastern Ontario	29.20	2015	Western Ontario	8.79
2006	Central Ontario	23.80	2021	Western Ontario	29.10	2013	Western Ontario	8.72
2007	Central Ontario	21.68	2018	Eastern Ontario	28.97	2005	Central Ontario	8.56
2004	Western Ontario	21.55	2012	Western Ontario	28.82	2004	Western Ontario	8.44
2008	Central Ontario	20.07	2016	Western Ontario	28.79	2014	Central Ontario	8.33
2005	Western Ontario	20.00	2013	Western Ontario	28.57	2007	Western Ontario	8.30
2004	Northern Ontario	19.04	2008	Eastern Ontario	28.54	2003	Central Ontario	8.26

Table 2: Top 10 Regions and Years with Highest Concentration of Each Pollutant

This table follows a similar format to the Table 1, listing the highest concentrations first. The concentrations of NO_x (in ppb) and PM_{2.5} (in µg/m₃) were highest in the early to mid-2000s, particularly in Western and Central Ontario, and have since declined. Meanwhile, O₃ (in ppb) levels are highest in Western Ontario dominating the top 10 with Northern Ontario not occupying a single spot. The O₃ concentrations show minor decrease, likely reflecting O₃ long lifespan in the atmosphere.

4.3 The Top 10 Years with Highest Concentration of Each Pollutant

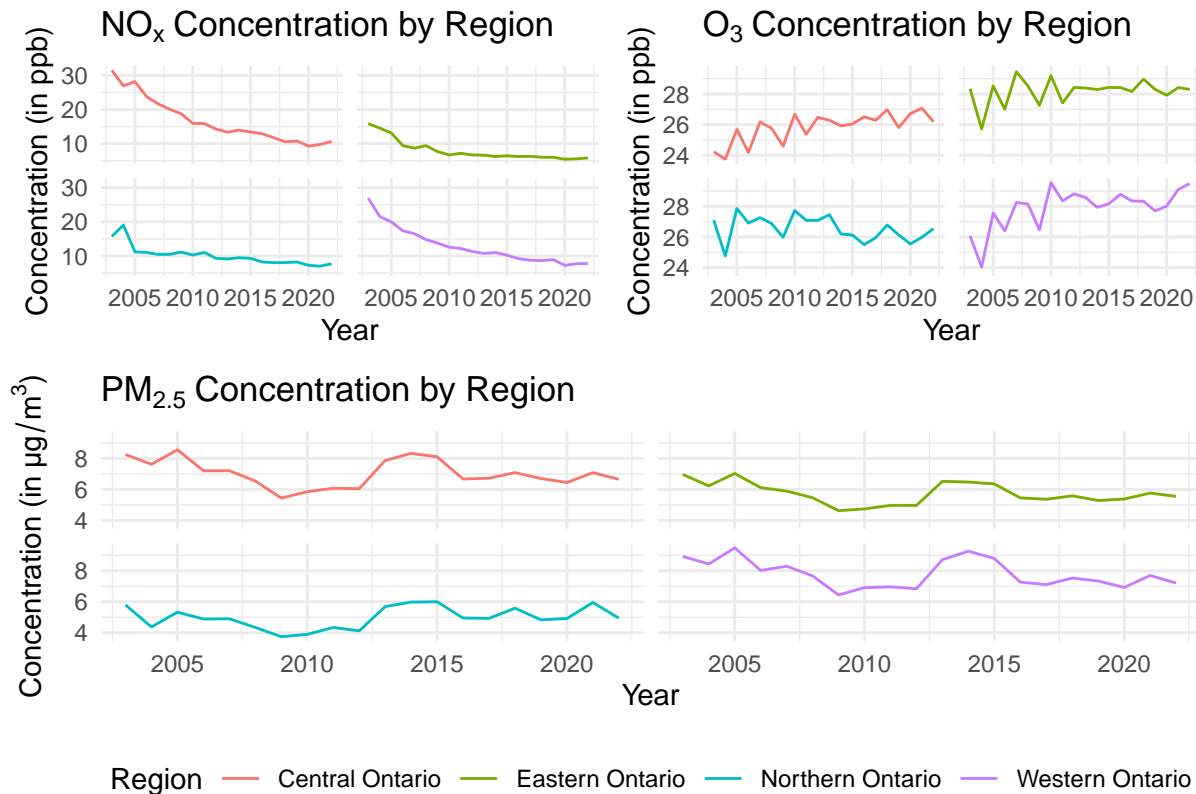
NO _x Table (in ppb)		O ₃ Table (in ppb)		PM _{2.5} Table (in µg/m ₃)	
Year	Conc.	Year	Conc.	Year	Conc.
2003	25.08	2010	28.41	2005	8.36
2004	23.42	2021	27.97	2003	8.04
2005	22.43	2018	27.88	2014	7.96
2006	17.87	2012	27.85	2015	7.73
2007	15.80	2007	27.83	2013	7.61
2008	15.04	2022	27.83	2004	7.30
2009	13.91	2013	27.73	2006	7.04
2011	12.36	2016	27.67	2007	7.03
2010	12.35	2017	27.43	2021	6.92
2012	11.23	2008	27.41	2018	6.78

Table 3: Top 10 Years with the Highest Concentration

The table reveals that NO_x levels peaked in 2003 – the first year of the dataset – and has steadily decreased since. Additionally, PM_{2.5} concentrations were highest in the mid-2000s before decreasing, and O₃ levels, which peaked around 2010–2012, have remained relatively high before a minor decrease in later years.

