DETECTION AND PREDICTION OF AIR POLLUTION LEVEL

A MAIN PROJECT REPORT

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF DEGREE OF

BACHELOR OF TECHNOLOGY

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of

APJ Abdul Kalam Technological University

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Certificate

This is to certify that the Main Project Report titled **"DETECTION AND PREDICTION OF AIR POLLUTION LEVEL"** is a bonafide record of the work carried out by **SRUTHI K S ,TESLIN ROSE P V ,VINI SASIDHARAN ,VISHNU V U** of Vidya Academy of Science & Technology, Thalakkottukara, Thrissur - 680 501 in partial fulfillment of the requirements for the award of **Degree of Bachelor of Technology** in **Computer Science and Engineering** of **APJ Abdul Kalam Technological University**, during the academic year 2019-2020. The Main Project report has been approved as it satisfies the academic requirements in the respect of main project work prescribed for the said degree.

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Undertaking

We, **SRUTHI K S, TESLIN ROSE P V, VINI SASIDHARAN, VISHNU V U**, hereby undertake that, the main project work entitled **"DETECTION AND PREDICTION OF AIR POLLUTION LEVEL"**, is carried out by us independently under the valuable guidance of **Ms. Nitha K P**, Asst. Prof., Dept. of Computer Science and Engineering, Vidya Academy of Science and Technology, Thalakkottukara, Thrissur, in partial fulfillment of the requirements for the award of degree of **Bachelor of Technology in Computer Science Engineering** of APJ Abdul Kalam Technological University, during the academic year 2019-2020.

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During the course of our main project work several persons collaborated directly and indirectly with us. Without their support it would be impossible for us to finish our work. That is why we wish to dedicate this section to recognize their support.

We want to start expressing our thanks to our project guide **Ms. Nitha K P**, Asst. Prof., Dept. of Computer Science and Engineering, because of his valuable advice and guidance towards this work. We received motivation, encouragement and hold up from his during the course of work.

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Last, but not the least we wish to express our gratitude to God Almighty for His abundant blessings without which this effort would not have been successful.

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Abstract

Air pollution has become an important public health concern The high concentration of fine particulate matter with diameter less than 2.5 μm (PM 2.5) is known to be associated with lung cancer, cardiovascular disease, respiratory disease, and metabolicdisease. Predicting Air Quality can help governments warn people at high risk, thus mitigating the complications.

In this work feature importance of air pollution, Implementing Random forest, XGBoost, CatBoost and Deep learning machine learning (ML) approaches. We use 8 features, including meteorological data, ground-measured PM 2.5 and gaseous pollutants. forecasting Air quality using deep learning technique LSTM and Prophet package by Facebook we can extract the trend yearly seasonality, and weekly seasonality of the time series

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Chapter 1

INTRODUCTION

1.1 General

As a consequence of urbanization and industrialization, air pollution has become one of the most important public health concerns. The PM 2.5 pollutant is defined as fine inhalable particles with diameters less than 2.5 μm. The association of high PM 2.5 concentration and cancer, cardiovascular disease, respiratory disease, metabolic disease, and obesity has been proven.

Particulate matter can be either human-made or naturally occur.Some examplesinclude dust, ash and sea-spray. Particulate matter (including soot) is emitted during the combustion of solid and liquid fuels, such as for power generation, domestic heating and in vehicle engines. Particulate matter varies in size. Different machine learning models have been applied to detect air pollution and predict PM2.5 levels based on a data set consisting of daily atmospheric conditions. Although several attempts have been made to predict PM 2.5 concentration, the relationship between features that influence PM 2.5 concentration prediction is still not well understood.

1.2 Objectives of the Work

This system exploits machine learning models to predict and forecast PM2.5 levels based on a data set consisting of atmospheric conditions in a specific city.

The proposed system does two tasks

- **(i)** predict the levels of PM2.5 based on given historical values.
- **(ii)** Forecast the level of PM2.5 for 7 days.

Random forest, Extreme gradient boost, CatBoost and Deep learning are employed to predict the level of PM 2.5 based on the previous readings. The primary goal is to predict the air pollution level in the City with the ground data set. Prophet and LSTM is used to forecast the PM2.5 level upto 7 Days.

1.3 Motivation for this work

PM is a complex mixture of solid and liquid particles suspended in air that is released into the atmosphere when coal, gasoline, diesel fuels and wood are burned. It is also produced by chemical reactions of nitrogen oxides and organic compounds that occur in the environment. Vegetation and livestock are also sources of PM. In big cities, production of PM is attributed to cars, trucks and coal-fired power plants.

The health effects of PM depend on several factors, including the size and composition of the particles, the level and duration of exposure, and the gender, age and sensitivity of the exposed individual. Symptoms of exposure may include persistent cough, sore throat, burning eyes and chest tightness. PM may also trigger asthma or lead to premature death, particularly in elderly individuals with pre-existing disease.3,4 In addition, people who are active outdoors are at higher risk, as physical activity increases the amounts of PM penetrating into the airways. People with disease (e.g. diabetes mellitus, malnutrition) are also at increased risk.5–7 A comprehensive review on diesel PM by Ristovski et al. was published in an earlier issue of this review series on air pollution and lung disease.

1.4 Methodologies Adopted

For the project, we evaluated several different types of prediction and forecast machine learning models which will be described below. We use Prophet and LSTM for forecasting air quality and XGBoost,Random Forest, CatBoost and Deep Learning for prediction.Data processing and matching is necessary because the data is obtained from different sources.Therefore, we intend to use interpolation to estimate and fill in the missing data.Data normalization is an important step for many machine-learning estimators. A correlation matrix can be used to investigate the dependence between multiple variables at the same time

1.5 Outline of the Report

This report contains 4 chapters. Chapter 1 gives the introduction to the project work and describes the objectives of the work. Literature survey is describes in Chapter 2. System Design is explained in the chapter 3 and Methodology is well explained in chater 4.

Chapter 2

LITERATURE REVIEW

2.1 A Machine Learning Approach for Air Quality Prediction: Model Regularization and Optimization

Dixian Zhu ,Changjie Cai , Tianbao Yang and Xun Zhou

In this paper, we tackle air quality forecasting by using machine learning approaches to predict the hourly concentration of air pollutants (e.g., ozone, particle matter (PM2.5) and sulfur dioxide). Machine learning, as one of the most popular techniques, is able to efficiently train a model on big data by using large-scale optimization algorithms. Although there exist some works applying machine learning to air quality prediction, most of the prior studies are restricted to several-year data and simply train standard regression models (linear or nonlinear) to predict the hourly air pollution concentration. In this work, we propose refined models to predict the hourly air pollution concentration on the basis of meteorological data of previous days by formulating the prediction over 24 h as a multi-task learning (MTL) problem. This enables us to select a good model with different regularization techniques. We propose a useful regularization by enforcing the prediction models of consecutive hours to be close to each other and compare it with several typical regularizations for MTL, including standard Frobenius norm regularization, nuclear norm regularization, and ‘2,1-norm regularization. Our experiments have showed that the proposed parameter-reducing formulations and consecutive-hour-related regularizations achieve better performance than existing standard regression models and existing regularizations.

