# Forecasting and time variability analysis of Ozone concentrations using nitrogen oxide and meteorological variables as predictors

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# **CEE 492 Final Project Selection**

#### 1. Dataset description:

The dataset used in this project is a CSV file about the air quality in northern Taiwan collected in 2015 [https://www.kaggle.com/datasets/nelsonchu/air-quality-in-northern-taiwan], which include air quality data and meteorological monitoring data for research and analysis, originally from Environmental Protection Administration, Executive Yuan, R.O.C. (Taiwan). There are 25 observation stations in total. Columns in this CSV file are the following:

- 1. Time The first column is the observation time of 2015
- 2. Station The second column is the station name, there are 25 observation stations, those stations are showing at the table  $\underline{1}$ .

Table 1: A table contain all stations in Taiwan.

		station		
Banqiao	Cailiao	Datong	Dayuan	Guanyin
Guting	Keelung	Longtan	Pingzhen	Sanchong
Shilin	Songshan	Tamsui	Taoyuan	Tucheng
Wanhua	Wanli	Xindian	Xinzhuang	Xizhi
Yangming	Yonghe	Zhongli	Zhongshan	Linkou

3. Items - From the third column to the last one

#### 4. item - unit - description

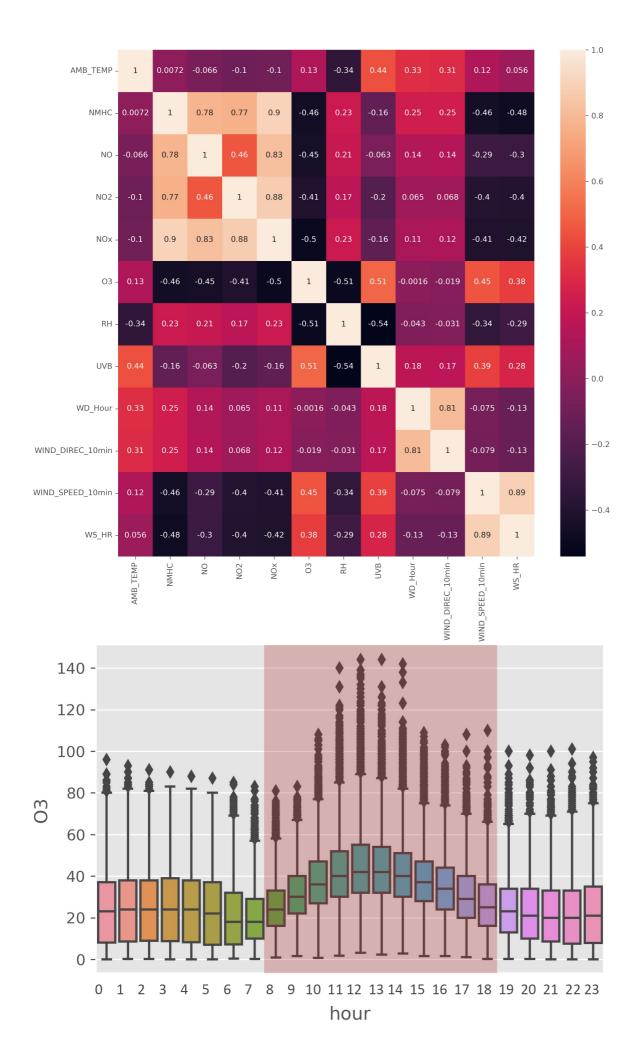
- SO<sub>2</sub> ppb Sulfur dioxide
- CO ppm Carbon monoxide
- O<sub>3</sub> ppb ozone
- PM<sub>10</sub> μg/m<sup>3</sup> Particulate matter
- PM<sub>2.5</sub> μg/m<sup>3</sup> Particulate matter
- NO<sub>x</sub> ppb Nitrogen oxides
- NO ppb Nitric oxide
- NO<sub>2</sub> ppb Nitrogen dioxide
- THC ppm Total Hydrocarbons
- NMHC ppm Non-Methane Hydrocarbon
- CH4 ppm Methane
- UVB UVI Ultraviolet index
- AMB\_TEMP Celsius Ambient air temperature
- RAINFALL mm
- RH % Relative humidity
- WIND\_SPEED m/sec The average of the last ten minutes per hour
- WIND\_DIREC degrees The average of the last ten minutes per hour
- WS\_HR m/sec The average of an hour
- WD\_HR degrees The average of an hour
- PH\_RAIN PH Acid rain
- RAIN\_COND μS/cm Conductivity of acid rain