5. Graphs

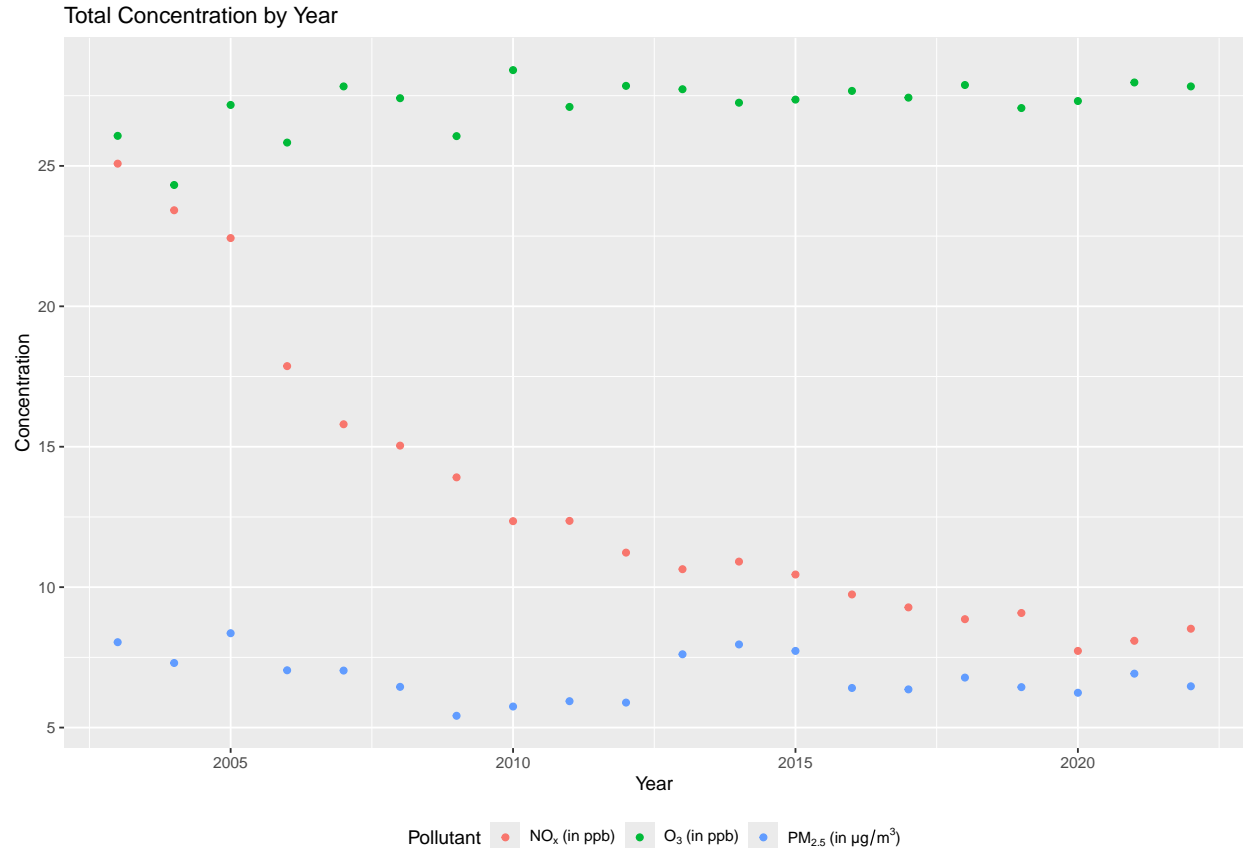
5.1 Line Charts of Yearly Concentration by Region



The Line Charts of Yearly Concentration by Region display the concentration of each pollutant faceted by region over 2003 till 2022. The x-axes represent the year and the y-axes represent the concentration of the pollutant at that year in its respective unit.

The graphs reveal a notable improvement in air quality over the years, with clear declines in both NO_x and PM_{2.5} levels across all regions, suggesting that emission controls and cleaner technologies have had a significant impact. NO_x concentrations show a consistent downward trend from higher levels in the early years, converging towards lower values by 2020, while PM_{2.5} levels exhibit a marked decrease, with the initial difference between regions decreasing over time. In contrast, O₃ concentrations appear relatively stable – with some fluctuations – which reflects the complex nature of ozone formation that depends on multiple factors such as sunlight, temperature, and precursor emissions.

