Capstone 1 - Statistical Data Analysis

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In the exploratory data analysis, we identified several features that were correlated with the Black Carbon (BC) and Nitrogen dioxide (NO2) concentrations. We observed strong positive or negative correlation for some features, and weak correlations for this rest. In this section, we perform statistical tests to identify the degree of correlation between the predictor and independent variable, and determine if there is multicollinearity between the predictor variables. We also identify the model that best fits the data for BC and NO2.

Identify features that have a high correlation, with a correlation coefficient above 0.9 or below -0.9, drop those features and fit a simple Linear Regression Model using OLS

Methodology:

First, we identify features that have a high correlation by setting a threshold of 0.9, and comparing each feature against all other features to check if the correlation matrix resulted in a value of >= 0.9 or <= -0.9, indicating a strong positive or negative correlation between features.

This test for multicollinearity will identify features that are highly correlated with each other. However, one of the assumptions of a linear regression model is that independent variables should be uncorrelated. Preserving highly correlated variables may result in coefficients from the regression not to be estimated precisely, and the standard errors are likely to be high.

Results:

BC Dataset:

By running the above test, we identified that for the BC dataset, the following features were not highly correlated

1. high-AsphaltPlant-10510811_dist
2. high-AsphaltPlant-808611_dist
3. high-AutoRepair-15714511_dist
4. Precip
5. Radiation
6. Maxtemp
7. Mintemp
8. Pressure
9. Number_intersections

Fitting a linear model using statsmodel with the above features resulted in the following summary statistics:

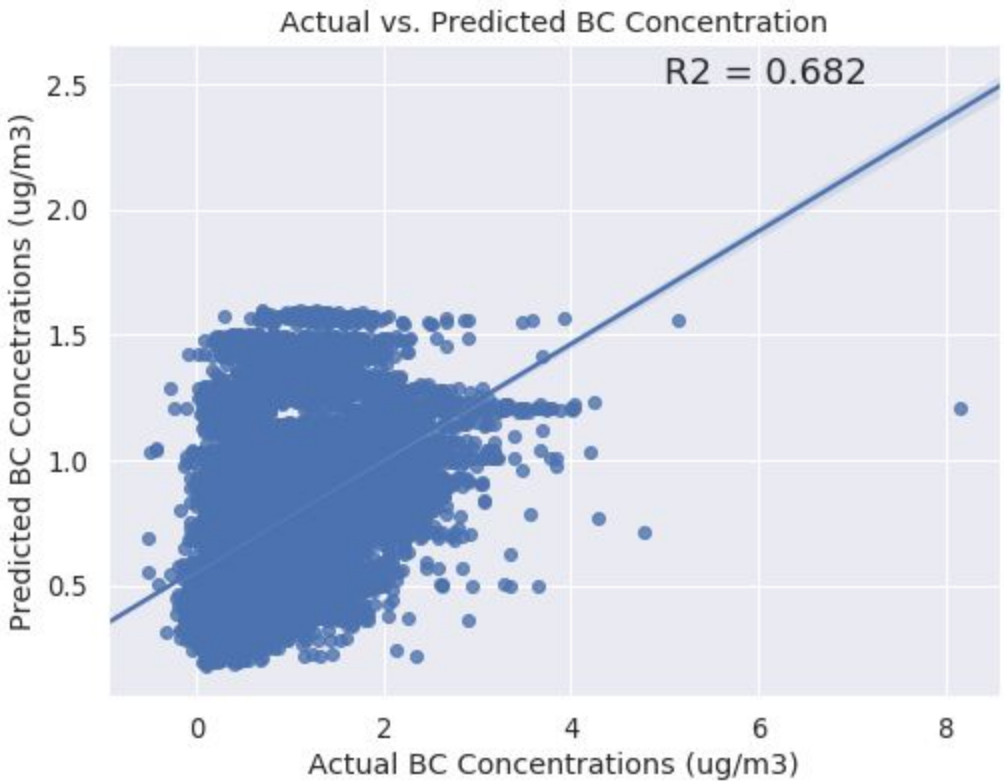
OLS Regression Results

Dep. Variable:	BC_Value	**R-squared (uncentered):**	0.682
Model:	OLS	**Adj. R-squared (uncentered):**	0.682
Method:	Least Squares	**F-statistic:**	5121.
Date:	Sun, 31 May 2020	**Prob (F-statistic):**	0.00
Time:	11:07:14	**Log-Likelihood:**	-16976.
No. Observations:	21488	**AIC:**	3.397e+04
Df Residuals:	21479	**BIC:**	3.404e+04
Df Model:	9		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
high-AsphaltPlant-10510811_dist	-0.0399	0.005	-8.699	0.000	-0.049	-0.031
high-AsphaltPlant-808611_dist	0.0155	0.004	4.270	0.000	0.008	0.023
high-AutoRepair-15714511_dist	0.0836	0.004	23.350	0.000	0.077	0.091
Precip	-2.7197	0.077	-35.422	0.000	-2.870	-2.569
Radiation	0.0899	0.002	36.860	0.000	0.085	0.095
Maxtemp	-1.5640	0.039	-40.448	0.000	-1.640	-1.488
Mintemp	0.2596	0.134	1.941	0.052	-0.003	0.522
Pressure	0.0039	0.002	2.092	0.036	0.000	0.008
number_intersections	-0.0121	0.001	-16.788	0.000	-0.013	-0.011

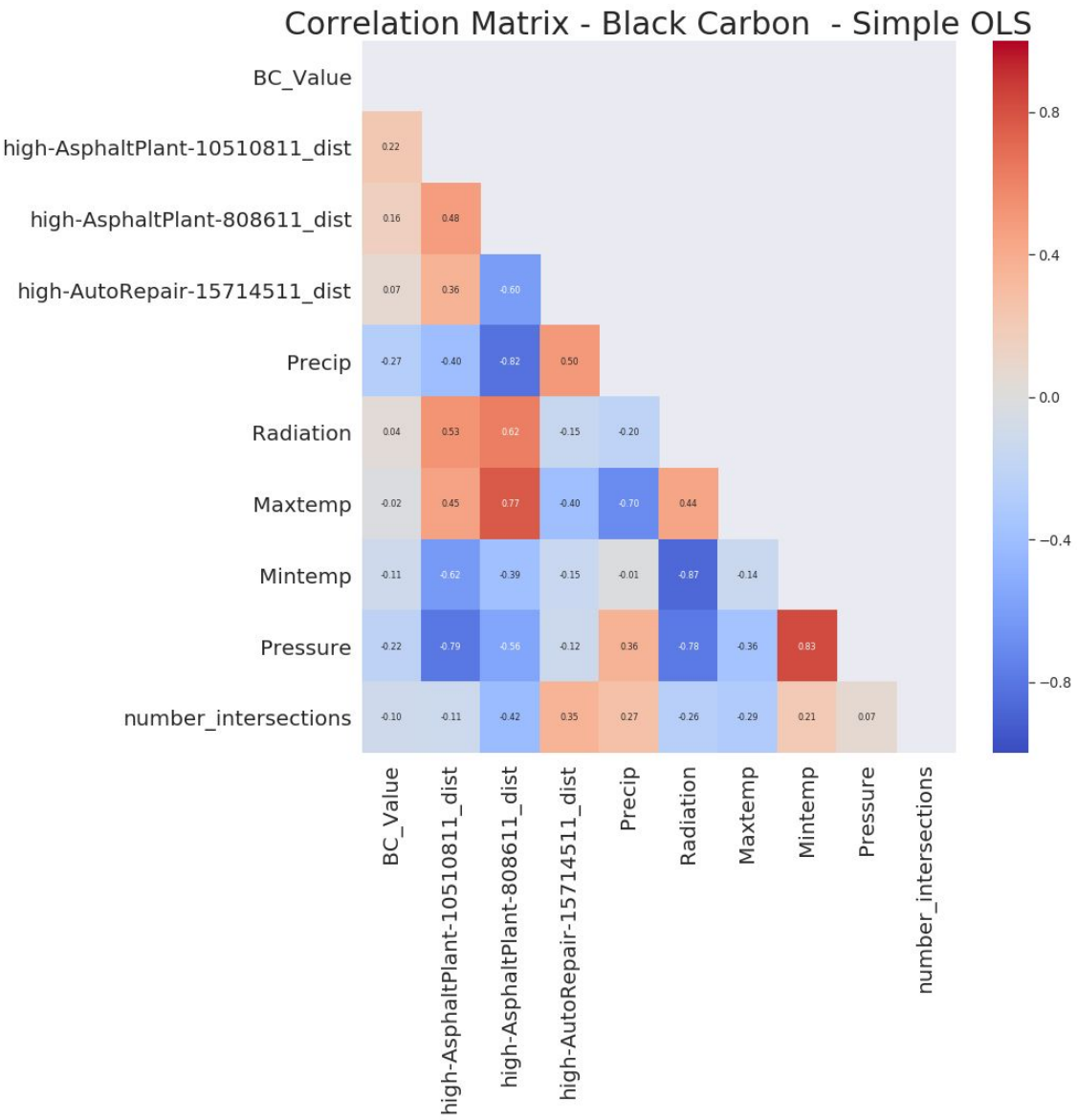
Omnibus:	5567.049	**Durbin-Watson:**	0.955
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	18211.398
Skew:	1.309	**Prob(JB):**	0.00
Kurtosis:	6.672	**Cond. No.**	3.97e+04

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 3.97e+04. This might indicate that there are
strong multicollinearity or other numerical problems.