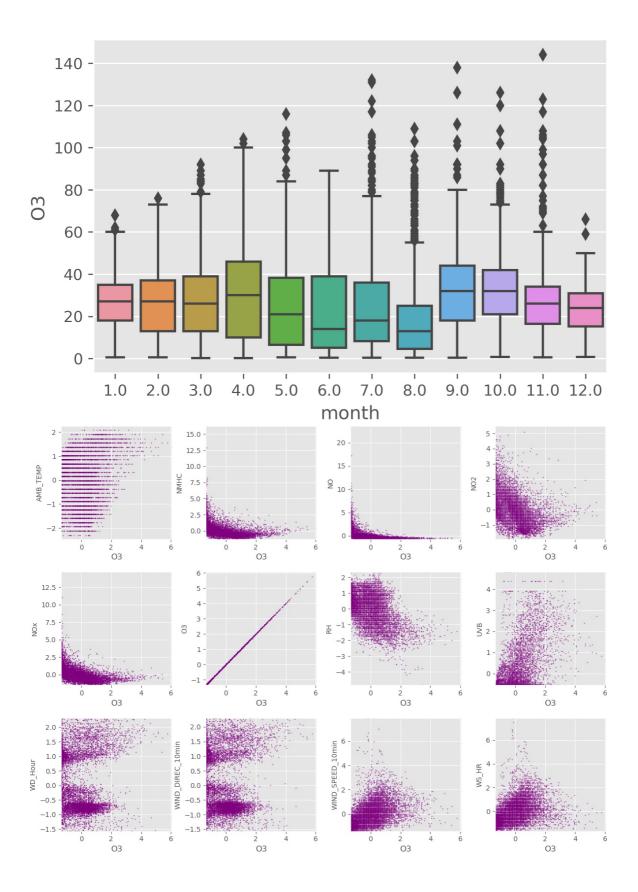
# **Proposal:**

The purpose of this project is to predict  $O_3$  concentrations using measurements of concentration of other pollutants and available meteorological measurements. Ozone might be formed when heat and sunlight cause chemical reactions between oxides of nitrogen ( $NO_x$ ) and Volatile Organic Compounds (VOC), which are also known as Hydrocarbons. Therefore it could be hypothesized that using measurements of  $NO_x$  as an independent variable a model could be developed to predict  $O_3$  concentrations. Additionally, meteorological variables such as air temperature, relative humidity(RH) and ultraviolet index (UVB - UVI) could be included as independent variables to assess their influence on temporal variability of ozone. As an additional step wind-related variables such as mean wind velocity and direction will be included to study their effect on temporal variability of ozone.

After the air quality data has been processed the strongest  $O_3$  predictors will be determined using PCA. PCA could be used to identify the main axes of variance within the dataset and explore underlying correlations that exist in a set of variables. Variables that are highly correlated cluster together. Using PCA 2D figures per each pair of variables are not needed, instead all the variables could be visualized simultaneously. Differences on PC1 are more important than differences on PC2. After plotting PCA plots, a heatmap could also be plotted to check the results. As additional criteria to identify the strongest predictors a LSTM network (long short-term memory network) can be used since the data used is time dependent. The network should contain several LSTM layers and fully-connected layers. The output should contain the pollution concentration and will point out the weights assigned to each correlated criterion, the values of such weights should also indicate what the strongest predictors are. Once the strongest predictors have been identified, genetic programming will be used to develop the models to predict  $O_3$  concentrations.