5.2 Scatter Plot of Overall Pollutant Concentration by Year

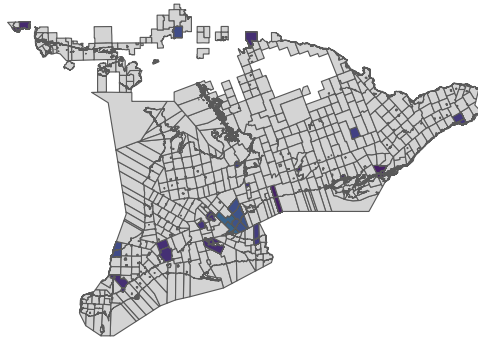


This Scatterplot of Overall Pollutant Concentration by Region displays the overall concentration, calculated by taking the mean of each year for all cities in the dataset, of each pollutant over 2003 till 2022. The x-axes represent the year and the y-axes represent the concentration of the pollutant at that year in its respective unit.

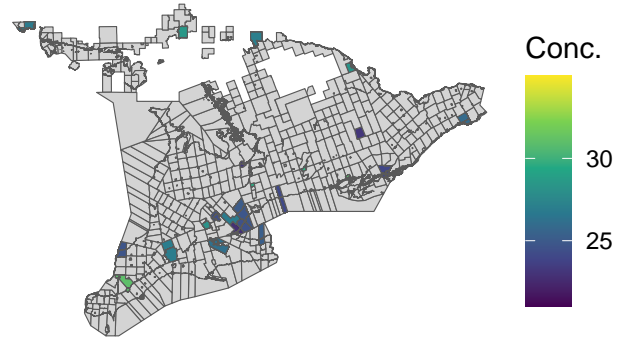
The plot reveals a downward trends of NO_x until 2020, with concentrations appearing to drop from around 25 ppb to near 8 ppb in 2020. This substantial decrease suggests that measures aimed at reducing emissions through regulations and increased standards have been effectively implemented over the years. On the other hand, PM_{2.5} and O₃ do not show a steady downward trend; instead, their concentrations fluctuate over the period analyzed. These fluctuations show the challenges in the efforts of controlling pollutants that are not directly emitted but are produced by chemical interactions in the atmosphere.

5.3 Heatmap

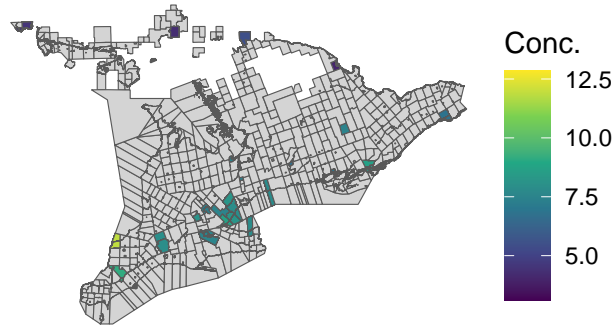
NO_x Concentration (in ppb)



O₃ Concentration (in ppb)



PM_{2.5} Concentration (in µg/m³)



The above graphs display the mean of each respective variable across Ontario cities. From these graphs, it can be surmised that NO_x is more concentrated in reporting cities than O₃, and both are more concentrated than PM_{2.5}.

6. Hypothesis Testing

Comparing the Pollutant Concentration in 2003 and 2022 in Each City

We would like to see if there is a difference between the mean pollutant level in each city in 2003 compared to 2022 (and if there is a difference, what kind of difference is present). For this test, since some cities stopped reporting over the years, we will only match up cities who have reported in both 2003 and 2022.

To achieve this, we will test the following hypothesis: - H_0 : the mean NOX level of cities in 2003 (μ_{2003}) is equal to the mean NOX level of cities in 2022 (μ_{2022}), i.e. $\mu_{2003} = \mu_{2022}$ or $\mu_{2003} - \mu_{2022} = 0$ - H_a : the mean NOX level of cities in 2003 (μ_{2003}) is not equal to the mean NOX level of cities in 2022 (μ_{2022}), i.e. $\mu_{2003} \neq \mu_{2022}$ or $\mu_{2003} - \mu_{2022} \neq 0$

To perform the test, we will perform a paired two sample t-test to see if the pollutant levels in each city has changes over the years. This can be done by taking the difference between the mean pollutant levels in each city in 2003 and in 2022 then performing a one sample t-test on the difference in mean pollutant levels.

```
##
## One Sample t-test
##
## data: values$diff
## t = 7.4834, df = 27, p-value = 4.748e-08
## alternative hypothesis: true mean is not equal to 0
## 95 percent confidence interval:
## 1.050617 1.844383
## sample estimates:
## mean of x
## 1.4475
```

Evaluation

The one sample t-test of the difference between the mean pollutant level in different cities in 2003 and 2022 shows a significant change in the mean pollutant levels in different cities over the years. The p-value of 4.748e-08 being less than 0.0001 suggests that there is significant evidence against the null hypothesis of there being no difference in the mean pollutant level in different cities over time. Likewise, since the null hypothesis of 0 is not within the 95% confidence interval of (1.050617, 1.844383), we have further evidence against the null hypothesis. Therefore, we can confidently reject the null hypothesis and conclude that over the years, there has been a change in the mean pollutant level in different cities in Canada.

