Final: PM2.5 Prediction with Machine Learning*

*For the fulfillment project proposal of AT82.01 Computer Programming for Data Science and Artificial Intelligence course by Dr. Chantri Polprasert

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Abstract—The project is to forecast PM2.5 based on weather data set collected from five weather stations in Bangkok. Using the scikit-learn library in Python, we created the Random Forest prediction model that can predict PM2.5 given the weather data. Then, we deployed the model into website created by Flask, to AWS for end-users to use.

Index Terms-Particulate Matters, PM2.5, Machine Learning

I. Introduction

A. Introduction to PM2.5

PM2.5, or Particulate Matter 2.5, is a critical measure of air quality that refers to tiny airborne particles or droplets with a diameter of 2.5 micrometers or smaller. These minuscule particles can originate from a variety of sources, including industrial emissions, vehicle exhaust, construction activities, natural dust, and even chemical reactions in the atmosphere. PM2.5 is significant because it has a substantial impact on both human health and the environment. Understanding PM2.5 levels is essential for assessing air quality, making informed policy decisions, and implementing measures to safeguard public well-being.



Fig. 1: PM 2.5 Impact on environment and humans [8]

B. Global Perspective View on PM2.5

A global perspective on PM2.5 levels is vital to comprehend the scale and variations in air quality across different regions. By monitoring PM2.5 on a global scale, we can identify trends, sources of pollution, and areas where air quality may be particularly hazardous. This global view often involves the use of satellites and international air quality monitoring networks. It helps nations collaborate in addressing transboundary air pollution and sharing information to mitigate the impact of airborne particles on a global scale.

C. Local Perspective View for Thailand

On a local level, such as within a country like Thailand, monitoring PM2.5 is crucial for assessing the immediate air quality conditions that people are exposed to. Local monitoring networks, government agencies, and environmental organizations collect data on PM2.5 levels to provide real-time information to citizens. This local perspective helps individuals make informed decisions about outdoor activities, and it assists policymakers in implementing measures to improve air quality and protect public health.



Fig. 2: PM 2.5 Impact in Thailand [9]

D. Why Do We Do PM2.5 Projects?

 Protecting Public Health: PM2.5 particles are so small that they can penetrate deep into the respiratory system, posing significant health risks. PM2.5 projects aim to reduce exposure to these particles and thereby protect the health of communities. High PM2.5 levels have been linked to respiratory diseases, cardiovascular issues, and even premature death.

- Environmental Impact: PM2.5 particles can also harm the environment. They can contribute to smog formation, damage ecosystems, and affect water quality. PM2.5 projects seek to reduce these environmental impacts.
- Policy and Regulation: Monitoring PM2.5 is essential for setting air quality standards and regulations. Governments and regulatory agencies use PM2.5 data to implement measures to limit emissions from various sources.
- 4) Awareness and Education: PM2.5 projects help raise public awareness about air quality issues. They encourage people to take action to reduce their own contributions to air pollution and to advocate for cleaner air.

In summary, PM2.5 projects serve the vital purpose of safeguarding both human health and the environment. They provide essential information for informed decision-making, regulation, and action at both the local and global levels. The business understanding are in Fig. 3.

II. PROBLEM STATEMENT

To predict the PM2.5 values based on given weather conditions and trends of the PM2.5, Temporal Trends PM2.5 (seasonal, monthly, daily, hourly), Correlations between weather parameters and PM2.5, Weather effects (wind speed and temperature) on PM2.5

III. RELATED WORKS

This project goal is to train the model to able to predict the PM2.5. Here the focus is on how other concerned in PM2.5 at different area and weather, some well-known techniques to make the model be able to predict desired target variables. Thus, These can make the model predicted the PM2.5 with high accuracy, precision, and recall.

Vahid Mehdipour [4] and his team from Tehran compared different methods for modeling PM2.5 in the capital city of Iran, Tehran. They proposed decision trees (DT), Bayesian Network (BN), and support vector machine (SVM). Using the data for over three periods, they concluded that PM10, NO_2 , SO_2 , and O_3 are critical factors for PM2.5 with the best model is SVM.

Delhi, another mega-city in India, also faced an enormous of air pollution because of rapid development for a while. Nidhi Sharma and her colleagues [6] forecast pollution load in an atmosphere using time-series regression forecasting. In the results, predicted trends are shown after 2017.