In this paper, we have developed efficient machine learning methods for air pollutant

prediction. We have formulated the problem as regularized MTL and employed advanced optimization algorithms for solving different formulations. We have focused on alleviating model complexity by reducing the number of model parameters and on improving the performance by using a structured regularizer. Our results show that the proposed light formulation achieves much better performance than the other two model formulations and that the regularization by enforcing prediction models for two consecutive hours to be close can also boost the performance of predictions. We have also shown that advanced optimization techniques are important for improving the convergence of optimization and that they speed up the training process for big data. For future work, we will further consider the commonalities between nearby meteorology stations and combine them in a MTL framework, which may provide a further boosting for the prediction.

2.2 A Deep Learning Approach for Forecasting Air Pollution in South Korea Using LSTM

Tien-Cuong Bui, Van-Duc Le, Sang K. Cha

Over the last few years, tackling air pollution is an urgent problem in South Korea. Much research is being conducted in environmental science to evaluate the severe impact of particulate matters on public health. Besides that, deterministic models of air pollutant behavior are also generated; however, these are both complex and often inaccurate. On the contrary, deep recurrent neural network reveals strong potential on forecasting outcomes of time-series data and has become more prevalent. This paper uses Recurrent Neural Networks and Long Short-Term Memory units as a framework for leveraging knowledge from time-series data of air quality and meteorological information. Finally, we investigate prediction accuracies of various configurations. This paper is a significant motivation for not only continuing researching on urban air quality but also helping the government leverage that insight to enact beneficial policies.

The goal of the presented work was to evaluate the effectiveness of encoder-decoder networks for building prediction machines with time series data. The proposed model shows significant results in prediction PM2.5 AQI of long future based on historical meteorological data. However, to enhance the accuracy of the prediction machine, the model needs to be evaluated more in the future. Finally, forecasting the status of air pollution

can help governments in policy-making and resource allocation.

2.3 Prediction Model of Air Pollutant Levels Using Linear Model with Component Analysis

Arie Dipareza Syafei, Akimasa Fujiwara, and Junyi Zhang

Abstract—The prediction of each of air pollutants as dependent variable was investigated using lag-1(30 minutes before) values of air pollutants (nitrogen dioxide, NO2, particulate matter 10um, PM10, and ozone, O3) and meteorological factors and temporal variables as independent variables by taking into account serial error correlations in the predicted concentration. Alternative variables selection based on independent component analysis (ICA) and principal component analysis (PCA) were used to obtain subsets of the predictor variables to be imputed into the linear model. The data was taken from five monitoring stations in Surabaya City, Indonesia with data period between March-April 2002. The regression with variables extracted from ICA was the worst model for all pollutants NO2, PM10, and O3 as their residual errors were highest compared with other models. The prediction of one-step ahead 30-mins interval of each pollutant NO2, PM10, and O3 was best obtained by employing original variables combination of air pollutants and meteorological factors. Besides the importance of pollutants interaction and meteorological aspects into the prediction, the addition spatial source such as wind direction from each monitoring station has significant contribution to the prediction as the emission sources are different for each station.

There is a concern of adverse effect to humans health due to high concentration of pollutants which exceed the standard value. These events occur often and people should get alerted when this happens, thus making the short-term prediction of pollutant become crucial. Linear models with original variables, ICs, and PCs extracted from six pollutants (NO, NO2, O3, SO2, CO, PM10 and meteorological factors (wind speed, solar gradiation, humidity and temperatures) were employed to predict 30-mins ahead of NO2, PM10, and O3. In addition, we include serial error correlation computation in the model for model accuracy. As expected, the presence of NO has positive correlation with NO2, aside with CO, wind speed and solar gradiation. Furthermore, it was shown that meteorologica factors have high role in the formation of O3. The faster wind speed will

reduce the concentration of NO2 while on the opposite will increase the concentration of O3. This pattern is also found for humidity. Since PM10 is relatively inert particle gas with less than 10um, using the 30-mins data we obtained, no significant correlation was found with other variables.

2.4 Industrial Air Pollution Prediction Using Deep Neural Network

Yu Pengfei, He Juanjuan, Liu Xiaoming, and Zhang Kai

In this paper, a deep neural network model is proposed to predict industrial air pollution, such as PM2.5 and PM10. The deep neural network model contains 9 hidden layers, each layer contains 45 neurons. The output of the hidden layer neurons is calculated using the ReLU activation function, which can effectively reduce the gradient elim- ination effect of the deep neural network. Twelve air pollutant indicators from industrial factories are collected as the input data, such as CO, NO2, O3, and SO2. About 180,000 real industrial air pollution data from Wuhan City are used to train and test the DNN model. Furthermore, the performance of our approach is compared with the SVM and Artifi- cial neural network methods, and the comparison result shows that our algorithm is accurate and competitive with higher prediction accuracy and generalization ability.

In this paper, we proposed a deep neural network model to predict industrial air pollutant. About 180,000 real industrial air pollution data from 2016 to 2018 in Wuhan are used to train, validate and test the model. We use ReLU non- linear activation function instead of the traditional Sigmoid activation function, effectively improve the training speed of the network, eliminating the gradient disappearance or gradient explosion phenomenon. We use the Batch Normal- ization method to improve the training accuracy and convergence speed of the network. Through the DropOff technology, effectively prevent the depth of the neural network over-fitting, improve the test data prediction accuracy. The per- formance of our approach is compared with the SVM and BP neural network, and the comparison result shows that our algorithm is accurate and competitive with higher prediction accuracy and generalization ability.

2.5 Air Pollution Forecasting Using a Deep Learning Model Based on 1D Convnets and Bidirectional GRU

QING TAO, FANG LIU , (Member, IEEE), YONG LI , (Senior Member, IEEE), DENIS SIDOROV, (Senior Member, IEEE)

Air pollution forecasting can provide reliable information about the future pollution situation, which is useful for an efficient operation of air pollution control and helps to plan for prevention. Dynamics of air pollution are usually reflected by various factors, such as the temperature, humidity, wind direction, wind speed, snowfall, rainfall, and so on, which increase the difficulty in understanding the change of air pollutant concentration. In this paper, a short-term forecasting model based on deep learning is proposed for PM2.5 concentration, and the convolutional-based bidirectional gated recurrent unit (CBGRU) method is presented, which combines 1D convnets (convolutional neural networks) and bidirectional GRU (gated recurrent unit) neural networks. The case is carried out by using the Beijing PM2.5 data set in UCI Machine Learning Repository. Comparing the prediction results with the traditional ones, it is proved that the error of the CBGRU model is lower and the prediction performance is better.