7. Bootstrapping

Estimating the Average Concentration of Pollutants in 2022

To estimate the average concentration of pollutants in 2022, we can use bootstrapping to find a 95% confidence interval of the mean pollutants of the cities.

In order to use bootstrapping to find a 95% confidence interval, we will repeatedly take samples of the pollutants filtered for only the year 2022 and calculate the mean of each sample. This process of re-sampling will be repeated 1000 times to produce a sampling distribution for each pollutant. From the sample distribution, we can find 2.5% and 97.5% quantile.

```
## 1 ) Mean NOx concentration of: 8.523611 , 95% confidence interval for NOx is
## [ 7.219514 , 10.024604 ]
##
## 2 ) Mean O3 concentration of: 27.833947 , 95% confidence interval for O3 is
## [ 27.101816 , 28.608401 ]
##
## 3 ) Mean PM2.5 concentration of: 6.474474 , 95% confidence interval for PM2.5 is
## [ 6.140158 , 6.821632 ]
```

Based on the result, we have:

- 1) A mean NO_x concentration of 8.523611. A 95% confidence interval of [7.219514 , 10.0246] for the concentration of NO_x . This means that out of 100 samples, 95 samples will have a mean NO_x concentration between [7.219514 , 10.0246].
- 2) A mean O_3 concentration of 27.83395. A 95% confidence interval of [27.10182 , 28.6084] for the concentration of O_3 . This means that out of 100 samples, 95 samples will have a mean O_3 concentration between [27.10182 , 28.6084].

- 3) A mean $PM_{2.5}$ concentration of 6.474474. A 95% confidence interval of [6.140158 , 6.821632] for the concentration of $PM_{2.5}$. This means that out of 100 samples, 95 samples will have a mean $PM_{2.5}$ concentration between [6.140158 , 6.821632].

8. Regression

8.1 Analyzing the Relationship Between Pollutants and Year

In order to analyze the relationship of a pollutant with other pollutants and the year, we would treat the year and two pollutants as continuous variables to fit a regression. For example, if we were examining the relationship between the overall yearly NO_x concentration and the year, the O_3 concentration and the overall yearly $PM_{2.5}$ concentration, we will take the logarithm of the NO_x concentration as the dependent variable and the year, the overall yearly O_3 concentration and the overall yearly $PM_{2.5}$ concentration all as the independent variable.

```
##
## Call:
## lm(formula = formula(log(Conc.NOX) ~ Year + Conc.PM25 + Conc.O3),
##     data = Combined_Yearly_Mean)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.137814 -0.034320 -0.005249  0.022683  0.173198
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 105.538569   7.485517  14.099 1.93e-10 ***
## Year        -0.050618   0.003861 -13.110 5.65e-10 ***
## Conc.PM25     0.062989   0.023487   2.682  0.0164 *
## Conc.O3      -0.058474   0.023494  -2.489  0.0242 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.08013 on 16 degrees of freedom
## Multiple R-squared:  0.9584, Adjusted R-squared:  0.9506
## F-statistic: 122.9 on 3 and 16 DF,  p-value: 2.925e-11
```

From the linear model, it suggests that there is a strong relationship between the logarithm of the NO_x concentration and the year, the $PM_{2.5}$ concentration and the O_3 concentration. In particular, by analyzing the p-values of each parameter, it can be seen that the year parameter is especially significant and that the mean $PM_{2.5}$ and O_3 levels have moderate significance on the logarithm of the mean NO_x concentration in comparison. The coefficient of determination (R^2) of 0.9584 suggests that 95.84% of the variables in the logarithm of the NO_x concentration can be explained by the model.

8.2 Interpreting regression parameters

Here, the regression parameters refer to the coefficients of the independent variables of the model.

- 1) Intercept:

- The intercept coefficient expresses the value of the dependent variable (logarithm of the NO_x concentration) when all other features are equal to 0. In this case, an intercept of ~ 105.54 suggests that the logarithm of the NO_x concentration is equal to ~ 105.54 when all independent variables are equal to 0.