Another interesting paper used Taiwan Air Quality Monitoring (TAQMN) data set. Doreswamy and his team [7] did the forecasting using also machine learning regression models. The data used are from 2012 to 2017. Models were evaluated by Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), and Coefficient of Determination (\mathbb{R}^2). They used Fourier arrangement and spline multinomial to fill the missing values in data set. The model they used are random forest regressor (RFR), gradient boosting regressor GBR), k neighbors regressor (KNR), MLP regressor (MLPR), and decision tree regressor CART. To select the best

model, they used cross-validation and determined that gradient boosting regressor model is better in forecasting air pollution in TAQMN data.

IV. DATASET

A. Description

The data set contains a record of PM2.5 per hour recorded in 2019 from 5 stations distributed in Bangkok as shown in Fig. 7. In total, 5 stations' data set for this project are given by Dr. Chantri via the Pollution Control Department of Thailand. The station are numbered as follows (5 from all 66 stations established in 2019).

- Station 03: Bang Khun Thian, Bangkok
- Station 50: Pathum Wan, Bangkok
- Station 52: Thonburi, Bangkok
- Station 53: Chok Chai, Bangkok
- Station 54: Din Daeng, Bangkok

The data set is in EXCEL spread sheet format.

B. Features

The dataset contains following features:

- · Date and time of record
- Various air quality parameters (CO, NO, NO₂, NOX, O₃, PM10, PM2.5)
- Meteorological data (wind speed, wind direction, temperature)

V. METHODOLOGY

To begin with, this project use scikit-learn [5] packages as it is simple and efficient tools for predictive data analysis. Next, we received data set, cleaned data, explored some data insights, pre-processed, selected the model, trained the model, evaluation, and deployed into simple website in AWS platform to demonstrate our powerful PM2.5 prediction.

A. Data Acquisition

To obtain the data set, Professor Chantri received the data set for us. These data sets came from the Pollution Control Department of Thailand (PCD) [2]. Generally, the data are recorded daily for public use. However, we can ask PCD for more details hourly records. Original data looks as shown in Fig. 8.

The original filename are in Thai. For better communicate between groups, we agreed to change into more accessible file names in English as shown in Fig. 9. We then imported the data set from each station, and stored in variables station03, station50, station52, station53, and station54, respectively.

B. Clean Data

As the original data were not generalized well and were really messy, we needed some cleaning process before analyzed with Exploratory Data Analysis in V-C. The process included here are:

- Dropped second level headers
- Renamed column names in Fig. 10

Title: PM2.5 Prediction with Machine Learning **(** 3. Value 1. Problem Statement 4. Data Acquisition Modeling What models are appropriate to use given What problem are you trying to solve? Where are you sourcing your data from **Propositions** What larger issues do the problem Is there enough data? Can you work with your outcomes? What are we trying to do address? for the end-user(s) of Linear Regression. And other kinds of the predictive system? Predict the PM2.5 trends with air data From Pollution Control Department. Yes, regression e.g., Random Forest Regression. What objectives are we from sensor. Because knowing high PM2.5 The is enough data from 5 stations serving? in prior can know what need to do in throughout 2019. And we can work with it. advance e.g., wearing masks, close the Give the model early window. warning system that end-user can know so they can prepare the protection and/or 2. Outcomes/Predictions 6. Model Evaluation 7. Data Preparation reduce the damage from What prediction(s) are you trying to make? How can you evaluate your model What do you need to do to your data in the small particle. order to run your model and achieve your Identify applicable predictor (X) and/or performance? target (y) variables. outcomes? Precision and Recall since heavy PM2.5 and non-heavy events is not the same Carbon monoxide (CO), humidity as Fill blank values, combine all data from amount. five stations. Combine date and time into predictor PM2.5 as target variable timestamp columns.