The results are compared with traditional mechine learning models and conventional deep learning models. The results show that the proposed method can be suitable and compet- itive on the PM2.5 data time series forecasting. To be more specific, compared with shallow machine learning models, such as DTR, SVR and GBR, deep learning-based methods exhibited better prediction performance. Furthermore, com- pared with GRU, bidirectional GRU has lower error value, which indicates that the use of bidirectional GRU can improve the prediction effect. This is because the bidirectional GRU processes the time series chronologically and antichrono- logically, it captures patterns that may be ignored by one- direction GRUs, improving feature learning capabilities in time series. In addition, compared with the other benchmark models, the accuracy of the CBGRU model is significantly improved, which shows that the convnets can help the GRU to obtain better prediction performance, because convnets uses its local feature learning ability and subsampling ability to obtain a sequence pattern that is more conducive to GRU processing.

Chapter 3

SYSTEM DESIGN

System design is the process of designing the elements of a system such as the architecture, modules and components, the different interfaces of those components and the data that goes through that system.

3.1 Prediction Model

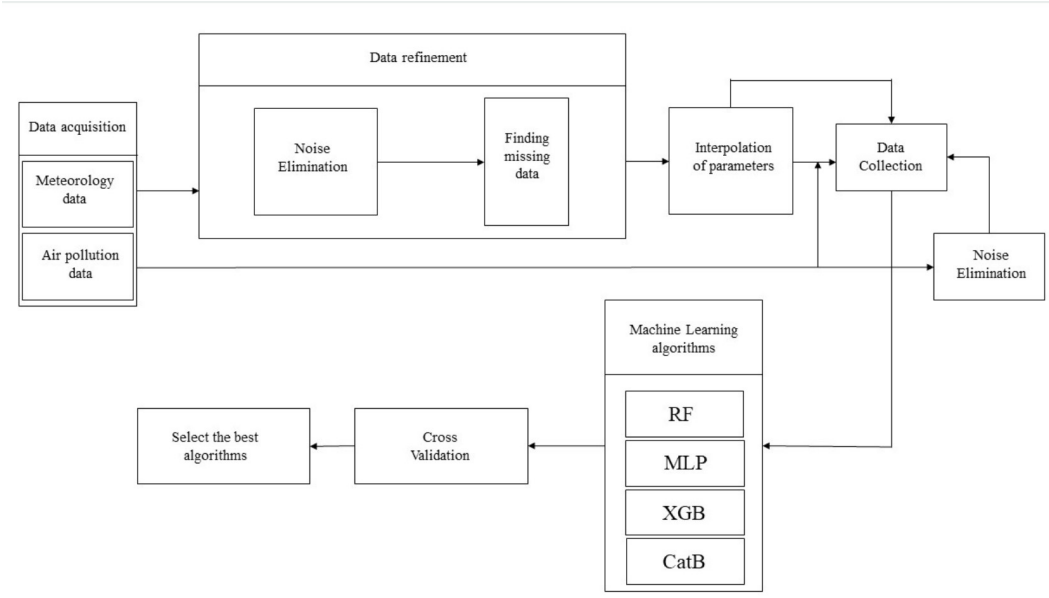

Figure 3.1: Prediction model

The data, which is a combination of both meteorological features and gaseous pollutants is randomly divided into two : Training set and Test set. Usually,it is divided as 70% for training and 30% for test set. Learn models using training set and test the model with test set,from that we select the most accurate model. During training process,the training set is trained using three machine learning algorithms.The algorithms used are : Random Forest, XGBoost, Deep Learning.

3.2 Forecast Model

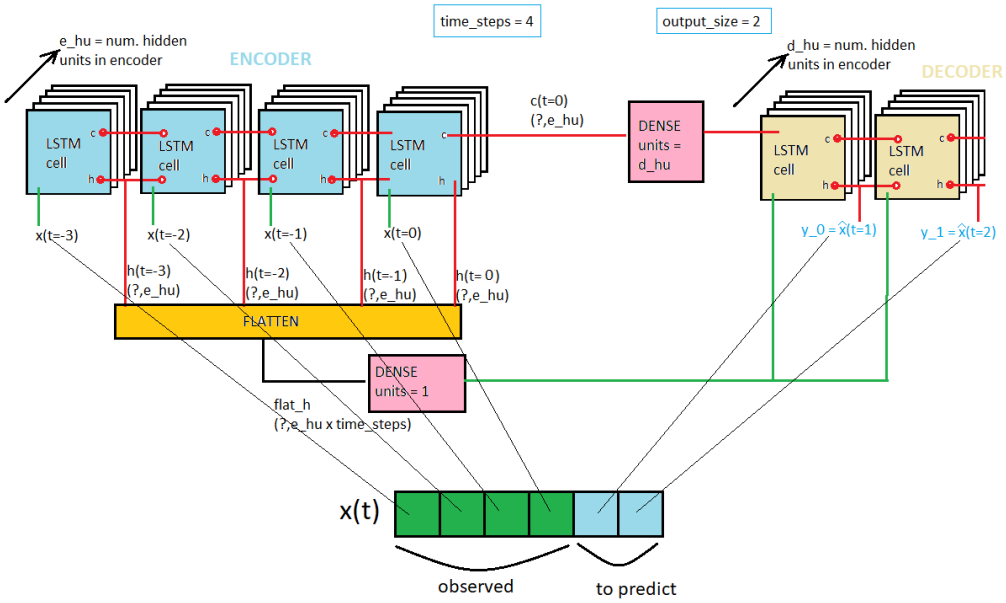

Figure 3.2: Architecture of the lstm

Time series forecasting (TSF) is the task of predicting future values of a given sequence using historical data. Recently, this task has attracted the attention of researchers in the area of machine learning to address the limitations of traditional forecasting methods, which are time-consuming and full of complexity. With the increasing availability of extensive amounts of historical data along with the need of performing accurate production forecasting, particularly a powerful forecasting technique infers the stochastic dependency between past and future values is highly needed. In this paper, we propose a deep learning approach capable to address the limitations of traditional forecasting approaches and show accurate predictions. The proposed approach is a deep long-short term memory (DLSTM) architecture, as an extension of the traditional recurrent neural network.