# **Exploratory Data Analysis:**





	Dependent Variable				Independent variable: Metereological variables								
Station	О3	NMHC	NO	NO2	NOx	Temperature	RH	UVB	W Direction 10 min	W Speed 10min	W Speed hourly	Wind Direction hourly	Average Fraction
Banqiao	0.991	0.984	0.966	0.966	0.966	0.991	0.991	0.991	0.991	0.991	0.991	0.991	0.984
Cailiao	0.978	0.000	0.958	0.958	0.958	0.977	0.978	0.000	0.977	0.977	0.977	0.977	0.794
Dayuan	0.988	0.000	0.975	0.975	0.975	0.980	0.955	0.000	0.852	0.910	0.922	0.922	0.770
Guanyin	0.980	0.000	0.969	0.969	0.969	0.973	0.980	0.000	0.977	0.980	0.979	0.977	0.798
Guting	0.988	0.966	0.983	0.983	0.983	0.985	0.983	0.000	0.985	0.985	0.985	0.985	0.901
Keelung	0.987	0.970	0.977	0.977	0.977	0.977	0.980	0.000	0.986	0.986	0.986	0.986	0.891
Linkou	0.973	0.000	0.966	0.966	0.966	0.973	0.973	0.000	0.972	0.972	0.964	0.972	0.793
Longtan	0.982	0.000	0.961	0.961	0.961	0.982	0.982	0.000	0.982	0.982	0.981	0.981	0.798
Pingzhen	0.988	0.000	0.968	0.968	0.968	0.988	0.988	0.000	0.983	0.988	0.988	0.988	0.802
Shilin	0.983	0.000	0.957	0.957	0.957	0.983	0.983	0.000	0.983	0.983	0.980	0.983	0.797
Songshan	0.985	0.967	0.976	0.976	0.976	0.985	0.985	0.000	0.984	0.984	0.984	0.984	0.891
Tamsui	0.961	0.000	0.956	0.956	0.956	0.000	0.000	0.961	0.000	0.000	0.000	0.000	0.348
Taoyuan	0.983	0.958	0.976	0.976	0.976	0.982	0.982	0.976	0.982	0.982	0.982	0.982	0.978
Tucheng	0.981	0.974	0.965	0.965	0.965	0.980	0.981	0.000	0.980	0.980	0.980	0.980	0.886
Wanhua	0.986	0.000	0.979	0.979	0.979	0.986	0.986	0.000	0.986	0.986	0.986	0.986	0.805
Wanli	0.984	0.000	0.976	0.976	0.976	0.983	0.976	0.000	0.976	0.982	0.983	0.975	0.800
Xindian	0.985	0.000	0.979	0.979	0.979	0.985	0.982	0.000	0.985	0.985	0.985	0.985	0.804
Xinzhuang	0.978	0.000	0.970	0.970	0.970	0.978	0.978	0.000	0.978	0.978	0.978	0.978	0.798
Xizhi	0.963	0.000	0.954	0.954	0.954	0.962	0.962	0.000	0.962	0.962	0.958	0.958	0.784
Yangming	0.979	0.000	0.964	0.964	0.964	0.979	0.979	0.000	0.000	0.000	0.000	0.000	0.441
Yonghe	0.987	0.972	0.978	0.978	0.978	0.984	0.987	0.000	0.987	0.987	0.987	0.987	0.893
Zhongli	0.988	0.973	0.967	0.967	0.967	0.986	0.986	0.000	0.986	0.986	0.985	0.985	0.890
Zhongshan	0.986	0.976	0.976	0.976	0.976	0.986	0.986	0.000	0.986	0.986	0.986	0.986	0.893

 Table 2: Descriptive statistics of features that compose in this analysis

	count	mean	std	min	25%	50%	75%	max
AMB_TEMP	8682	1.18E-15	1.00	-2.47	-0.89	0.15	0.68	2.25
NMHC	8619	-4.74E-15	1.00	-1.32	-0.62	-0.30	0.29	16.26
NO	8462	3.20E-15	1.00	-0.75	-0.50	-0.32	0.05	23.55
NO2	8462	1.56E-15	1.00	-1.94	-0.78	-0.10	0.57	5.48
NOx	8462	1.62E-15	1.00	-1.54	-0.69	-0.20	0.42	14.67
О3	8685	-8.78E-16	1.00	-1.35	-0.80	-0.07	0.54	6.06
RH	8684	-1.56E-15	1.00	-4.85	-0.75	0.17	0.76	2.35
UVB	8684	3.53E-15	1.00	-0.56	-0.56	-0.56	0.12	4.81
WD_Hour	8680	2.64E-16	1.00	-1.58	-0.78	-0.59	1.01	2.32
WIND_DIREC_10min	8682	6.96E-16	1.00	-1.56	-0.78	-0.58	1.01	2.31
WIND_SPEED_10min	8682	-6.21E-15	1.00	-1.43	-0.72	-0.18	0.53	7.92
WS_HR	8680	-2.83E-15	1.00	-1.67	-0.80	-0.12	0.56	7.86

# **Predictive Modeling**

The independent variables were segmented in pollutants and meteorological measurements. In order to visualize how the measurements change throughout the year the values were average per month. Then the resulting values were standardized using their mean. Once the values were standardized they were plotted against time.