A plot of the actual vs predicted BC concentration shows that a **linear regression model does a decent job** of predicting concentrations for BC, especially when the concentrations are below 1.5 ug/m3, but does not do a good job at higher concentrations.

Correlation heatmap of the above selected features is shown here:



NO2 Dataset:

Applying the above test for the NO2 dataset, we identify the following features were not highly correlated

1. high-AsphaltPlant-10510811_dist
2. high-AsphaltPlant-808611_dist
3. high-FoodPlant-340611_dist
4. Precip
5. Radiation
6. Maxtemp
7. Mintemp
8. Pressure
9. number_intersections

Fitting a linear model using statsmodel with the above features resulted in the following summary statistics:

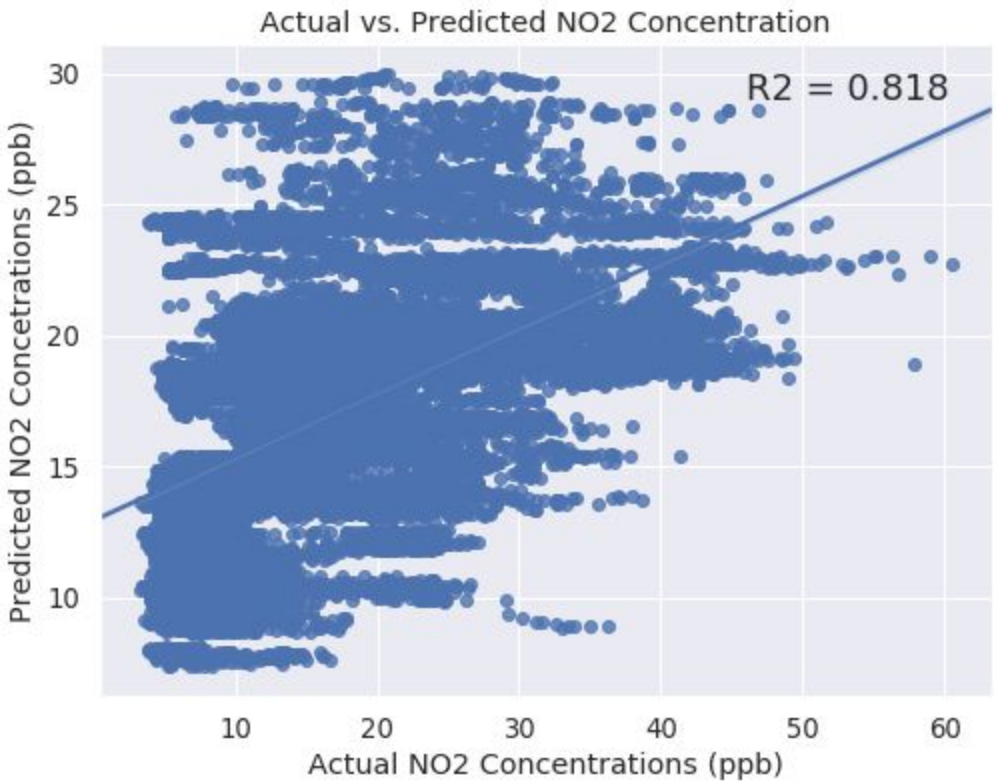
OLS Regression Results

Dep. Variable:	NO2_Value	**R-squared (uncentered):**	0.818
Model:	OLS	**Adj. R-squared (uncentered):**	0.818
Method:	Least Squares	**F-statistic:**	1.075e+04
Date:	Sun, 31 May 2020	**Prob (F-statistic):**	0.00
Time:	11:07:23	**Log-Likelihood:**	-76254.
No. Observations:	21488	**AIC:**	1.525e+05
Df Residuals:	21479	**BIC:**	1.526e+05
Df Model:	9		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
high-AsphaltPlant-10510811_dist	0.1445	0.072	2.017	0.044	0.004	0.285
high-AsphaltPlant-808611_dist	-0.1970	0.057	-3.447	0.001	-0.309	-0.085
high-FoodPlant-340611_dist	0.9573	0.057	16.924	0.000	0.846	1.068
Precip	-43.8396	1.213	-36.156	0.000	-46.216	-41.463
Radiation	1.6794	0.038	43.681	0.000	1.604	1.755
Maxtemp	-29.0032	0.610	-47.551	0.000	-30.199	-27.808
Mintemp	8.8408	2.111	4.189	0.000	4.704	12.978
Pressure	0.0129	0.029	0.442	0.658	-0.044	0.070
number_intersections	-0.0728	0.011	-6.411	0.000	-0.095	-0.051

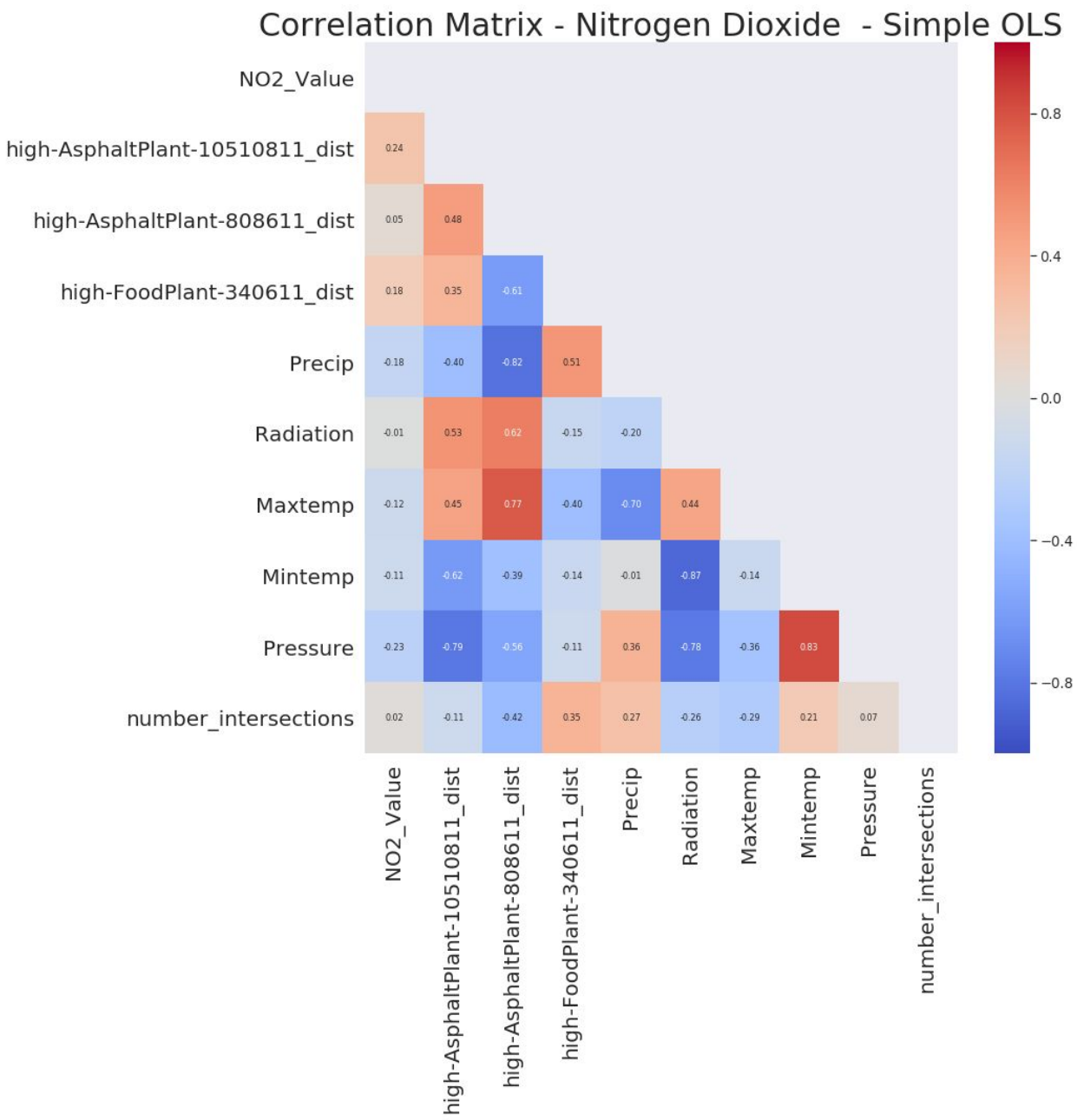
Omnibus:	1881.925	**Durbin-Watson:**	0.815
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	2437.379
Skew:	0.772	**Prob(JB):**	0.00
Kurtosis:	3.579	**Cond. No.**	3.97e+04

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 3.97e+04. This might indicate that there are strong multicollinearity or other numerical problems.