2) Year, Mean $\text{PM}_{2.5}$ Concentration, and Mean O_3 Concentration:

- The coefficient for Year expresses the linear effect of the Year parameter; specifically, a coefficient of -0.050621 suggests that as the Year increases by 1, the logarithm of the NO_x concentration decreases by 0.050621 . Similarly, a coefficient for the $\text{PM}_{2.5}$ level of 0.062955 and a coefficient for the O_3 level of -0.058456 suggests that as the $\text{PM}_{2.5}$ concentration increases by 1 and the O_3 level increases by 1 there will be an increase in the logarithm of the NO_x level by 0.062955 and a decrease in the logarithm of the NO_x level by 0.058456 , respectively.

Overall, this model suggests a strong linear relationship between the logarithm of the mean NO_x level and the year, the mean $\text{PM}_{2.5}$ level and the mean O_3 level. In other words, this model also explains that the NO_x concentration has an exponential relationship with the features used, in particular an exponential decay relationship with the year.

9. Cross Validation

Previously, we analyzed the regression parameters to see how well our model performed on our data set. In this case, we will further analyze the relationships of pollutants with each other and the year by performing cross validation.

Specifically, we will analyze the relationship between $\text{PM}_{2.5}$ and the other pollutants alongside the year by using k-fold cross validation. To perform k-fold cross validation, we will split the data set into k even pieces and use each i^{th} fold to check the validity of our model that is trained on the remaining $k - 1$ folds by taking predictions using the data in the i^{th} fold. This process will be repeated for each fold of the data set, a mean squared error (MSE) will be calculated for each fold, and an average of the MSE's will be taken at the end.

The average MSE is: 0.5452378

Conclusion on Results

The average MSE from the k-fold cross validation was 0.5452296 which is relatively low and maybe indicate the moderate predicting power of the linear model where the $\text{PM}_{2.5}$ level was the dependent variable with year, NO_x concentration and the O_3 concentration were the independent variables. This suggests that there is likely a linear relationship between the $\text{PM}_{2.5}$ concentration, the year, NO_x concentration and O_3 concentration.

10. Summary of Research

Below are the key findings from the analysis:

- Our investigation into the trends of NO_x (in ppb), O_3 (in ppb), and $\text{PM}_{2.5}$ (in $\mu\text{g}/\text{m}^3$) in Ontario from 2003 to 2022 has yielded several important insights into both temporal and spatial patterns in air quality across the province.
- The annual mean concentrations reveal that NO_x levels peaked in 2003 and have steadily declined over the years, with a marked reduction by 2020. $\text{PM}_{2.5}$ concentrations also significantly declining from the early to mid-2000s, suggesting effective emission controls and cleaner technologies.

- O₃ levels have remained relatively stable, with only minor fluctuations around 2010–2012, largely because O₃ is a secondary pollutant formed by chemical reactions that depend on environmental and chemical factors.
- Analysis of the top 10 cities by mean concentration shows that major urban centers—such as Toronto and Hamilton—consistently rank among the highest for NO_x, while Sarnia, Windsor, and Hamilton stand out for PM_{2.5}. Smaller or semi-rural communities (e.g., Port Stanley, Tiverton) tend to show the highest O₃ levels.
- The scatter plots and regression analyses indicate a strong correlation between NO_x and the other pollutants when viewed over time. Both NO_x and PM_{2.5} exhibit clear downward trends, whereas O₃ remains more variable.
- A regression model using the logarithm of NO_x as the dependent variable confirms that PM_{2.5}, O₃, and the year are significant predictors ($R^2 = 0.96$). This underscores how reducing primary pollutants (NO_x) can improve PM_{2.5} levels but has a less pronounced impact on O₃, given the latter's complex atmospheric formation.
- Extrapolating from current trends suggests that NO_x and PM_{2.5} concentrations will continue to decline if emission controls and cleaner technologies persist. However, O₃ may remain relatively stable unless additional targeted measures are implemented.