Chapter 4

METHODOLOGIES

4.1 Data Pre-processing

Data pre-processing is a process of cleaning the raw data i.e. the data is collected in the real world and is converted to a clean data set. In other words, whenever the data is gathered from different sources it is collected in a raw format and this data isn't feasible for the analysis.Therefore, certain steps are executed to convert the data into a small clean data set, this part of the process is called as data pre-processing.

Data processing and matching is necessary because the data was obtained from different sources. Daily climatic data was downloaded from the IMO portal. There are a few missing values or in some cases, full day missing records. Therefore, we used imputation by predictive mean matching to estimate and fill in the missing data. The time format of the data was not in good format and thus was converted to be compatible with the other data. Missing values for short or long periods are a common problem in air pollution monitoring stations. This happens when there is a critical failure or temporary power cutoff. There are many missing values that cannot be compensated by interpolation.

4.1.1 Data Distribution

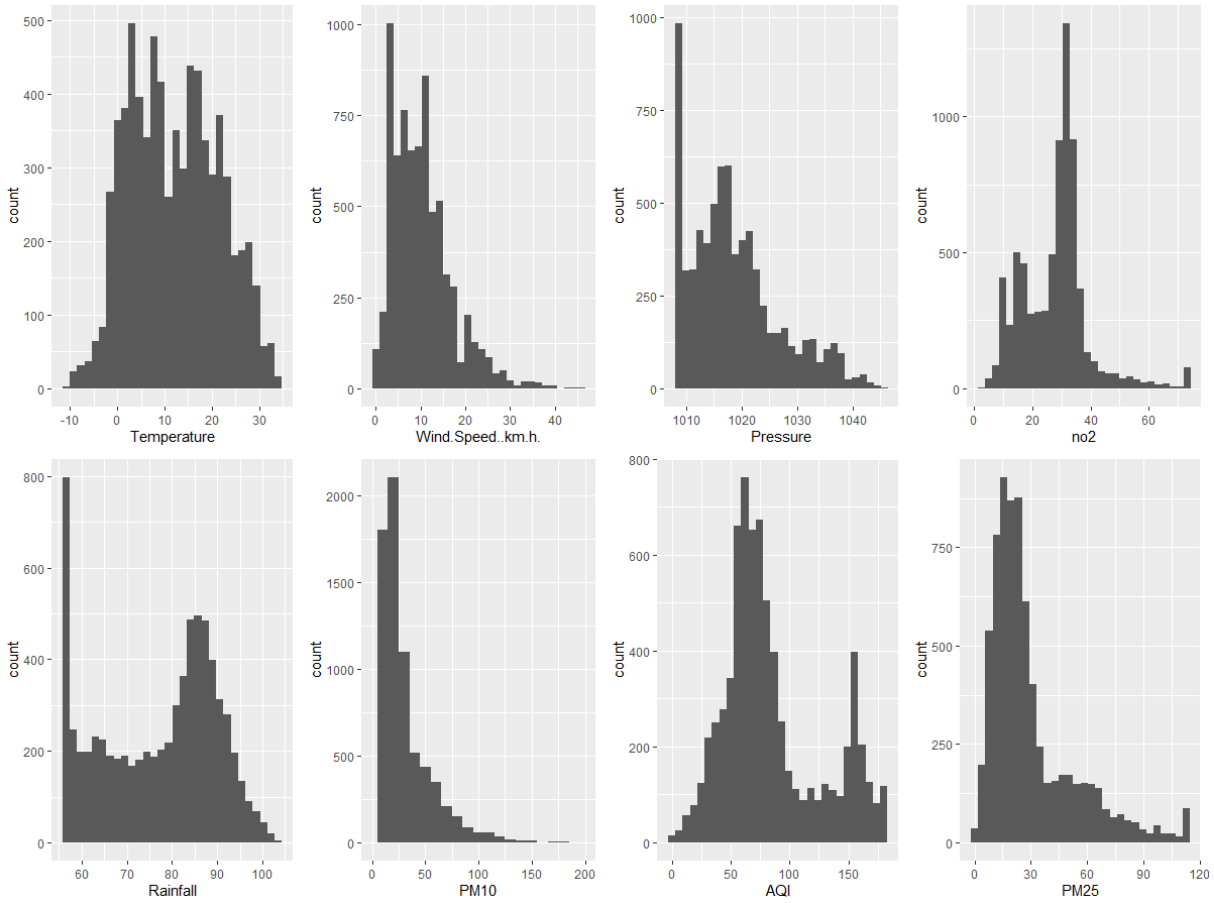

Figure 4.1: Static Analysis

Outliers are extreme values that deviate from other observations on data , they may indicate a variability in a measurement, experimental errors or a novelty. In other words, an outlier is an observation that diverges from an overall pattern on a sample.we can find outliers by checking histograms or densiity plot of the data.

4.1.2 Correlation

Correlation is a measure of how strongly one variable depends on another.Correlation is a bivariate analysis that measures the strength of association between two variables and the direction of the relationship. In terms of the strength of relationship, the value of the correlation coefficient varies between +1 and -1. A value of +1 or -1 indicates a perfect degree of association between the two variables.

Spearman rank correlation

Spearman rank correlation is a non-parametric test that is used to measure the degree of association between two variables. The Spearman rank correlation test does not carry any assumptions about the distribution of the data and is the appropriate correlation analysis when the variables are measured on a scale that is at least ordinal.The assumptions of the Spearman correlation are that data must be at least ordinal and the scores on one variable must be monotonically related to the other variable