Modified from Bill Schmarzo's Machine Learning Canvas and Jasmine Vasandani's Data Science Workflow Canvas for CP-DSAI @AIT

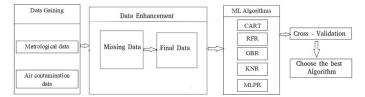
Fig. 3: Project Canvas



Fig. 4: Area of interest, Tehran, Iran [4]



Fig. 5: trend of SO_2 in $\mu g/m^3$ [6]



Date: 18 Oct 2023

Fig. 6: Proposed prediction pipeline model for air pollution [7]



Fig. 7: Weather Stations Location

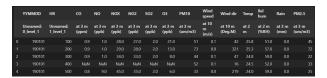


Fig. 8: Original sensor data from Thonburi station, Bangkok

- · Added Province and District columns
- Merged all fives stations into single DataFrame
- Merged Date and Time columns and converged into Timestamp (datetime formatting)
- · Reordered the columns
- Checked and edited data types of columns (dtypes)
- · Replaced string values in numerical columns

```
rename columns
df_52.rename(columns = {'YYMMDD':'yymmdd',
                      'HR':'hr',
                      'CO':'CO',
                        NO ':'NO'
                        NOX ':'NOX'
                        NO2':'NO2',
                        SO2 ': 'SO2'
                        Wind speed': 'wind_speed',
                        Wind dir': 'wind_dir',
                       'PM10':'pm10',
                       'PM2.5':'pm2.5'
                        Temp':'temp',
                        Rel hum': 'humidity',
                        Rain':'rain'
                       }, inplace = True)
```

Fig. 10: Renaming all column names

C. Exploratory Data Analysis (EDA)

For this task, we just exploring the data to see if there are potential problems in the data set (outliers, mislabeled data, unwanted correlations between variables/samples, etc.). However, no actual work done in here. The steps includes identifying missing values and deciding how to handle them, whether by imputing missing values, removing rows with missing values, or using other strategies.

Then, after we did some more cleansing and format the data, we could show some insights in the data as shown in Fig. 11.

Fig. 11: data after do some cleansing before put into EDA

At first, We do uni-variate analysis, plotting to see the trend of average PM2.5 daily in all 5 stations in Fig. 12. PM2.5 is quite high in the first two months. Then it drops dramatically at each its lowest in September. Then, it starts rising again

up until the end of December. Additionally, we also did some histogram plot to see the distribution of PM2.5 in Fig. 13. It normal range is from between 15 to 35 most of the times. Then, we did some scatter plot to see more insight between PM2.5 and PM10 of that predictor in Fig. 14. As predicted, it shows that PM2.5 strongly related to PM10. Furthermore, if these two are high, CO value will also be high too.

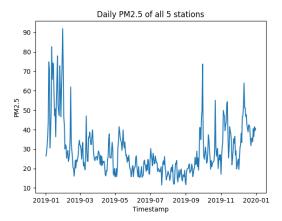


Fig. 12: Daily mean PM2.5 of all station

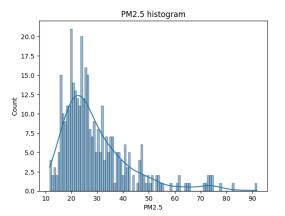


Fig. 13: PM2.5 histogram

Next, we compared PM2.5 from each station and do some kernel density estimate (kde) distribution in Fig. 15 and Fig. 16, respectively. Since all stations are relatively in the same province, Bangkok, PM2.5 values should be in the same trends most of the time. However, in kde plot for visualizing the distribution of observations in a dataset, analogous to a histogram, it shows that stations has 2 different distributions of the PM2.5 values. Showing that the kde distribution of Bang Khun Thian is similar with Din Daeng. The other group is Chok Chai, Pathum Wan, and Thonburi. Also, we do some scatter on PM2.5 for each station and it's quite messy in Fig. 17. In this figure, even though not clearly see at first, if NO_2 increases, it tends to increase the minimum PM2.5 value boundary. This indicates that NO_2 has some effects to PM2.5.