11. Appendix

```
# Loading libraries
library(tidyverse)
library(readxl)
library(patchwork)
library(lubridate)
library(kableExtra)
library(ggplot2)
library(lubridate)
library(knitr)
library(stringr)
library(gridExtra)
library(sf)
library(viridis)
library(purrr)
library(cowplot)

# Reading in all data excel files
NOX <- read_excel("./data/NOX.xlsx", skip = 3)
O3 <- read_excel("./data/O3.xlsx", skip = 3)
PM25 <- read_excel("./data/PM25.xlsx", skip = 5)
# 1. Description of the Dataset Columns
names(NOX)
# 2. Background of the Data: No code for this section
# 3. Overall Research Question
# Create a dataframe that contains the mapping of each city to it's region
city_to_region <- data.frame(City = c(
  # Western Ontario
  "Windsor West", "Windsor Downtown", "Windsor North", "Grand Bend", "London",
  "Chatham", "Sarnia", "Brantford", "Kitchener",
```

```

"St. Catharines", "St. Catherines", "Port Stanley", "Essex", "Hamilton Mountain",
"Hamilton Downtown", "Hamilton West", "Guelph",
# Central Ontario
"Toronto Downtown", "Toronto East", "Toronto North", "Toronto West", "Burlington",
"Oakville", "Oshawa", "Brampton", "Mississauga",
"Newmarket", "Milton", "Etobicoke West", "Stouffville", "Barrie", "Parry Sound",
"Peterborough",
# Eastern Ontario
"Ottawa Downtown", "Ottawa Central", "Kingston", "Tiverton", "Belleville",
"Cornwall", "Dorset", "Petawawa", "Morrisburg",
# Northern Ontario
"Sudbury", "Sault Ste. Marie", "North Bay", "Thunder Bay"
), Region = c(
  rep("Western Ontario", 17),
  rep("Central Ontario", 15),
  rep("Eastern Ontario", 10),
  rep("Northern Ontario", 4)), stringsAsFactors = FALSE)
# Mutate datasets to have numeric means, years, and only contain data from 2003 onwards
NOX = NOX %>% mutate(Mean = as.numeric(Mean)) %>%
  filter(Year >= 2003)
O3 = O3 %>% mutate(Mean = as.numeric(Mean)) %>%
  filter(Year >= 2003)
PM25 = PM25 %>% mutate(Mean = as.numeric(Mean)) %>%
  mutate(Year = as.integer(Year)) %>% filter(Year >= 2003)
# Remove all rows with a non-numeric mean
O3 = O3 %>% drop_na(Mean)
NOX = NOX %>% drop_na(Mean)
PM25 = PM25 %>% drop_na(Mean)
# Join all data to city-region-mapping to convert cities into regions
NOX = NOX %>% left_join(city_to_region, by = "City")
O3 = O3 %>% left_join(city_to_region, by = "City")
PM25 = PM25 %>% left_join(city_to_region, by = "City")

# Make tables
# Mean per years for that particulate matter
NOX_City_mean <- NOX %>% group_by(City) %>% summarise(Conc. = mean(Mean))
O3_City_mean <- O3 %>% group_by(City) %>% summarise(Conc. = mean(Mean))
PM25_City_mean <- PM25 %>% group_by(City) %>% summarise(Conc. = mean(Mean))

# 4. Tables
# 4.1 The Top 10 Cities With the Highest Pollutant Concentration
# Display tables of most relevant cities from datasets arranged in descending order
NOX_table <- kable(NOX_City_mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
O3_table <- kable(O3_City_mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
PM25_table <- kable(PM25_City_mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
# Summarise data by determining the mean of each region over all years
NOX_Region = NOX %>% group_by(Year, Region) %>% summarise(Conc. = mean(Mean))
O3_Region = O3 %>% group_by(Year, Region) %>% summarise(Conc. = mean(Mean))
PM25_Region = PM25 %>% group_by(Year, Region) %>% summarise(Conc. = mean(Mean))