Once again, the above plot shows that the simple linear model does a decent job of predicting concentrations below 30 ppb, but does not perform well at high concentrations.

A correlation heatmap of selected features is shown here:



Summary:

The OLS for both the BC and NO2 datasets results in a model with a decent R2 value indicating that linear regression model may result in the good fit, at least with just the features that are not highly correlated. However, these features have a very high Variance Inflation Scores resulting in multicollinearity. We can try better algorithms that may result in a better fit.

Step Forward Approach with VIF Scores and R2 estimation

The approach here is to start with the feature that results in the best R2 value, and then loop through all the features by adding features sequentially. Each time a new feature is added, we calculate the R2 for the new model, and determine if the new R2 is higher than the previously estimated R2 value. If the R2 is higher, then we calculate the VIF scores with addition of each feature. If the VIF score of any of the features increases above threshold of 10, then we drop the newly added feature. This process continues until we determine the best set of features that results in highest R2 value, and VIF scores < 10.

A VIF is the quotient of the variance in a model with multiple terms by the variance of a model with one term alone. It quantifies the severity of multicollinearity in an ordinary least squares regression analysis.

Methodology:
Prior to applying the VIF methodology, the column names for the predictor variables were transformed to the format Q('column name') since some column names contain numbers. The data was then split into test, train dataset to get the best generalizable features.

The first step is to loop through all the features, and fit a simple OLS model for each feature individually. Determine the feature that results in the largest R2 value. Next, we loop through the features again, and recalculate the R2 value for the addition of each new feature. If the R2 value for the model with newly added feature is larger than the previously estimated R2, we calculate the VIF scores and determine if all the VIF scores are below 10. If ***any*** score exceeds 10, then we drop the newly added feature.

Finally, we recalculate VIF score for the remaining features, and fit an OLS on the remaining features.

Results:

BC dataset:
For the BC dataset, only 'Radiation' as a feature was selected and the OLS fit resulted in an R2 value of 0.593 for the training data and 0.584 for the test data.

Results of the OLS model fit with the selected features are shown below.

Training data:

```
(     VIF Factor        features
 0  46676.348204       Intercept
 1      1.000000  Q('Radiation'), <class 'statsmodels.iolib.summary.Summary'>
 """
                                OLS Regression Results
==============================================================================
Dep. Variable:               BC_Value   R-squared (uncentered):                   0.593
Model:                            OLS   Adj. R-squared (uncentered):              0.593
Method:                 Least Squares   F-statistic:                         2.190e+04
Date:                Sun, 14 Jun 2020   Prob (F-statistic):                       0.00
Time:                        23:17:33   Log-Likelihood:                         -13655.
No. Observations:               15041   AIC:                                    2.731e+04
Df Residuals:                   15040   BIC:                                    2.732e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                     coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Q('Radiation')     0.0021   1.42e-05    147.979      0.000       0.002       0.002
==============================================================================
Omnibus:                     3927.252   Durbin-Watson:                   2.017
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             8782.050
Skew:                           1.502   Prob(JB):                         0.00
Kurtosis:                       5.234   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
""")
```

Test data:

```
(     VIF Factor        features
 0  46894.386704       Intercept
 1      1.000000  Q('Radiation'), <class 'statsmodels.iolib.summary.Summary'>
 """
                                OLS Regression Results
==============================================================================
Dep. Variable:               BC_Value   R-squared (uncentered):                   0.584
Model:                            OLS   Adj. R-squared (uncentered):              0.584
Method:                 Least Squares   F-statistic:                              9059.
Date:                Sun, 14 Jun 2020   Prob (F-statistic):                       0.00
Time:                        23:18:10   Log-Likelihood:                         -6045.7
No. Observations:                6447   AIC:                                    1.209e+04
Df Residuals:                    6446   BIC:                                    1.210e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                     coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Q('Radiation')     0.0021   2.24e-05     95.176      0.000       0.002       0.002
==============================================================================
Omnibus:                     2496.187   Durbin-Watson:                   1.995
Prob(Omnibus):                  0.000   Jarque-Bera (JB):            12776.889
Skew:                           1.804   Prob(JB):                         0.00
Kurtosis:                       8.877   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
""")
```

NO2 dataset:

For the NO2 dataset, only ‘Radiation’ as a feature was selected and the OLS fit resulted in an R2 value of 0.759 for the training data and 0.757 for the test data.

Results of the OLS model fit with the selected features are shown below.

Training data:

```
(     VIF Factor        features
 0  46676.348204       Intercept
 1      1.000000  Q('Radiation'), <class 'statsmodels.iolib.summary.Summary'>
 """
                            OLS Regression Results
==============================================================================
Dep. Variable:              NO2_Value   R-squared (uncentered):                   0.759
Model:                            OLS   Adj. R-squared (uncentered):              0.759
Method:                 Least Squares   F-statistic:                          4.748e+04
Date:                Sun, 14 Jun 2020   Prob (F-statistic):                        0.00
Time:                        23:25:17   Log-Likelihood:                         -55437.
No. Observations:               15041   AIC:                                  1.109e+05
Df Residuals:                   15040   BIC:                                  1.109e+05
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                     coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Q('Radiation')     0.0499      0.000    217.896      0.000       0.049       0.050
==============================================================================
Omnibus:                     1777.290   Durbin-Watson:                   2.016
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             2467.291
Skew:                           0.969   Prob(JB):                         0.00
Kurtosis:                       3.425   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
""")
```

Test data:

```
(     VIF Factor        features
 0  46894.386704       Intercept
 1      1.000000  Q('Radiation'), <class 'statsmodels.iolib.summary.Summary'>
 """
                            OLS Regression Results
==============================================================================
Dep. Variable:              NO2_Value   R-squared (uncentered):                   0.757
Model:                            OLS   Adj. R-squared (uncentered):              0.757
Method:                 Least Squares   F-statistic:                          2.004e+04
Date:                Sun, 14 Jun 2020   Prob (F-statistic):                        0.00
Time:                        23:26:25   Log-Likelihood:                         -23872.
No. Observations:               6447   AIC:                                  4.775e+04
Df Residuals:                   6446   BIC:                                  4.775e+04
Df Model:                          1
Covariance Type:            nonrobust
==============================================================================
                     coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Q('Radiation')     0.0504      0.000    141.555      0.000       0.050       0.051
==============================================================================
Omnibus:                      732.467   Durbin-Watson:                   1.995
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1003.036
Skew:                           0.950   Prob(JB):                    1.56e-218
Kurtosis:                       3.348   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
""")
```

Summary:

The stepforward approach with VIF and R2 estimation resulted in the selection of only one single feature, which is Radiation. This feature seems to result in the highest R2 with concentration, and addition of other features to the model does not improve performance.