Fig. 9: Rename filenames from Thai to English for easy access

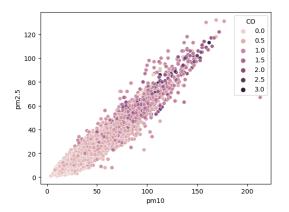


Fig. 14: Scatter plot of PM2.5-PM10 and colored by CO

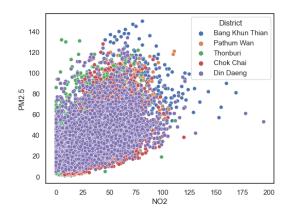


Fig. 17: Scatter plot of PM2.5- NO_2 and colored by District

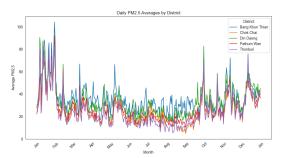


Fig. 15: PM2.5 for each stations

Lastly, We did multivariate analysis. We did the correlation heat map plot to see potential for predictor to use in Fig. 18a. It can be seen that CO, NO, NO_2 , NOX, SO_2 , and PM10 have potential to be the predictor for PM2.5 as target variable. We also computed the predictive power score (PPS) in Fig. 18b, which calculate how strong each predictor can predict

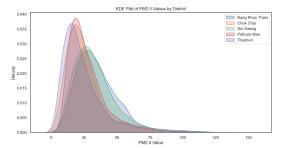


Fig. 16: kde distribution for each stations

other (target) variables. This time, PPS states that only NO_2 and PM10 has some predictive power for PM2.5. We created the violin plot to see the distribution, outliers, mean, and minimum and maximum range for each numerical variables as shown in Fig. 19. We see that most of all variables are not normal distribution, but we need to confirmed again with the probability plot before we decide to use what method for scaling. We also have some interesting test that, wind direction and wind speed is somewhat contribute to PM2.5. In additions, it can also show that most of the time, where wind are coming from which direction in Fig. 20.

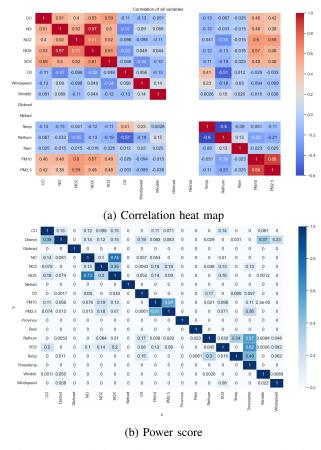


Fig. 18: Correlation and Power score between variables

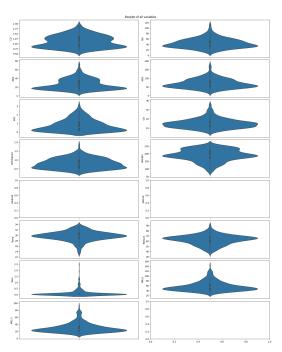


Fig. 19: Violin plot of all variables

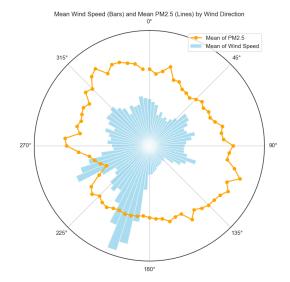


Fig. 20: Mean Wind Speed and Mean PM2.5 by Wind Direction

D. Pre-processing

After explored what our data set looks like, we did preprocessing - the steps required to go from raw data to a format suitable to input to your ML model [1].

- 1) Remove Unnecessary Columns: These columns will be removed:
 - 'Globrad' and 'Netrad' will be removed because 100 % are NaN (Not a Number), they don't have any reference numbers to fill.
 - 'SO2' will also be removed because not enough data. Only less than 20 % entries are not enough to fill the rest more than 80 % of the missing values.
 - 'Province' has only single unique value, Bangkok. No variation anyway.
 - 'Timestamp' will also be dropped in this stage assuming time-independent.
- 2) Train-test Split: We split data set into train and test set with test ratio of 0.2 with fixed random state. In order to make train and test set has the same data from each station equally, we defined stratify by District column. We checked that train set are equally distributed on District in Fig 21. The traintest split need to be random (shuffled). If not, it'll be ordered chronologically and station-orderly, making the last station has limited train data. The train test split settings is shown in Fig. 22. After that, we then imputed, encoded, and scaled the data.