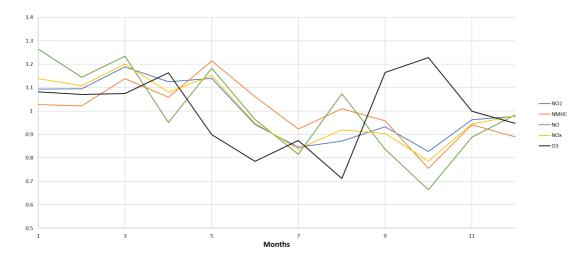


Figure 1: Standardized pollutants and ozone monthly concentration changes

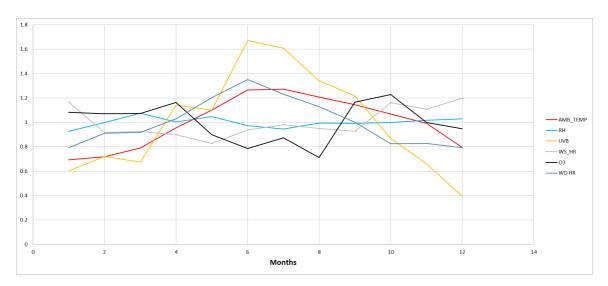


Figure 2: Standardized meteorological measurements and standardized ozone monthly concentration changes

As seen in the previous figure, O3 peaked in the months when concentration of the nitrogen based pollutants and non-methane hydrocarbons dropped. This is especially the case for NO concentrations (green line). This pattern of corresponding decreasing pollutant concentrations and increasing ozone could suggest that the pollutant concentrations are negatively correlated with ozone concentrations. This is also consistent with figure 1 (correlation plot)

In regards to the meteorological variables, UVB (ultraviolet index) and air temperature peak in the same months. Both temperature and UVB experience and increase in their values from the beginning of the year peaking in June. After June, both values experience a steady decrease. No discernable pattern can be observed in terms of the relation of the latter two variables and ozone concentrations.

Wind direction values are telling of changes in direction with respect to yearly average direction. The increase or decrease of the values shown in figure 3 correspond to a relative shift in direction of the wind compared to the yearly wind direction. These shifts in the direction of the wind can be used later on the forecasting of O3 concentration. Wind direction could help elucidate if O3 concentration from upwind neighboring locations could affect O3 values in the location of interest, Banquiao.

The exploratory data analysis suggests that in order to forecast ozone concentration the model inputs i.e. independent variables will have to be averaged over the month. Furthermore, such monthly mean values will have to be standardized using the mean annual corresponding values. Once the data has been standardized it will be used to train a model.

As a first iteration, a linear model with multiple independent variables will be optimized using available standardized measurements of ozone. A first model will be produced only using standardized pollutant values, and a second model will include as additional variables wind direction and upwind station standardized ozone concentrations from corresponding upwind stations. If the linear model mean square error, computed using predictions of ozone and observation, is below 0.5 a more involved model will be used. Two candidates for the second iteration of the predictive model will be considered. A fully connected neural network and a model produced with genetic programming packages in python for model discovery. In order to train the neural network pollutant measurements as well as from 9 out of the 12 months will be used as well as the corresponding mean wind direction values of Banquiao coupled with the ozone measurements from the 6 neighboring stations shown below. In order to validate the model, 12 the remaining data will be used.



**Figure 3:** Geographic location of 7 stations we focused on

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**Bold text** 

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#### Strikethrough

- 1. Ordered list item
- 2. Ordered list item
  - a. Sub-item
  - b. Sub-item
    - i. Sub-sub-item
- 3. Ordered list item
  - a. Sub-item
- List item
- · List item
- · List item

subscript: H<sub>2</sub>O is a liquid

superscript: 2<sup>10</sup> is 1024.

unicode superscripts<sup>0123456789</sup>

#### unicode subscripts<sub>0123456789</sub>

A long paragraph of text. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Putting each sentence on its own line has numerous benefits with regard to <u>editing</u> and <u>version</u> <u>control</u>.

Line break without starting a new paragraph by putting two spaces at end of line.

# **Document organization**

Document section headings:

# **Heading 1**

# **Heading 2**

# **Heading 3**

# **Heading 4**

Heading 5

**Heading 6** 



#### Horizontal rule:

Heading 1's are recommended to be reserved for the title of the manuscript.