Lasso Regularization with GridSearch

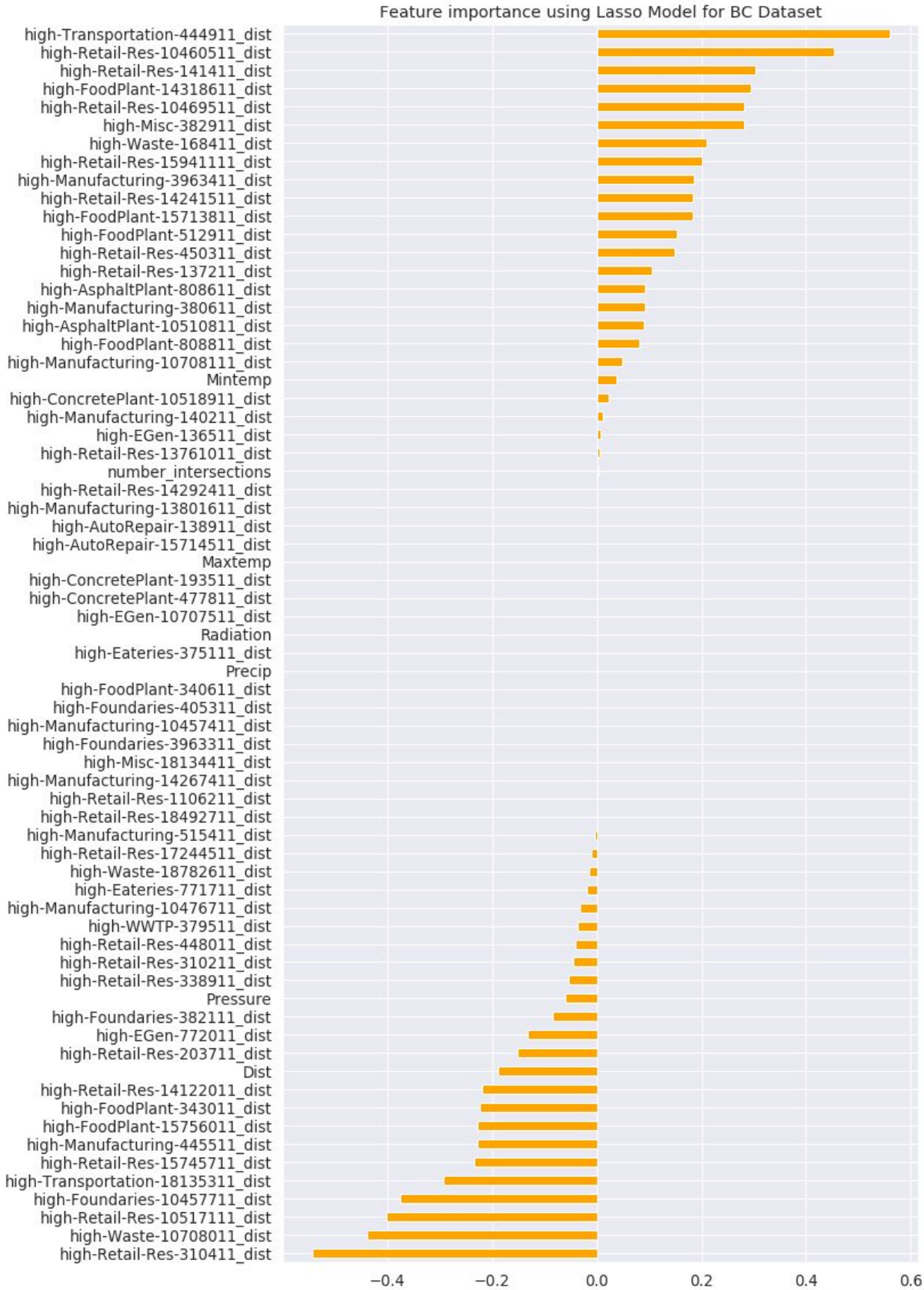
Methodology:
In this method, we do feature selection using Lasso Regularization. The lasso regularization will penalize a feature's coefficient by making it 0, if a feature is irrelevant. In this case, all features with coefficient = 0 can be removed from the model. In this approach, we first split the data into test and train set, perform a 5-fold Lasso cross validation on the training data. We then determine the optimal value for alpha that gives the best fit for the training data, use that value of alpha to refit the training data and predict on the test set. We compute the mean squared error on the test data, and the model score. Once the features are determined by Lasso, we again apply the step forward feature selection approach with R2 and VIF estimation to select features that are not highly collinear.

Results:

BC dataset:
For the BC dataset,

```
Best Alpha using LassoCV =  0.00015274253372807208
MSE on test data =  0.07799639454945655
Best score using LassoCV:  0.5345421171448599
```

The features that were selected are as follows. In total, Lasso picked 49 features out of the 68 features, as shown below:


Feature importance using Lasso Model for BC Dataset
high-Transportation-444911_dist
high-Retail-Res-10460511_dist
high-Retail-Res-141411_dist
high-FoodPlant-14318611_dist
high-Retail-Res-10469511_dist
high-Misc-382911_dist
high-Waste-168411_dist
high-Retail-Res-15941111_dist
high-Manufacturing-3963411_dist
high-Retail-Res-14241511_dist
high-FoodPlant-15713811_dist
high-FoodPlant-512911_dist
high-Retail-Res-450311_dist
high-Retail-Res-137211_dist
high-AsphaltPlant-808611_dist
high-Manufacturing-380611_dist
high-AsphaltPlant-10510811_dist
high-FoodPlant-808811_dist
high-Manufacturing-10708111_dist
Mintemp
high-ConcretePlant-10518911_dist
high-Manufacturing-140211_dist
high-EGen-136511_dist
high-Retail-Res-13761011_dist
number_intersections
high-Retail-Res-14292411_dist
high-Manufacturing-13801611_dist
high-AutoRepair-138911_dist
high-AutoRepair-15714511_dist
Maxtemp
high-ConcretePlant-193511_dist
high-ConcretePlant-477811_dist
high-EGen-10707511_dist
Radiation
high-Eateries-375111_dist
Precip
high-FoodPlant-340611_dist
high-Foundaries-405311_dist
high-Manufacturing-10457411_dist
high-Foundaries-3963311_dist
high-Misc-18134411_dist
high-Manufacturing-14267411_dist
high-Retail-Res-1106211_dist
high-Retail-Res-18492711_dist
high-Manufacturing-515411_dist
high-Retail-Res-17244511_dist
high-Waste-18782611_dist
high-Eateries-771711_dist
high-Manufacturing-10476711_dist
high-WWTP-379511_dist
high-Retail-Res-448011_dist
high-Retail-Res-310211_dist
high-Retail-Res-338911_dist
Pressure
high-Foundaries-382111_dist
high-EGen-772011_dist
high-Retail-Res-203711_dist
Dist
high-Retail-Res-14122011_dist
high-FoodPlant-343011_dist
high-FoodPlant-15756011_dist
high-Manufacturing-445511_dist
high-Retail-Res-15745711_dist
high-Transportation-18135311_dist
high-Foundaries-10457711_dist
high-Retail-Res-10517111_dist
high-Waste-10708011_dist
high-Retail-Res-310411_dist
−0.4
−0.2
0.0
0.2
0.4
0.6

Results of the OLS model fit for BC:

OLS Regression Results

Dep. Variable:	BC_Value	**R-squared (uncentered):**	0.827
Model:	OLS	**Adj. R-squared (uncentered):**	0.827
Method:	Least Squares	**F-statistic:**	2099.
Date:	Sun, 31 May 2020	**Prob (F-statistic):**	0.00
Time:	11:13:46	**Log-Likelihood:**	-10408.
No. Observations:	21488	**AIC:**	2.091e+04
Df Residuals:	21439	**BIC:**	2.131e+04
Df Model:	49		
Covariance Type:	nonrobust		

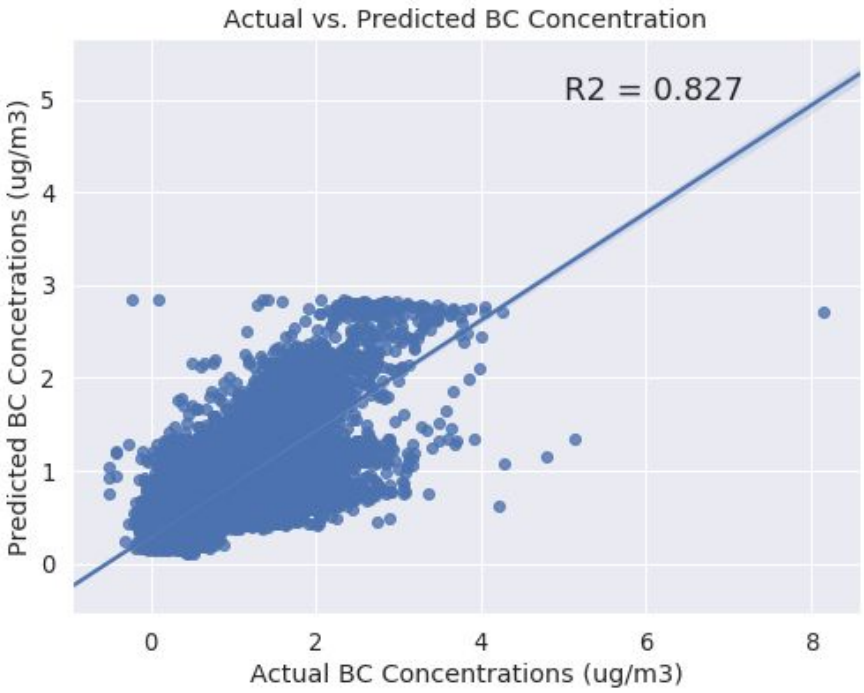
	coef	std err	t	P>|t|	[0.025	0.975]
high-AsphaltPlant-10510811_dist	4.0567	0.436	9.295	0.000	3.201	4.912
high-AsphaltPlant-808611_dist	-41.9524	3.269	-12.835	0.000	-48.359	-35.546
high-ConcretePlant-10518911_dist	-1.0495	0.095	-11.074	0.000	-1.235	-0.864
high-EGen-136511_dist	4.4218	0.398	11.120	0.000	3.642	5.201
high-EGen-772011_dist	-0.9109	0.106	-8.580	0.000	-1.119	-0.703
high-Eateries-771711_dist	4.5713	0.659	6.935	0.000	3.279	5.863
high-FoodPlant-14318611_dist	15.2293	1.193	12.762	0.000	12.890	17.568
high-FoodPlant-15713811_dist	-0.3450	0.094	-3.684	0.000	-0.529	-0.161
high-FoodPlant-15756011_dist	-2.8975	0.524	-5.528	0.000	-3.925	-1.870
high-FoodPlant-343011_dist	-1.6590	0.178	-9.327	0.000	-2.008	-1.310
high-FoodPlant-512911_dist	-4.0435	0.833	-4.851	0.000	-5.677	-2.410
high-FoodPlant-808811_dist	0.5232	0.082	6.355	0.000	0.362	0.685
high-Foundaries-10457711_dist	-4.4442	1.363	-3.260	0.001	-7.116	-1.772
high-Foundaries-382111_dist	0.2678	0.113	2.372	0.018	0.047	0.489
high-Manufacturing-10476711_dist	3.1388	0.230	13.655	0.000	2.688	3.589
high-Manufacturing-10708111_dist	0.4735	0.197	2.408	0.016	0.088	0.859
high-Manufacturing-140211_dist	1.2277	0.833	1.474	0.140	-0.405	2.860