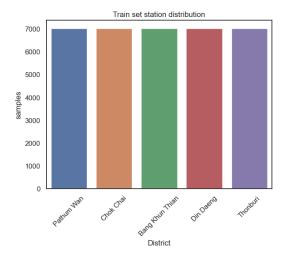


Fig. 21: Train set District (station) distribution check

Fig. 22: Train test split

3) Replace missing values (Imputation): Since all columns are received from sensor data. Assuming that all data were calibrated correctly, we filled with forward fill, and some for backward fill. The imputation process is shown in Fig. 23. The reason we did imputed step separately, not included in Pipeline is because in SimpleImputer(), there's no forward fill and backward fill option available. Due to shuffle option in V-D2, the index are now not in order because of randomly shuffled, and are not in chronological order any more. So, the forward fill will fill wrongly. Thus, After the train_test_split, do .reindex method to make it in order of station and chronologically again (not exact) but it stills better, after that, do forward fill and backward fill.

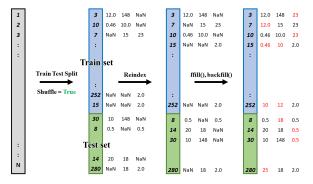


Fig. 23: Imputation process

4) Scaling: Every numerical columns come at different ranges in Fig. 24. So we need to do the scaling, otherwise the

model may neglect some of the predictor(s) and pass some of them.

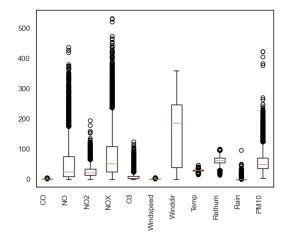


Fig. 24: Predictor variables at different scales

In order to select the appropriate scaler type, we need to check at probability plot of each predictor separately. If it was a normal distribution, we'd scale it with StandardScaler(). If it was not, we'll scale it with MinMaxScaler(). Luckily, we can check the normal distribution using a probability plot from the stats library in Fig. 25. In this case, NO_2 should use MinMaxScaler() because this indicates NO_2 is not in a normal distribution. In the other case when using StandardScaler(), we can see on the probability plot of Fig. 26 that the data mostly fitted with the mean line, indicating that it was a normal distribution.

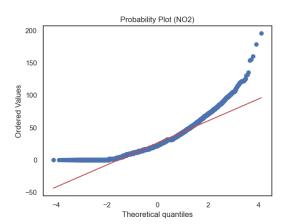


Fig. 25: Probability Plot for NO_2

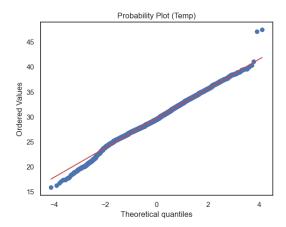


Fig. 26: Probability Plot for temperature

- 5) Encoding: In this data set, only the District is encoded. This does not have any order meaning e.g. Thonburi does not have any higher or lower hierarchy than Bang Khun Thian, so we'll encode with One-Hot Encoder.
- 6) Creating Preprocess Pipeline: This pipeline will include only Scaling and Encoding since replacing (filled) missing values was done in step before. We used ColumnTransformer() to ensure that each column receive the correct pre-process step.

TABLE I: Preprocess Pipeline Summary

Column	Pipeline Step(s)		
Name	Standard Scale	MinMax Scale	OneHot Encoder
CO	√		
NO		√	
NO2		√	
NOX		√	
O3		√	
Windspeed		√	
Winddir		√	
Temp	√		
Relhum	√		
Rain	√		
PM10 ^a		√	
District			√

^aPM.10 will be dropped in other scenario.

E. Modeling

The model we selected came from most in regression models available in scikit-learn.

- 1) Linear Regression will be used for basic prediction of PM2.5. It is the baseline for our goals. In addition, it is the most simple one among others. However, it can't be comprehended with outliers.
- 2) Ridge Regression
- 3) Lasso Regression
- 4) Gradient Boosting Regression
- 5) Histogram-based Gradient Boosting Regression Tree
- 6) ϵ -support Vector Regression (SVR)
- 7) K Neighbor Regression
- 8) Decision Tree Regression
- 9) Random Forest Regression

10) AdaBoost Regression

To select the best model for this purpose, we did k-fold cross-validation with k = 5. After we got the best model, we did a grid search with cross-validation to find the best hyper-parameters for that model with k-folds k = 10. Then, we gave the best model and best hyper-parameters to train on the whole training set again, including the validation set.

F. Training

Training will be done by the scikit-learn .fit method. We trained the best model with the best hyper-parameters with all training sets, unlike in cross-validation where some parts of the training set were separated into the validation sets.