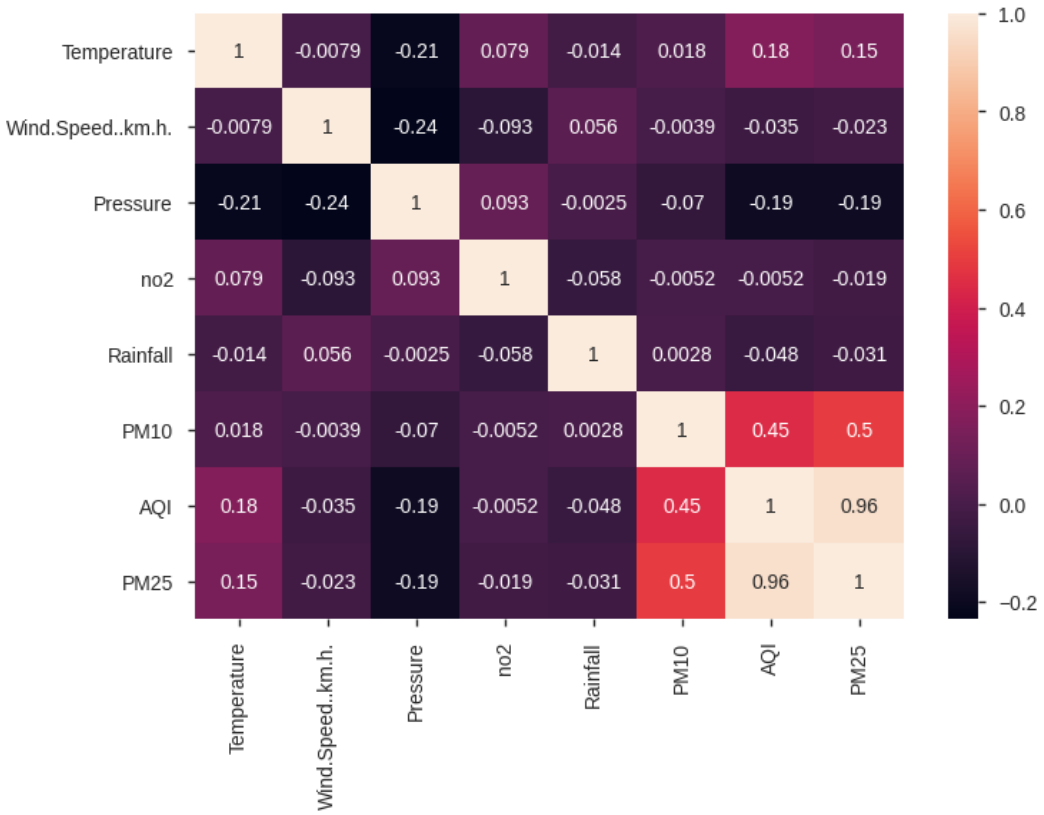

Figure 4.2: Correlation

4.1.3 Normalization

Normalization is a technique often applied as part of data preparation for machine learning. The goal of normalization is to change the values of numeric columns in the dataset to a common scale, without distorting differences in the ranges of values. For machine learning, every dataset does not require normalization. It is required only when features have different ranges.Data normalization is an important step for many machine-learning estimators, particularly when dealing with deep learning. The preferred range of features

for most ML approaches is between -1 to 1. Features with a wider range can cause instability during the model training Standardization was used to standardize the features by deducting the mean and scaling the data, with the variance of feature. After applying standard normalizations,train and test datasets were prepared. Dataset records were shuffled and split to 70% for the train and 30% for the test.

Z-Score

Z-score normalization is also known as zero-mean normalization. Z-score normalization technique normalizes the input values in the dataset using mean and standard deviation. The mean and standard deviation for each feature vector is calculated across the training dataset. This normalization technique determines whether an input value is below or above the average value. It will be very useful to normalize the dataset when the attribute's maximum or minimum values are unknown and outliers dominate the input values.

4.1.4 Imputation

Imputation is a term replace the missing values by some predictable which said to be plausible values in the dataset. It makes use of observed supporting information for cases with non-response maintain high accuracy.

Prediction mean matching Imputation

Predictive mean matching imputation is hot deck imputation within classes where the classes are defined based on the range of the predicted values from the imputation model. This method achieves a more even spread of donor values for imputation within classes, which reduces the variance of the imputed estimator. Donor values within classes may be drawn with or without replacement, where without replacement is expected to lead to a further reduction in the variance.

4.2 Prediction

4.2.1 Random Forest Modeling

Random forests are a combination of tree predictors such that each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest. The generalization error for forests converges a.s. to a limit as the number of trees in the forest becomes large. The generalization error of a forest of tree classifiers depends on the strength of the individual trees in the forest and the correlation between them.

Random Forests are trained via the bagging method. Bagging or Bootstrap Aggregating, consists of randomly sampling subsets of the training data, fitting a model to these smaller data sets, and aggregating the predictions. This method allows several instances to be used repeatedly for the training stage given that we are sampling with replacement. Tree bagging consists of sampling subsets of the training set, fitting a Decision Tree to each, and aggregating their result. In the Random Forests algorithm, each new data point goes through the same process, it visits all the different trees in the ensemble, which are were grown using random samples of both training data and features. Depending on the task at hand, the functions used for aggregation will differ. For Classification problems, it uses the mode or most frequent class predicted by the individual trees, whereas for Regression tasks, it uses the average prediction of each tree.

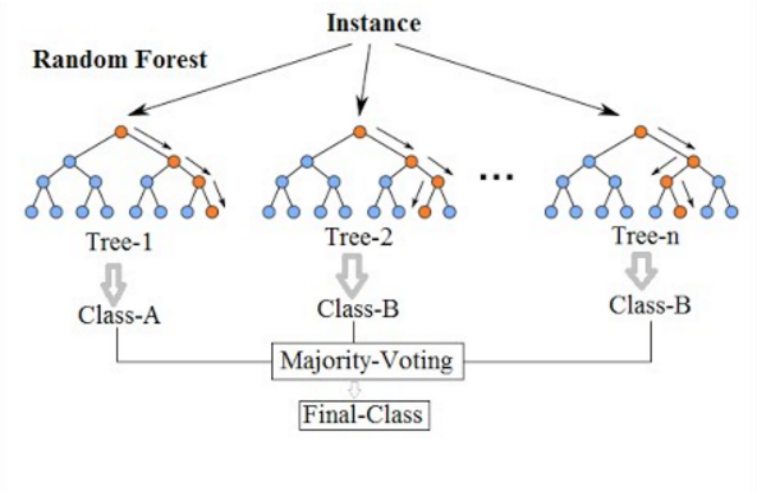

Figure 4.3: Random Forest

Procedure

Random forest is a supervised ensembling learning method, introduced by Ho [6], that acts based on decision trees. it is very flexible and fast. To conduct RF analysis, it is necessary to adjust a model's hyperparameters. A grid search for model performance optimization was carried out with the 10-fold cross-validation technique based on the R square metric.

Parameter	Range	Optimum value
mtry	0-15	3
ntree	0-1000	500

Figure 4.4: Table: Random Forest Parameters

K-fold Cross Validation

The objective is to choose different partitions of training set and validation set, and then average the result, so that the result will not be biased by any single partition.In k-fold cross-validation, the original sample is randomly partitioned into k equal sized subsamples. Of the k subsamples, a single subsample is retained as the validation data for testing the model, and the remaining subsamples are used as training data. The cross-validation process is then repeated k times, with each of the k subsamples used exactly once as the validation data. The k results can then be averaged to produce a single estimation. The advantage of this method over repeated random sub-sampling is that all observations are used for both training and validation, and each observation is used for validation exactly once. 10-fold cross-validation is commonly used, but in general k remains an unfixed parameter. The ntree parameter specifies the number of trees to grow. In the random forests literature, this is referred to as the ntree parameter. Larger number of trees produce more stable models and covariate importance estimates, but require more memory and a longer run time. For small datasets, 50 trees may be sufficient. For larger datasets, 500 or more may be required. The mtry parameter specifies the number of variables available for splitting at each tree node. In the random forests literature, this is referred to as the mtry parameter. The default value of this parameter depends on which R package is used to fit

the model:

RandomForest - For classification models, the default is the square root of the number of predictor variables (rounded down). For regression models, it is the number of predictor variables divided by 3 (rounded down).