high-Manufacturing-380611_dist	2.2972	0.328	7.010	0.000	1.655	2.939
high-Manufacturing-3963411_dist	10.2872	1.892	5.437	0.000	6.579	13.996
high-Manufacturing-445511_dist	21.6157	4.852	4.455	0.000	12.106	31.125
high-Manufacturing-515411_dist	-1.4269	0.419	-3.407	0.001	-2.248	-0.606
high-Misc-382911_dist	0.2670	0.038	7.094	0.000	0.193	0.341
high-Retail-Res-10460511_dist	1.4084	0.284	4.966	0.000	0.852	1.964
high-Retail-Res-10469511_dist	1.7054	0.103	16.523	0.000	1.503	1.908
high-Retail-Res-10517111_dist	35.1287	3.896	9.016	0.000	27.492	42.766
high-Retail-Res-137211_dist	0.8309	0.080	10.365	0.000	0.674	0.988
high-Retail-Res-13761011_dist	0.5070	0.107	4.750	0.000	0.298	0.716
high-Retail-Res-14122011_dist	-0.5406	0.055	-9.804	0.000	-0.649	-0.432
high-Retail-Res-141411_dist	0.3273	0.040	8.281	0.000	0.250	0.405
high-Retail-Res-14241511_dist	0.5724	0.106	5.385	0.000	0.364	0.781
high-Retail-Res-15745711_dist	-0.0809	0.107	-0.754	0.451	-0.291	0.129
high-Retail-Res-15941111_dist	0.1098	0.099	1.111	0.267	-0.084	0.304
high-Retail-Res-17244511_dist	-11.4232	3.319	-3.442	0.001	-17.928	-4.919
high-Retail-Res-203711_dist	34.4138	2.578	13.351	0.000	29.361	39.466
high-Retail-Res-310211_dist	0.3069	0.060	5.112	0.000	0.189	0.425
high-Retail-Res-310411_dist	-27.4632	1.394	-19.703	0.000	-30.195	-24.731
high-Retail-Res-338911_dist	-9.9571	1.077	-9.248	0.000	-12.068	-7.847
high-Retail-Res-448011_dist	-21.4297	2.174	-9.855	0.000	-25.692	-17.168
high-Retail-Res-450311_dist	0.3393	0.026	13.079	0.000	0.288	0.390
high-Transportation-18135311_dist	-1.0254	0.107	-9.554	0.000	-1.236	-0.815
high-Transportation-444911_dist	2.6736	0.415	6.449	0.000	1.861	3.486
high-WWTP-379511_dist	0.0058	0.167	0.035	0.972	-0.322	0.334
high-Waste-10708011_dist	-13.0775	2.679	-4.882	0.000	-18.328	-7.827
high-Waste-168411_dist	1.0897	0.102	10.725	0.000	0.891	1.289
high-Waste-18782611_dist	-3.8877	1.119	-3.474	0.001	-6.081	-1.694
Mintemp	1.0414	0.116	9.004	0.000	0.815	1.268
Pressure	-0.0284	0.002	-17.120	0.000	-0.032	-0.025
Dist	-0.1226	0.015	-8.152	0.000	-0.152	-0.093
number_intersections	0.0018	0.001	2.057	0.040	8.62e-05	0.004

Omnibus:	7523.079	**Durbin-Watson:**	1.483
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	55141.437
Skew:	1.493	**Prob(JB):**	0.00
Kurtosis:	10.258	**Cond. No.**	2.19e+06

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 2.19e+06. This might indicate that there are
strong multicollinearity or other numerical problems.

A scatter plot of the predicted vs actual concentrations are shown below, with an R2 value of 0.827.



This indicates that the Lasso regression approach outperforms both the simple OLS and the Step forward VIF approach.

However, most of the correlation coefficients are really high and the OLS model indicates that there is strong multicolinearity present. To overcome this, once again we perform a stepforward VIF approach, where we start with the 49 features that were selected by the Lasso model, and sequentially add features that results in the maximum R2 and lowest VIF scores.

Results of the step forward VIF approach for Lasso:

Only the ‘Mintemp’ feature is selected by the step forward VIF approach and the R2 for the training set was 0.592, and the test set was 0.583.

NO2 dataset:

For the NO2 dataset,

```
Best Alpha using LassoCV =  0.00038952008419926016
MSE on test data =  0.20860434953284926
Best score using LassoCV:  0.6395777236551858
```

The features that were selected are as follows. In total, the lasso approach selected 42 features out of 61 features.


Feature importance using Lasso Model for NO2 Dataset
high-Transportation-444911_dist
high-Retail-Res-10460511_dist
high-Misc-18132711_dist
high-WWTP-379511_dist
high-Misc-382911_dist
high-FoodPlant-512911_dist
high-Manufacturing-13983311_dist
high-Retail-Res-127511_dist
high-AsphaltPlant-10510811_dist
high-EGen-136511_dist
high-Manufacturing-140211_dist
high-Retail-Res-18697911_dist
high-Retail-Res-200611_dist
high-Retail-Res-18495611_dist
Mintemp
number_intersections
high-Misc-15974511_dist
high-Manufacturing-10457511_dist
high-Eateries-771711_dist
high-Retail-Res-13761011_dist
high-Manufacturing-3963411_dist
high-FoodPlant-808811_dist
high-Manufacturing-14267411_dist
Precip
high-Manufacturing-445511_dist
high-Manufacturing-14182811_dist
Radiation
high-Foundaries-405311_dist
high-Manufacturing-4955911_dist
high-Foundaries-382111_dist
Maxtemp
high-FoodPlant-340611_dist
high-FoodPlant-14318611_dist
high-EGen-10707511_dist
high-AutoRepair-195711_dist
high-Retail-Res-310411_dist
high-Retail-Res-10517111_dist
high-Retail-Res-18496511_dist
high-Waste-10708011_dist
high-Retail-Res-18135811_dist
high-Retail-Res-15745711_dist
high-Retail-Res-13825511_dist
high-Retail-Res-310211_dist
Pressure
high-Retail-Res-18697211_dist
high-Retail-Res-18133511_dist
high-Eateries-375111_dist
high-Retail-Res-448011_dist
high-Manufacturing-14071611_dist
high-Retail-Res-7845611_dist
high-Retail-Res-338911_dist
high-Misc-13985611_dist
high-Retail-Res-14122011_dist
Dist
high-FoodPlant-804911_dist
high-Retail-Res-15721111_dist
high-AsphaltPlant-808611_dist
high-Manufacturing-773811_dist
high-WWTP-203811_dist
−1.0
−0.5
0.0
0.5
1.0
1.5

Results of the OLS model fit:

OLS Regression Results

Dep. Variable:	NO2_Value	**R-squared (uncentered):**	0.912
Model:	OLS	**Adj. R-squared (uncentered):**	0.911
Method:	Least Squares	**F-statistic:**	5268.
Date:	Sun, 31 May 2020	**Prob (F-statistic):**	0.00
Time:	11:13:52	**Log-Likelihood:**	-68511.
No. Observations:	21488	**AIC:**	1.371e+05
Df Residuals:	21446	**BIC:**	1.374e+05
Df Model:	42		
Covariance Type:	nonrobust		