G. Evaluation

After training the model, we plan to evaluate the model using Mean Squared Error (MSE) and \mathbb{R}^2 score as shown in (3) and (4). \mathbb{R}^2 score was selected because it can tell how much proportion of the whole data set this regression model explained. This evaluation process was nicely provided by scikit-learn for easy implementation directly from the pipeline we created. The overall process from selecting the model until the evaluation is shown in Fig. 27.

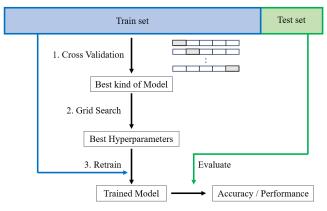


Fig. 27: Training Process

The evaluation matrix scores we tried to use are Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), Mean Squared Error (MSE), and Coefficient of Determination (R^2 score).

$$MAE = \frac{\sum_{i=1}^{m} |x_i - \hat{x}_i|}{m} \tag{1}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{m} (x_i - \hat{x}_i)^2}{m}}$$
 (2)

$$MSE = \frac{1}{m} \sum_{i=1}^{m} (x_i - \hat{x}_i)^2$$
 (3)

$$R^{2} = \left[\frac{1}{M} \frac{\sum_{j=1}^{M} [(Y_{j} - \overline{Y})(X_{j} - \overline{X})]}{\sigma_{n} \sigma_{r}}\right]^{2}$$
(4)

where,

m and M are the number of observations

- $\hat{x_i}$ is the predicted value
- x_i is the actual value
- σ_x is the standard deviation of the observation X
- σ_y is the standard deviation of the observation Y
- X_i is the observed values
- \overline{X} is the mean of the observed values
- Y_i is the calculated values
- \overrightarrow{Y} is the mean of the calculated values.

H. Deployment

The deployment will use a microweb framework, Flask, and some basic HTML to show the results. The steps are as follows:

- 1) Deploy model in local host.
 - a) Develop Machine Learning model.
 - b) Convert model file to pickle object (.pkl) or joblib (.model).
 - c) Create one Flask website app (app.py), tutorial from [13].
 - d) In the Flask app, load the model object and create a form for user input.
 - e) Create a prediction method in app.py to make a prediction.
 - f) Test deployment on local host port 8080, tutorial from [15].
- 2) Upload all codes to Github https://github.com/BaiPorAndFern/CP_pm2.5_prediction.
- 3) Deploy the model on Amazon Web Service (AWS).
 - a) Create an account.
 - b) Create Administration-to-Customer (A2C) instance
 - c) Edit security group in Inbound rules, Adding TCP port 8080.
 - d) Download PuTTY private keygen (.ppk file).
 - e) Download and install Putty [10] and WinSCP [11].
 - f) Upload Flask website to EC2 using WinSCP. Note that before uploading, you must activate the key pair by double-clicking on it in Fig. 28.
 - g) Install necessary packages on the virtual machine:
 - sudo apt-get update,
 - sudo apt-get install python3-pip, and
 - pip3 install numpy flask scikit-learn
 - h) run the main.py python main.py.

The overall process for deployment is shown in Fig. 29.

VI. RESULTS

This project uses a total of 11 features from 5 weather stations data set. After pre-processing was done, we began using some part of the data set, the train set, to select the model and its hyperparameters. In Fig. 30, the model selection result was shown. The result showed the validation \mathbb{R}^2 score, ranked from highest to lowest. Hence, the Random Forest regression

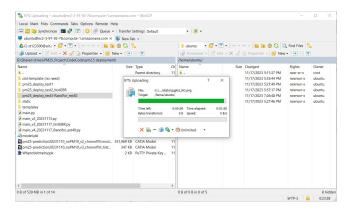


Fig. 28: Upload to AWS using WinSCP [11]

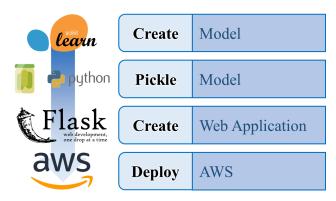


Fig. 29: Deployment Steps

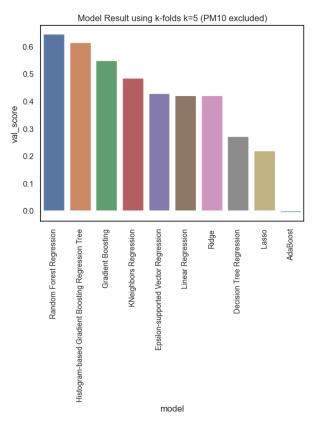


Fig. 30: Model Selection

was selected because of its performance with the highest \mathbb{R}^2 score of 0.645.