Party - The default is always 5.

There is extensive discussion in the literature about the influence of mtry. Cutler et al. (2007) reported that different values of mtry did not affect the correct classification rates of their model and that other performance metrics (sensitivity, specificity, kappa, and ROC AUC) were stable under different values of mtry. On the other hand, Strobl et al. (2008) reported that mtry had a strong influence on predictor variable importance estimates. We make use of grid search to tune the parameters mtry and ntree, for obtaining accurate predictions from our model.

Accuracy

Accuracy is a nice metric for classification, but it doesn't really make sense in the context of regression. Instead, we will use root mean square error (RMSE) to estimate how well our random forest was able to predict our test set outcomes. RMSE or Root Mean Squared Error is the average deviation of the predictions from the observations. It is useful to get a gross idea of how well (or not) an algorithm is doing, in the units of the output variable.

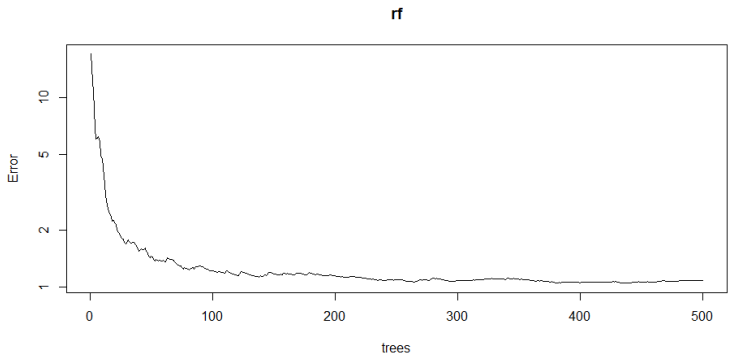

Figure 4.5: Plot of number of trees vs Error

The variables importance measures can be plotted using the function varImpPlot(),as shown in the fisgure below:

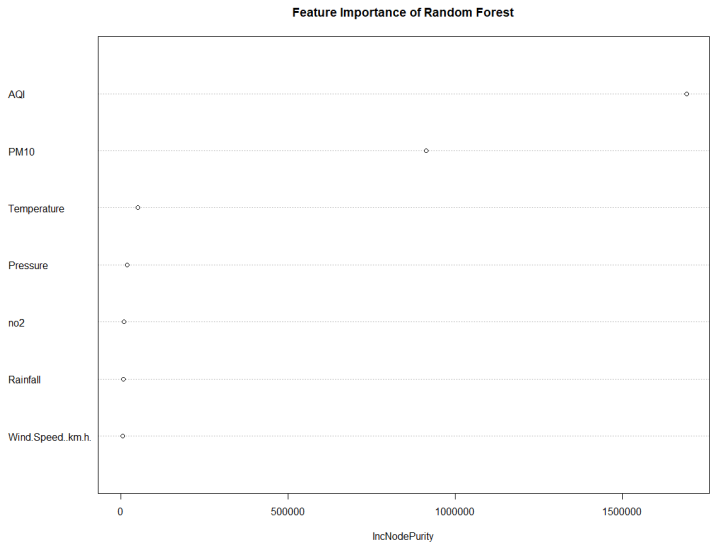

Figure 4.6: Feature Impotance

A histogram representation to show the frequency of the trees with particular number of nodes in our random forest model:

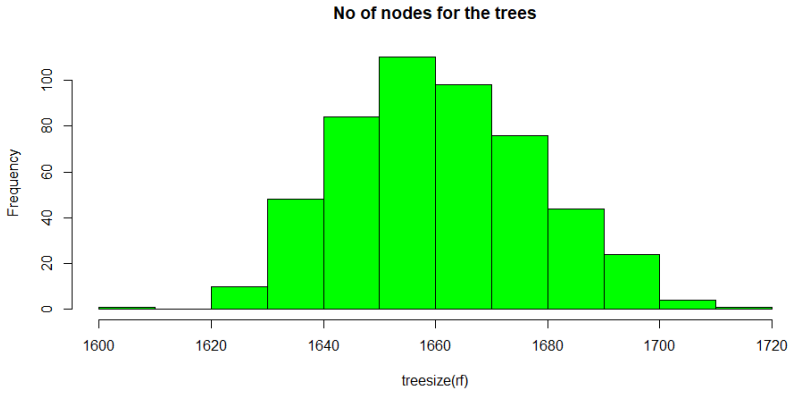

Figure 4.7: Histogram

4.2.2 Deep Learning

Deep learning is one of the machine learning methods that is based on its ancestor—the Artificial Neural Network (ANN). The most beautiful thing about Deep Learning is that it is based upon how we, humans, learn and process information. Everything we do, every memory we have, every action we take is controlled by our nervous system which is composed of neurons! The simplest of the ANNs can be created from three layers of "neurons". The input layer, the hidden layer and the output layer. Information flows from the input layer, through the hidden layer to the output layer and then out.