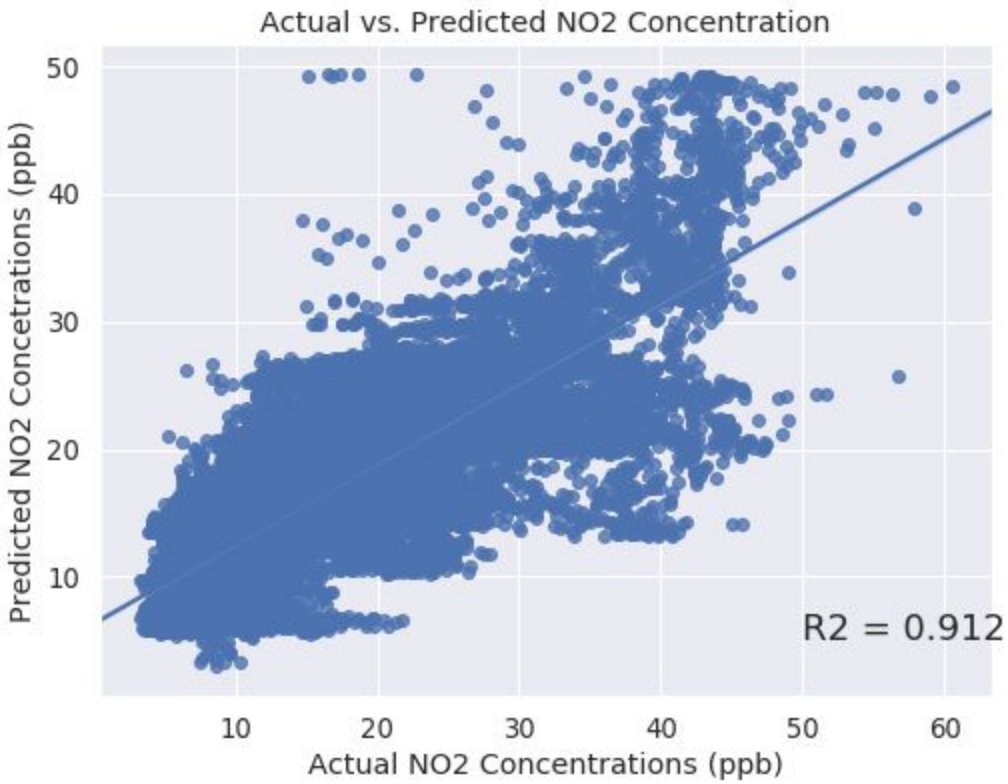
	coef	std err	t	P>|t|	[0.025	0.975]
high-AsphaltPlant-10510811_dist	32.3134	2.068	15.622	0.000	28.259	36.368
high-AsphaltPlant-808611_dist	-8249.1066	1179.534	-6.994	0.000	-1.06e+04	-5937.132
high-EGen-136511_dist	37.1751	3.570	10.413	0.000	30.178	44.173
high-Eateries-375111_dist	4945.4679	731.520	6.761	0.000	3511.634	6379.301
high-Eateries-771711_dist	-16.3971	3.835	-4.276	0.000	-23.913	-8.881
high-FoodPlant-512911_dist	-74.7029	11.637	-6.420	0.000	-97.512	-51.894
high-FoodPlant-804911_dist	-39.5776	4.700	-8.421	0.000	-48.789	-30.366
high-FoodPlant-808811_dist	-11.2241	2.503	-4.483	0.000	-16.131	-6.317
high-Manufacturing-10457511_dist	9.1533	2.327	3.934	0.000	4.593	13.714
high-Manufacturing-13983311_dist	13.4396	0.718	18.713	0.000	12.032	14.847
high-Manufacturing-140211_dist	32.5681	4.404	7.395	0.000	23.936	41.201
high-Manufacturing-14071611_dist	732.8911	86.306	8.492	0.000	563.725	902.057
high-Manufacturing-14267411_dist	-4.7073	1.479	-3.182	0.001	-7.607	-1.808
high-Manufacturing-3963411_dist	148.9537	25.301	5.887	0.000	99.362	198.545
high-Manufacturing-773811_dist	-81.1912	3.262	-24.888	0.000	-87.586	-74.797
high-Misc-13985611_dist	-17.7073	2.432	-7.281	0.000	-22.474	-12.940
high-Misc-15974511_dist	-18.6592	2.763	-6.753	0.000	-24.075	-13.243
high-Misc-18132711_dist	18.4679	1.443	12.794	0.000	15.639	21.297
high-Misc-382911_dist	2.1365	0.513	4.166	0.000	1.131	3.142
high-Retail-Res-10460511_dist	-8.7317	6.954	-1.256	0.209	-22.363	4.900
high-Retail-Res-127511_dist	3.4740	1.077	3.225	0.001	1.362	5.586

high-Retail-Res-13761011_dist	-8.7124	1.868	-4.664	0.000	-12.374	-5.051
high-Retail-Res-13825511_dist	-549.0568	80.329	-6.835	0.000	-706.508	-391.605
high-Retail-Res-14122011_dist	-4.4559	0.681	-6.539	0.000	-5.792	-3.120
high-Retail-Res-15721111_dist	-52.3147	3.257	-16.060	0.000	-58.699	-45.930
high-Retail-Res-18133511_dist	7.1740	4.101	1.749	0.080	-0.864	15.212
high-Retail-Res-18495611_dist	5.0519	1.102	4.584	0.000	2.892	7.212
high-Retail-Res-18697211_dist	1.1972	1.982	0.604	0.546	-2.688	5.083
high-Retail-Res-18697911_dist	-0.9889	1.588	-0.623	0.533	-4.101	2.123
high-Retail-Res-200611_dist	-1.8877	1.461	-1.292	0.196	-4.751	0.975
high-Retail-Res-310211_dist	3.4964	1.734	2.017	0.044	0.098	6.894
high-Retail-Res-338911_dist	343.1114	48.150	7.126	0.000	248.733	437.490
high-Retail-Res-448011_dist	295.8299	41.376	7.150	0.000	214.730	376.929
high-Retail-Res-7845611_dist	3214.2432	443.922	7.241	0.000	2344.123	4084.364
high-Transportation-444911_dist	80.2390	4.880	16.441	0.000	70.673	89.805
high-WWTP-203811_dist	-796.7642	98.315	-8.104	0.000	-989.468	-604.060
high-WWTP-379511_dist	10.4299	1.830	5.699	0.000	6.842	14.017
Precip	3.2921	2.402	1.370	0.171	-1.416	8.000
Mintemp	12.1718	2.307	5.277	0.000	7.650	16.693
Pressure	-0.2900	0.033	-8.854	0.000	-0.354	-0.226
Dist	-2.2286	0.417	-5.350	0.000	-3.045	-1.412
number_intersections	0.1638	0.013	12.745	0.000	0.139	0.189

Omnibus:	3716.569	**Durbin-Watson:**	1.331
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	8745.204
Skew:	0.986	**Prob(JB):**	0.00
Kurtosis:	5.425	**Cond. No.**	3.34e+07

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 3.34e+07. This might indicate that there are
strong multicollinearity or other numerical problems.

A plot of the predicted vs actual concentrations are shown below, and the model has an R2 value of 0.912.



The above approach indicates that the Lasso approach outperforms the simple OLS and the stepforward VIF methodology, resulting in a much better prediction, even at high concentrations.

However, most of the correlation coefficients are really high and the OLS model indicates that there is strong multicolinearity present. To overcome this, once again we perform a stepforward VIF approach, where we start with the 42 features that were selected by the Lasso model, and sequentially add features that results in the maximum R2 and lowest VIF scores.

Results of the step forward VIF approach for Lasso:
Similar to the BC dataset, only min temp was selected as feature and R2 value for the training set was 0.759, and test set was 0.756.

Summary:
The lasso approach results in a much better model fit than simple OLS. But the features selected by the lasso model are still highly correlated with each other which may not result in a great fit for a validation set. The step forward VIF approach with lasso resulted in the selection of features that had lower model coefficients, and also gave us some insight on feature importance.

Feature Selection Using Random Forest

Feature selection using the Random Forest approach comes under the category of embedded methods as it combines qualities of filter and wrapper methods. Feature selection in random forest is done by building sevel decision trees, and each tree is built over a random extraction of the observations from the dataset and a random extraction of the features. Not every tree sees all the features or all the observations, and this guarantees that the trees are de-correlated and therefore less prone to over-fitting.