We now have the algorithm to train. Then, we need to adjust its hyper-parameters to reach its optimal performance. The results from fine-tuning hyper-parameters in Fig. 31 showed that, among others, Random Forest Regression with $n_{estimators} = 200$ is the best with R^2 score of 0.648. However, it does not differ much from $n_{estimators} = 40$, but very different at the size of the model object. Thus, we select $n_{estimators} = 40$.

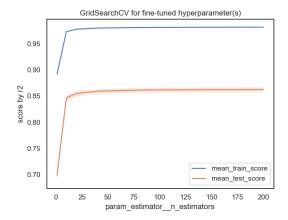


Fig. 31: Fine-tuned Hyper-parameter

After obtaining the optimal model possible, we trained it to the whole training set and evaluated using an unseen test set. The model shows the result of MSE and R^2 score of 162.97 and 0.443, respectively. In this step, we found out that the most important feature was NO_2 . Results come from pipeline build-in attributes feature_importances_ and all features rank is shown in Fig. 32.

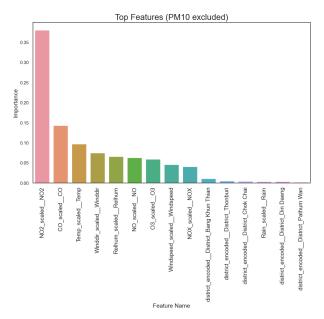


Fig. 32: Feature Importance

Then, after the model was trained, we tested on another sample of unseen data, excluded from our data set. The model showed that it can accept all input we gave to the model and made PM2.5 prediction results as shown in Fig. 33. We observed that, among other stations, Bang Khun Thian, if selected, will be sensitive to predicted PM2.5 the most. This can be traced back to feature importance in Fig. 32 that shows Bang Khun Thian is the most important district.

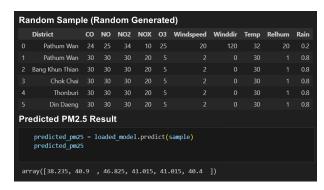


Fig. 33: Test Model

VII. CONCLUSIONS AND FUTURE WORKS

In this project, we deploy the random forest regression model that can accept the new sample, and give a prediction of what pm2.5 will be, given the features. The model was initialized using a trained model from 5 weather stations in Bangkok.

The main benefit of this project is predicting the PM2.5 value based on given weather conditions, specializing scikit-learn library to create a machine learning model to achieve that task, and deploying it to the website for end-users to use. This model can also be used with other station data too, to further enhance the performance of the model, making it able to predict various data from other places.

The future works can be that the model used does not include time series. This can be improved by including a Timestamp in the analytics and using a time-series algorithm like an Auto-Regressive Integrated Moving Average (ARIMA). Since the problem involves forecast with time series, this model can be used.

Also, We can add the Air Quality Index (AQI) based on the Thailand Air Pollution Department criterion as shown in Fig. 34 into prediction results and add recommendations related to the predicted PM2.5 value, giving the users more on how should they act and prepared (Decision-Making).

Another thing that can be improved is changing the evaluation score. Using R^2 score alone can sometimes mislead the users if more features are added. R^2 score will always increase if more features are added, regardless of whether these features are significant or not. So using the adjusted R^2 score would be more adjusted to the real scenario. Now, adding an unnecessary variable will often decrease the adjusted R^2 score as there are now indicators of non-significant terms included in the model.

Lastly, including more weather data and PM2.5 from other stations and other provinces would give more in-depth details on PM2.5 data in Thailand and will strengthen the model further in predicting PM2.5 in more diverged places.



Fig. 34: US AQI levels, equivalent PM2.5 standards by $\mu g/m^3$, and health recommendations for each level. [3]

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