```

```

# 4.2 The Top 10 Regions and Years with Highest Concentration of Each Pollutant
# Display tables from datasets of the most relevant regions arranged in descending order
NOX_tab <- kable(NOX_Region %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
O3_tab <- kable(O3_Region %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
PM25_tab <- kable(PM25_Region %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")

# 4.3 The Top 10 Years with Highest Concentration of Each Pollutant
# Summarise data by determining mean of all regions/cities over every year
NOX_Yearly_Mean = NOX %>% group_by(Year) %>% summarise(Conc. = round(mean(Mean), 2))
O3_Yearly_Mean = O3 %>% group_by(Year) %>% summarise(Conc. = round(mean(Mean), 2))
PM25_Yearly_Mean = PM25 %>% group_by(Year) %>% summarise(Conc. = round(mean(Mean), 2))
# Display tables from datasets of the yearly mean of each respective particle
NOX_tab <- kable(NOX_Yearly_Mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
O3_tab <- kable(O3_Yearly_Mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")
PM25_tab <- kable(PM25_Yearly_Mean %>% mutate(Conc. = round(Conc., 2)) %>%
  arrange(desc(Conc.)) %>% head(10), "latex")

# 5. Graphs
# 5.1 Line Charts of Yearly Concentration by Region
# Display graphs of concentration of each respective particle over the years per region
plot_NOX <- ggplot(NOX_Region, aes(x = Year, y = Conc., col = Region)) +
  geom_line() +
  facet_wrap(~ Region) +
  labs(title = expression(NO[x] ~ "Concentration by Region"), x = "Year",
    y = "Concentration (in ppb)") +
  theme_minimal() +
  theme(legend.position = "none", strip.text = element_blank())

plot_O3 <- ggplot(O3_Region, aes(x = Year, y = Conc., col = Region)) +
  geom_line() +
  facet_wrap(~ Region) +
  labs(title = expression(O[3] ~ "Concentration by Region"), x = "Year",
    y = "Concentration (in ppb)") +
  theme_minimal() +
  theme(legend.position = "none", strip.text = element_blank())

plot_PM25 <- ggplot(PM25_Region, aes(x = Year, y = Conc., col = Region)) +
  geom_line() +
  facet_wrap(~ Region) +
  labs(title = expression(PM[2.5] ~ "Concentration by Region"), x = "Year",
    y = expression("Concentration (in " * g / m^3 * ")")) +
  theme_minimal() +
  theme(legend.position = "none", strip.text = element_blank())

(plot_NOX | plot_O3) / plot_PM25 +
  plot_layout(guides = "collect") & theme(legend.position = "bottom")

# 5.2 Scatter Plot of Overall Pollutant Concentration by Year

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# Store all yearly means for each respective particle
Yearly_Means = list(NOX_Yearly_Mean, PM25_Yearly_Mean, O3_Yearly_Mean)
# Merge all data by year
Combined_Yearly_Mean = reduce(Yearly_Means, full_join, by = "Year")
# Rename columns for ease of use
Combined_Yearly_Mean = Combined_Yearly_Mean %>%
  rename(Conc.NOX = Conc..x, Conc.PM25 = Conc..y, Conc.O3 = Conc.)
# Reshape data into longer format
Graphing_Yearly_Means <- Combined_Yearly_Mean %>%
  pivot_longer(cols = starts_with("Conc."),
    names_to = "Pollutant",
    values_to = "Value")
# Graph yearly mean concentration of each particle over time
ggplot(Graphing_Yearly_Means,
  aes(x = Year, y = Value,
    col = factor(Pollutant,
      levels = c("Conc.NOX", "Conc.O3", "Conc.PM25")))) +
  geom_point() +
  labs(col = "Pollutant", y = "Concentration", title = "Total Concentration by Year ") +
  # scale_color_discrete(labels = c(expression(NO[x] ~ "(in ppb)"),
  #   expression(O[3] ~ "(in ppb)"), expression(PM[2.5] ~ "(in " ~ g/m^3 *
  #   ")")) + theme(legend.position = "bottom")

# 5.3 Heatmap of Mean Particle Concentration over all Time Accross Ontario
group_cities <- function(data, exclude_cities){
  grouped_data <- data %>%
    filter(!City %in% exclude_cities) %>%
    # Exclude the cities from the dataset
    bind_rows(
      data %>%
        # Get only the two cities we want, group their year rows, get their means and turn them into one
        filter(City %in% exclude_cities) %>%
        group_by(Year) %>%
        # take mean of each column accross the row
        summarise(across(where(is.numeric), ~mean(.x, na.rm = TRUE)), .groups = "drop") %>%
        # fix the city name to be a combo of all cities
        mutate(City = paste(exclude_cities, collapse = "-"))
    )
  return(grouped_data)
}
NOX_LL <- read_excel("./data/NOX.xlsx", skip = 3) %>% mutate(Mean = as.numeric(Mean)) %>%
  filter(Year >= 2003) %>% drop_na(Mean) %>%
  mutate(Year = as.integer(Year)) %>%
  group_by(Year, City) %>%
  summarise(Mean = mean(Mean, na.rm = TRUE))
# Load Ontario shapefile
Ontario <- st_read("data/shape")
Ontario <- Ontario %>%
  rename(City = NAME)
# Change CRS for Ontario
st_crs(Ontario) <- 4326
# Store city groupings
subgroupings = list(c("Toronto Downtown", "Toronto East", "Toronto West", "Toronto North"),

```

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        c("Hamilton Downtown", "Hamilton West", "Hamilton Mountain"),
        c("Windsor Downtown", "Windsor West"),
        c("Ottawa Downtown", "Ottawa Central"))
# Define the function
process_and_plot <- function(data, data_name) {
  # Group subcities into one city
  for (subgroup in subgroupings) {
    data <- group_cities(data, subgroup)
  }
  # Convert city name to uppercase
  data$City <- toupper(as.character(data$City))
  # Join each data set with the shapefile
  merged_data <- Ontario %>%
    left_join(data, by = "City") %>%
    st_as_sf()
  # Filter out any remote data point outliers
  coords <- st_coordinates(merged_data)
  merged_data <- merged_data %>%
    mutate(max_lat = map_dbl(geometry, ~ max(st_coordinates(.x)[,2]))) %>%
    filter(max_lat <= 47) %>%
    select(-max_lat)
  # Select only relevant columns in data
  merged_data <- merged_data %>%
    select(Year, City, Mean, SHAPE_Area, SHAPE_Leng, geometry)
  # Plot
  return( ggplot() +
    geom_sf(data = merged_data, aes(fill = Mean)) +
    scale_fill_viridis_c() +
    theme_minimal() +
    labs(
      title = paste("Mean Value of", data_name, "Over Time"),
      fill = "Mean Value"
    )
  )
}

# Datalist
datalist <- list(
  list(NOX_LL, "NOX"),
  list(O3, "O3"),
  list(PM25, "PM25")
)

result_list <- list() # Create an empty list
# Loop through and call the function

for (i in seq_along(datalist)) {
  # Process each item and store the result
  p <- process_and_plot(datalist[[i]][[1]], datalist[[i]][[2]])
  result_list[[i]] <- p
}