Heading 2's are recommended for broad sections such as Abstract, Methods, Conclusion, etc.

Heading 3's and Heading 4's are recommended for sub-sections.

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Bare URL link: https://manubot.org

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# Referencing figures, tables, equations

Figure 4

Figure 5

```
Figure 6

Figure 7

Table 3

Equation 1

Equation 2
```

# **Quotes and code**

Quoted text

Quoted block of text

Two roads diverged in a wood, and I—I took the one less traveled by, And that has made all the difference.

Code in the middle of normal text, aka inline code.

Code block with Python syntax highlighting:

```
from manubot.cite.doi import expand_short_doi

def test_expand_short_doi():
    doi = expand_short_doi("10/c3bp")
    # a string too long to fit within page:
    assert doi == "10.25313/2524-2695-2018-3-vliyanie-enhansera-copia-i-
        insulyatora-gypsy-na-sintez-ernk-modifikatsii-hromatina-i-
        svyazyvanie-insulyatornyh-belkov-vtransfetsirovannyh-geneticheskih-
        konstruktsiyah"
```

Code block with no syntax highlighting:

```
Exporting HTML manuscript
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```

# **Figures**



**Figure 4:** A square image at actual size and with a bottom caption. Loaded from the latest version of image on GitHub.



**Figure 5: An image too wide to fit within page at full size.** Loaded from a specific (hashed) version of the image on GitHub.



Figure 6: A tall image with a specified height. Loaded from a specific (hashed) version of the image on GitHub.



**Figure 7:** A vector .svg image loaded from GitHub. The parameter sanitize=true is necessary to properly load SVGs hosted via GitHub URLs. White background specified to serve as a backdrop for transparent sections of the image.

# **Tables**

**Table 3:** A table with a top caption and specified relative column widths.

Bowling Scores	Jane	John	Alice	Bob
Game 1	150	187	210	105
Game 2	98	202	197	102
Game 3	123	180	238	134

**Table 4:** A table too wide to fit within page.

		Digits 1-33	Digits 34-66	Digits 67-99	Ref.
ķ	oi	3.14159265358979323 846264338327950	28841971693993751 0582097494459230	78164062862089986 2803482534211706	piday.org
E	9	2.71828182845904523 536028747135266	24977572470936999 5957496696762772	40766303535475945 7138217852516642	nasa.gov

**Table 5:** A table with merged cells using the attributes plugin.

	Colors		
Size	Text Color	Background Color	
big	blue	orange	
small	black	white	

# **Equations**

A LaTeX equation:

$$\int_0^\infty e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \tag{1}$$

An equation too long to fit within page:

$$x = a + b + c + d + e + f + g + h + i + j + k + l + m + n + o + p + q + r + s + t + u + v + w + x + y + z + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9$$
(2)

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# **1** Blue Banner

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**♦ Light Red Banner** useful for *warnings* - <u>manubot.org</u>

## References

#### 1. Sci-Hub provides access to nearly all scholarly literature

Daniel S Himmelstein, Ariel Rodriguez Romero, Jacob G Levernier, Thomas Anthony Munro, Stephen Reid McLaughlin, Bastian Greshake Tzovaras, Casey S Greene *eLife* (2018-03-01) <a href="https://doi.org/ckcj">https://doi.org/ckcj</a>

DOI: <u>10.7554/elife.32822</u> · PMID: <u>29424689</u> · PMCID: <u>PMC5832410</u>

#### 2. Reproducibility of computational workflows is automated using continuous analysis

Brett K Beaulieu-Jones, Casey S Greene

Nature biotechnology (2017-04) <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6103790/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6103790/</a>

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Douglas Heaven

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DOI: 10.1038/d41586-019-00447-9 · PMID: 30718888

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cOAlition S

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Peter Suber

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Journal of The Royal Society Interface (2018-04) <a href="https://doi.org/gddkhn">https://doi.org/gddkhn</a>

DOI: <u>10.1098/rsif.2017.0387</u> · PMID: <u>29618526</u> · PMCID: <u>PMC5938574</u>

#### 8. Open collaborative writing with Manubot

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PLOS Computational Biology (2019-06-24) https://doi.org/c7np

DOI: 10.1371/journal.pcbi.1007128 · PMID: 31233491 · PMCID: PMC6611653