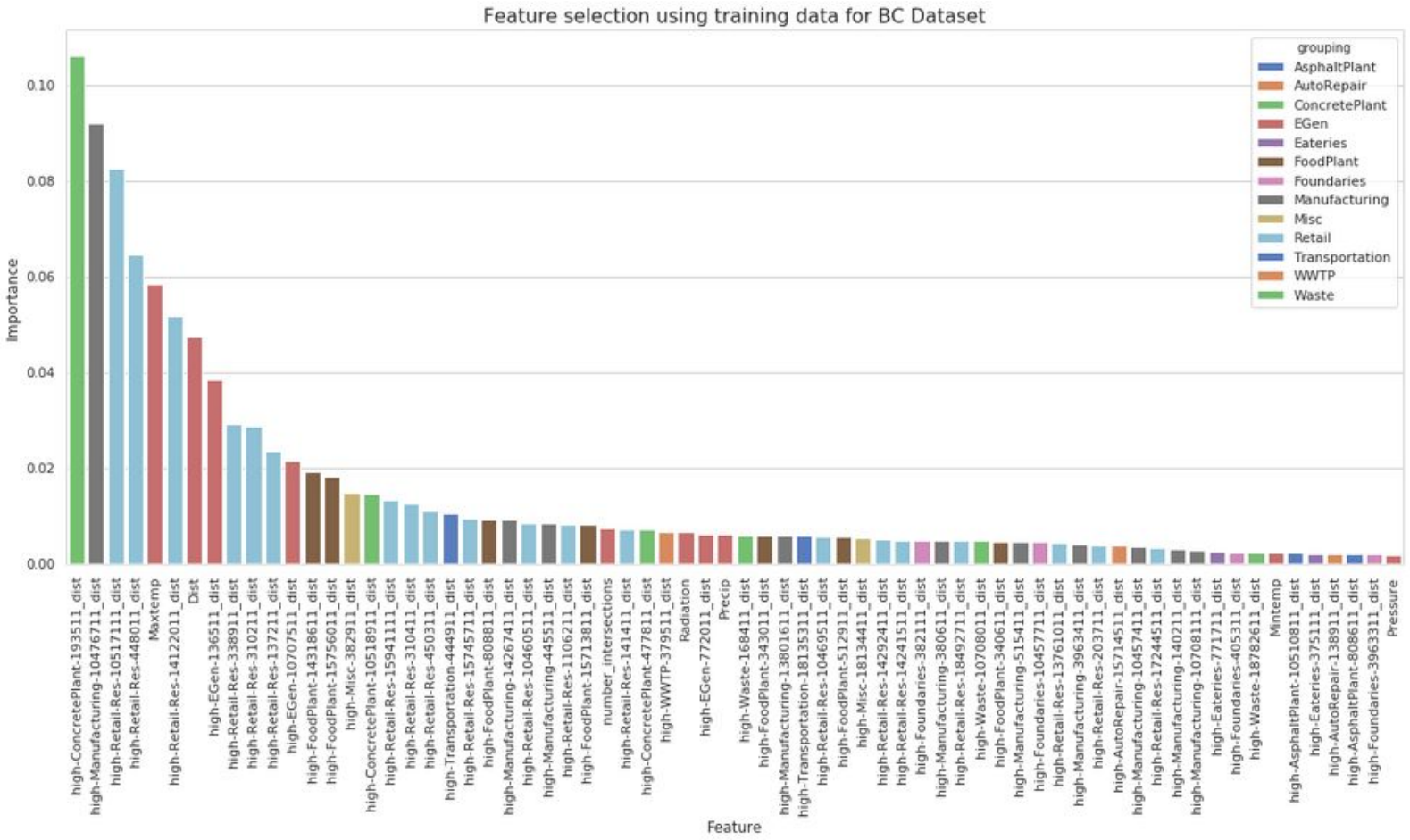
Methodology:

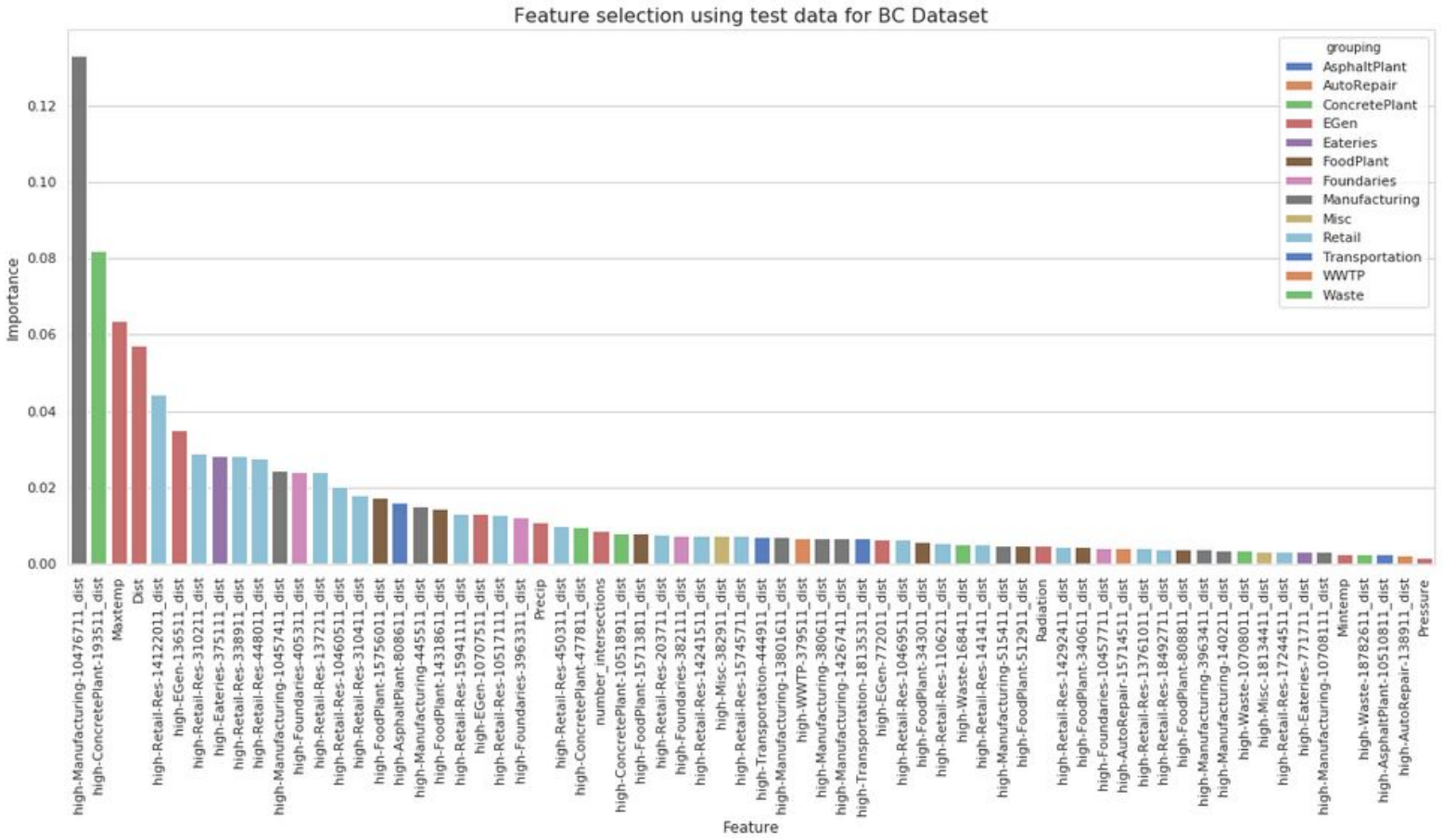
Once again, we split the data into test and train set and apply the RandomForestRegressor() function, and the feature importance attribute to understand the importance of features. Here, n_estimators is set at 100.