# TODO: render the graphs side by side
plot_grid(result_list[[1]], result_list[[2]])
# 6. Hypothesis Testing

```

```

# Estimating the average of the Mean NOX over year X
# Set random seed so that results are reproduceable
set.seed(123)

# Filter datasets for only the year 2022
NOX_2022 <- NOX %>% filter(Year == 2022) %>% select(Mean)
O3_2022 <- O3 %>% filter(Year == 2022) %>% select(Mean)
PM25_2022 <- PM25 %>% filter(Year == 2022) %>% select(Mean)

# Bootstrap function that will repeated take samples
boot_function <- function() {
  boot_sample_NOX = sample_n(NOX_2022, nrow(NOX_2022), replace=T)
  boot_sample_O3 = sample_n(O3_2022, nrow(O3_2022), replace=T)
  boot_sample_PM25 = sample_n(PM25_2022, nrow(PM25_2022), replace=T)
  return (c(mean(boot_sample_NOX$Mean), mean(boot_sample_O3$Mean),
            mean(boot_sample_PM25$Mean)))
}

# Combine all bootstrap means into a dataframe
bootstrap_bar = as.data.frame(replicate(1000, boot_function()))
columns = c("NO", "O2083", "PM20802085")
for (i in 1:3) {
  # Flatten rows of dataframe into a column vectors
  vec = as.vector(as.matrix(bootstrap_bar[i,]))
  # Find the 2.5% and 97.5% quantile
  conf = quantile(vec, c(0.025, 0.975))
  cat("95% confidence interval for", columns[i], "is", "[", conf[1], ",",
      conf[2], "]", "\n")
}

# 7. Bootstrapping
# Estimating the Average Concentration of Pollutants in 2022
# Estimating the average of the Mean NOX over year X
# Set random seed so that results are reproduceable
set.seed(123)

# Filter datasets for only the year 2022
NOX_2022 <- NOX %>% filter(Year == 2022) %>% select(Mean)
O3_2022 <- O3 %>% filter(Year == 2022) %>% select(Mean)
PM25_2022 <- PM25 %>% filter(Year == 2022) %>% select(Mean)

# Bootstrap function that will repeated take samples
boot_function <- function() {
  boot_sample_NOX = sample_n(NOX_2022, nrow(NOX_2022), replace=T)
  boot_sample_O3 = sample_n(O3_2022, nrow(O3_2022), replace=T)
  boot_sample_PM25 = sample_n(PM25_2022, nrow(PM25_2022), replace=T)
  return (c(mean(boot_sample_NOX$Mean), mean(boot_sample_O3$Mean), mean(boot_sample_PM25$Mean)))
}

# Combine all bootstrap means into a dataframe
bootstrap_bar = as.data.frame(replicate(1000, boot_function()))
columns = c("NOX", "O3", "PM25")
datasets = c(NOX_2022, O3_2022, PM25_2022)

```

```

for (i in 1:3) {
  # Flatten rows of dataframe into a column vectors
  vec = as.vector(as.matrix(bootstrap_bar[i,]))
  # Find the 2.5% and 97.5% quantile
  conf = quantile(vec, c(0.025, 0.975))
  cat(i, " ", "Mean", columns[i], "concentration of:", mean(datasets[i]$Mean), ",",
      "95% confidence interval for", columns[i], "is", "[", conf[1], ",", conf[2], "]", "\n")
}

# 8. Regression
# 8.1 Analyzing the Relationship Between Pollutants and Year
NOX_other_pollutant_model = lm(formula(log(Conc.NOX)~Year + Conc.PM25 + Conc.O3),
                                data = Combined_Yearly_Mean)
summary(NOX_other_pollutant_model)
# 8.2 Interpreting regression parameters: No code for this section
# 9. Cross Validation
set.seed(123)
k_fold_mse = rep(0, 5)
# Split data into 5 folds
Combined_Yearly_Mean <- Combined_Yearly_Mean %>%
  mutate(group_ind = sample(c(1:5),size=nrow(Combined_Yearly_Mean), replace=TRUE))

for (i in 1:5) {
  # train on fold all fold not i then test on fold i
  train_set <- Combined_Yearly_Mean %>% filter(group_ind != i)
  test_set <- Combined_Yearly_Mean %>% filter(group_ind == i)
  NOX_other_pollutant_model = lm(formula(Conc.PM25~Year + Conc.NOX + Conc.O3), data = train_set)
  pred = predict(NOX_other_pollutant_model, newdata=test_set)
  # mse = mean((test_set$Conc.PM25 - pred)^2)
  k_fold_mse[i] = mse
}
cat("The average MSE is:", mean(k_fold_mse), "\n")
# 10. Summary of Research: No code for this section

```