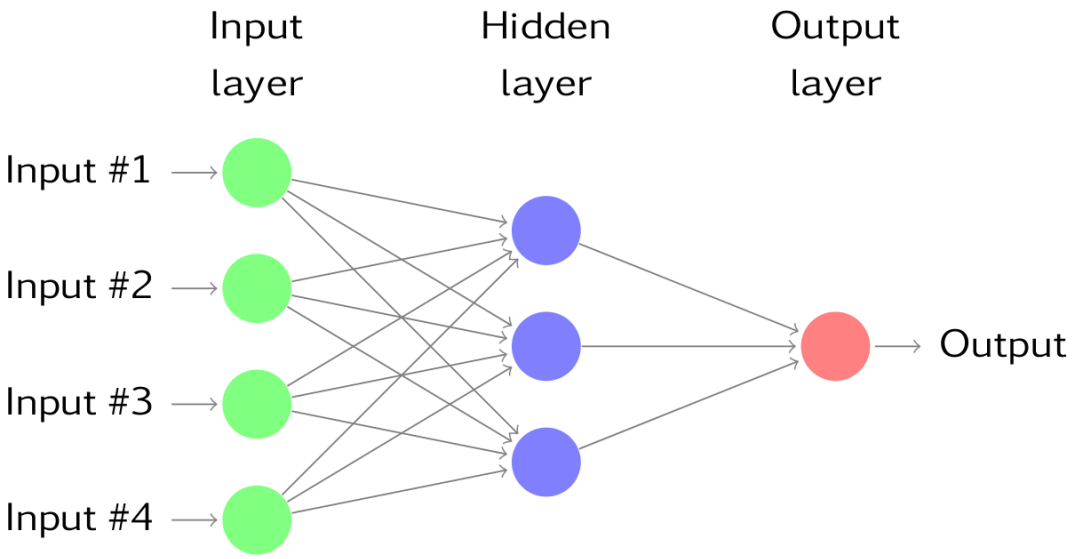

Figure 4.8: Simple Artificial Neural Network

When a neural network is being trained. it is provided with a set of inputs as well as their corresponding outputs. It runs the inputs through the neurons on each of the layers of the network, and using the parameters above, each neuron transforms the input in some way and forwards it to the next layer and so on. The result that it receives on the output layer is then compared to the outputs supplied above and it checks how far apart the two are and accordingly adjusts the parameters on each of the neurons through special algorithmsdesigned to bring the actual and produced outputs as close to each other as possible. It learns to adjust its weights and threshold values to arrive at the correct output. This is what we call as "learning" for the artificial neural network. This process is repeated a (very high) number of times until the produced and expected outputs are as

close as possible. That completes the training.when new inputs are supplied to the neural network, we can confidently say that the predicted outputs of the network will be fairly close to the actual outputs. Such ANNs can be used in predicting based upon certain features and classifying objects and images.

Such neural networks which consist of more than three layers of neurons (including the input and output layer) are called as Deep Neural Networks. And training them is called as Deep Learning.

Multilayer Perceptron

A multilayer perceptron (MLP) is a class of feedforward artificial neural network (ANN). To measure the performance of the regressor the loss function is defined Sometimes the problem of overfitting and underfitting occurs at the time of training the model. In order to train the network, an optimization procedure is required for this. We need loss function and an optimizer. This procedure will find the values for the set of weights, W that minimizes the loss function.

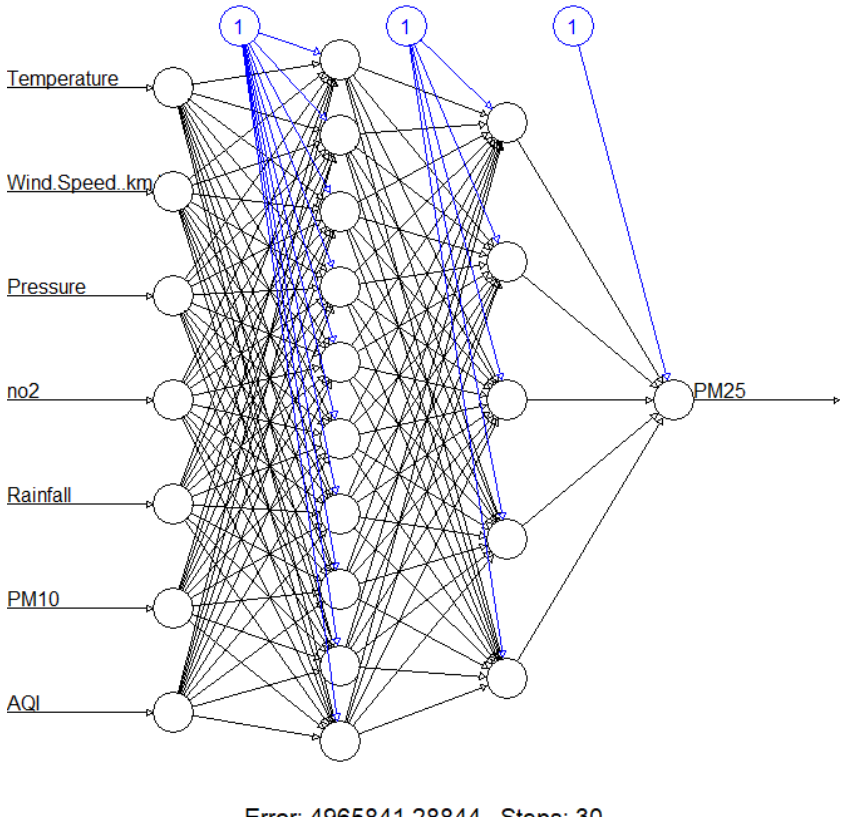

Figure 4.9: Neural Network Model

Procedure: AQI is set as the dependent variable,and the rest of the features are set as the independent variables.The data is converted into a matrix form,and is split into two independent samples, training and testing, 70 percent and 30 percent respectively.The test and train samples are then normalised, using Z Normalization.The tuned model has two hidden layer, with ten and five neurons. The activation function used in Rectified Linear Unit (relu). The input layer has one neuron each for the independent variables,and the output layer has one neuron for response. As we are using regression and the output variable is numeric, mse is used as the loss function ,and rmsprop is used as the optimizer function and mae is used as the metric function , to compile the model.To fit the model,the training data is used ,which is run over a 100 epochs,then to evaluate the model ,the testing data is used. The test data is used for getting the prediction.

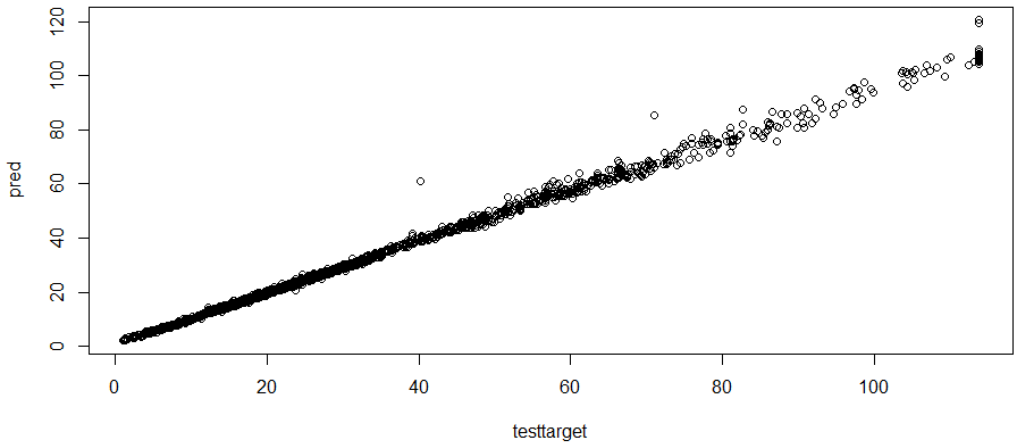

Figure 4.10: Predicted vs Testtarget Plot

4.2.3 XGBoost modelling

XGBoost is an ensemble learning algorithm that follows the principle of boosting. Boosting is a general term in ML where multiple weak learners such as regression trees are ensembled to create a single strong learner. The basic idea behind this procedure is to learn sequentially in which the current regression tree is fitted to the residuals (errors) from the previous trees. This new regression tree is then added to the fitted model to update the residuals. It is worth noting that statistical learning approaches that learn slowly such as boosting tend to perform well . The principle of gradient boosting further enhances the flexibility of the boosting algorithm by constructing the new regression trees to be maximally correlated to the negative of the gradient of the loss function. XGBoost is based on a gradient boosting algorithm proposed by Tianqi Chen .The XGBoost similar to the random forest is tuned using hyperparameters. A grid search on hyperparameters with 10-fold cross-validation was carried out to find the best model based on R square metrics.

Parameter	Range	Optimum value
n_estimators	70-5000	1500
max_depth	0-10	6
gamma	0.1-1	0.0468
min_child_weight	3-10	8

Table : XgBoost Parameters

Figure 4.11: Parameters

The root mean square value of xgboost is obtained as 0.7457792.

Cross validation in xgboost

Cross validation is a statistical method to evaluate machine learning models on unseen data. It comes in handy when the dataset is limited and prevents overfitting by not taking an independent sample (holdout) from training data for validation. By reducing the size of training data, we are compromising with the features and patterns hidden in the data which can further induce errors in our model. This is similar to cross_val_score functionality provided by the caret library. XGBoost uses built-in cross validation function cv(): xgb.cv()

2. k-fold Cross-validation — In k-fold cross-validation, data is shuffled and divided into k equal sized subsamples. One of the k subsamples is used as a test/validation set and remaining (k -1) subsamples are put together to be used as training data. Then we fit a model using training data and evaluate using the test set. This process is repeated k times so that every data point stays in validation set exactly once. The k results from each model should be averaged to get the final estimation. The advantage of this method is that we significantly reduce bias and variance and also increase the robustness of the model.

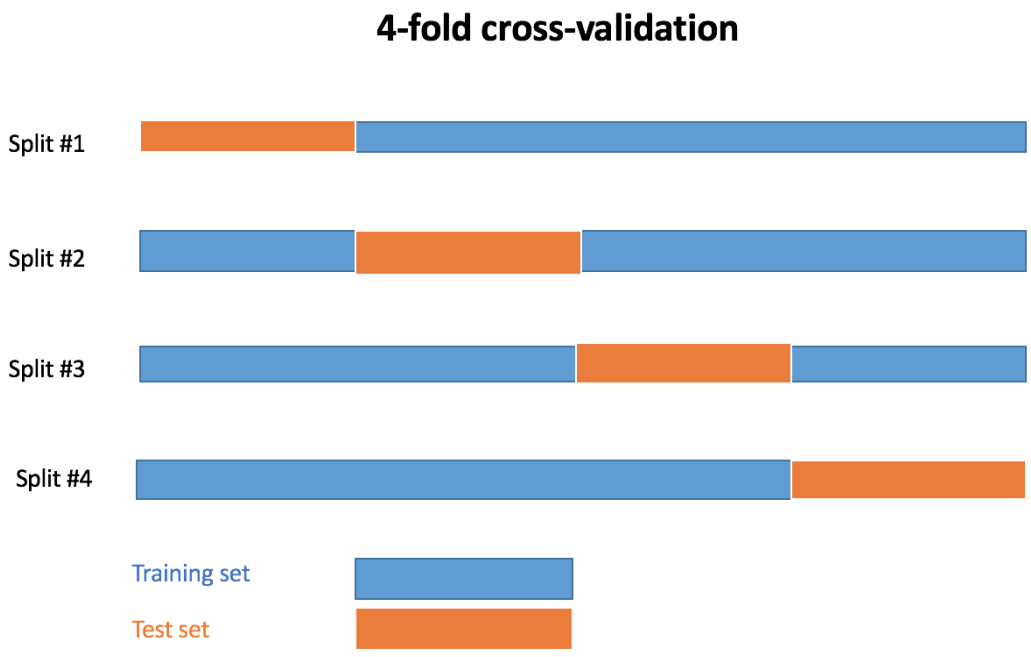

Figure 4.12: cross-validation

Feature Importance

Although it is important to be proficient in understanding the inner workings of the algorithm, Just showing that the algorithm predicts well is not enough. You have to attribute the predictions to the elements of the input data that contribute to your accuracy. feature importances which helps us explain the predictive power of the features in the dataset.

Sometimes it is just as important to understand how the features in our model contribute to prediction. The feature importances from xgboost are calculated based on the training data given to the model, not on predictions on a test dataset.by getting a better understanding of the model's logic you can not only verify it being correct but also work on improving the model by focusing only on the important variables

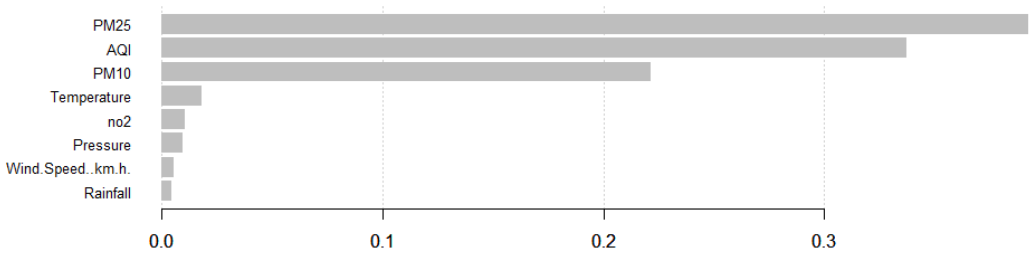

Figure 4.13: Feature Importance of xgBoost

4.2.4 CatBoost modelling

CatBoost is a new gradient boosting decision tree (GBDT) algorithm that can handle categorical features well. "CatBoost" name comes from two words "Category" and "Boosting". This algorithm is different from traditional GBDT algorithms. One main difference between CatBoost and other boosting algorithms is that the CatBoost implements symmetric trees. CatBoost is an ensemble of symmetric decision trees, whose symmetry structure endows it fewer parameters, faster training and testing, and higher accuracy. In addition, CatBoost replaces the gradient estimation method of the traditional gradient boosting algorithm with ordered boosting, thereby reducing the bias of the gradient estimation and improving the generalization capability The root mean square value of catboost is obtained as 0.6030147.

Parameters	Value
Iteration	1500
Learning rate	0.01
Depth	10
:Loss fuction	RMSE
Random seed	55
od type	Iter

Figure 4.14: Parameters

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