Results:

BC dataset:

Graphs below show the feature importance for training and test data

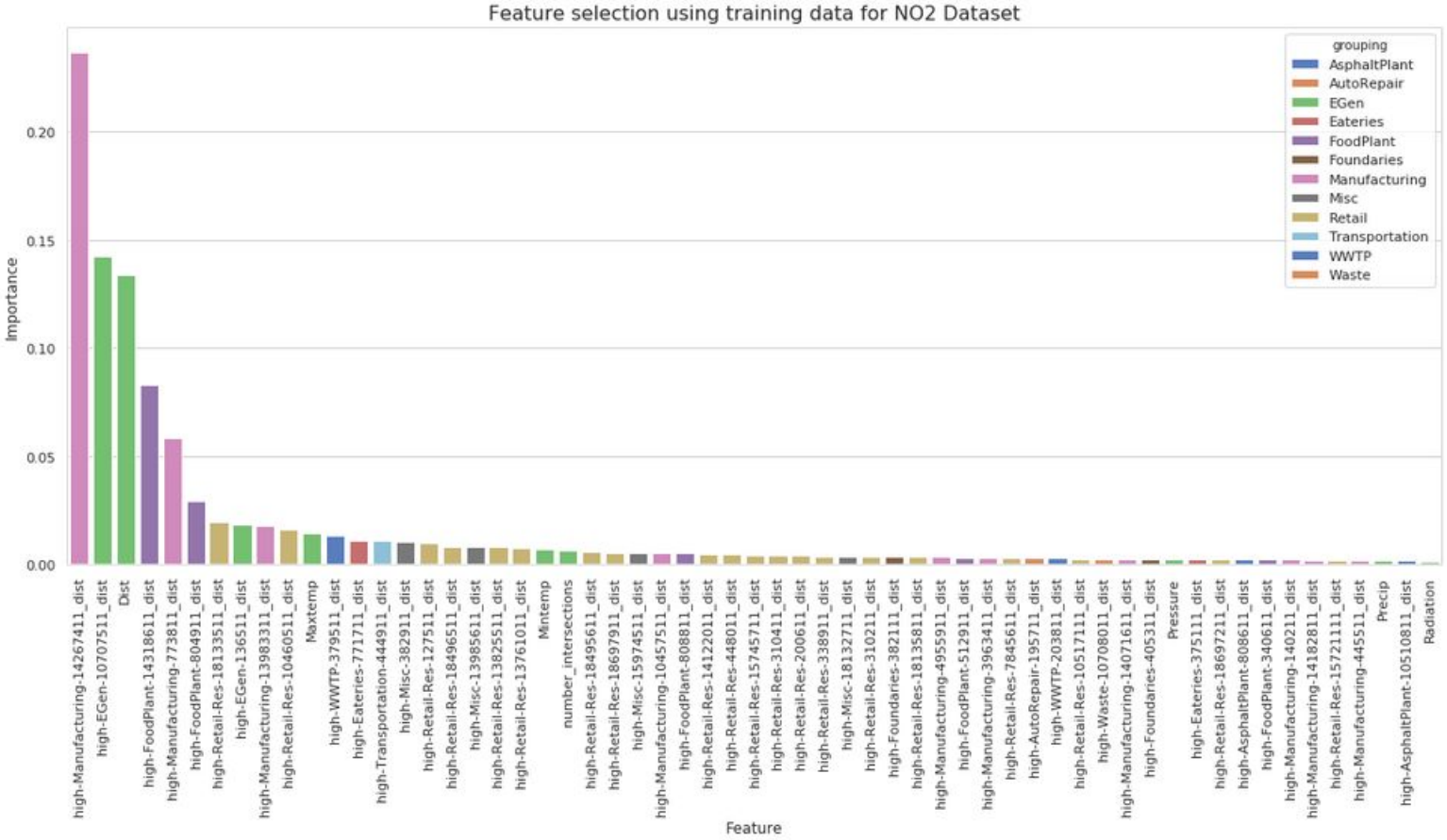


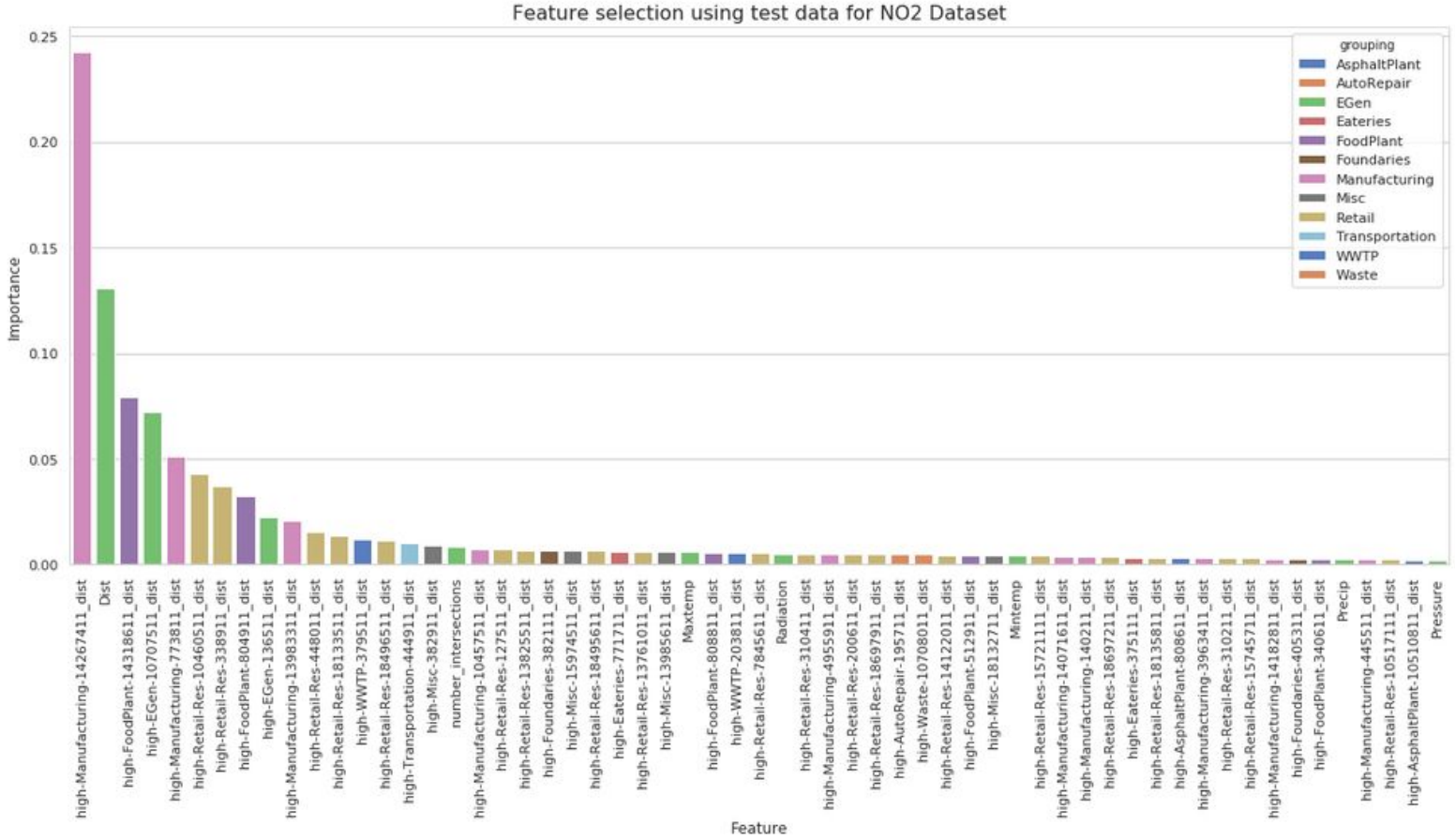


Results show that for the BC dataset, **'Manufacturing-10476711', 'ConcretePlant-193511'** are the top two features.

NO2 dataset:

Graphs below show the feature importance for training and test data. Results show that for the NO2 dataset, **'Manufacturing-14267411', 'Dist', 'EGen-10707511' and 'FoodPlant-14316811'** are the top few features.


Feature selection using training data for NO2 Dataset
Importance
0.00
0.05
0.10
0.15
0.20
grouping
AsphaltPlant
AutoRepair
EGen
Eateries
FoodPlant
Foundaries
Manufacturing
Misc
Retail
Transportation
WWTP
Waste
high-Manufacturing-14267411_dist
high-EGen-10707511_dist
Dist
high-FoodPlant-14318611_dist
high-Manufacturing-773811_dist
high-FoodPlant-804911_dist
high-Retail-Res-18133511_dist
high-EGen-136511_dist
high-Manufacturing-13983311_dist
high-Retail-Res-10460511_dist
Maxtemp
high-WWTP-379511_dist
high-Eateries-771711_dist
high-Transportation-444911_dist
high-Misc-382911_dist
high-Retail-Res-127511_dist
high-Retail-Res-18496511_dist
high-Misc-13985611_dist
high-Retail-Res-13825511_dist
high-Retail-Res-13761011_dist
Mintemp
number_intersections
high-Retail-Res-18495611_dist
high-Retail-Res-18697911_dist
high-Misc-15974511_dist
high-Manufacturing-10457511_dist
high-FoodPlant-808811_dist
high-Retail-Res-14122011_dist
high-Retail-Res-448011_dist
high-Retail-Res-15745711_dist
high-Retail-Res-310411_dist
high-Retail-Res-200611_dist
high-Retail-Res-338911_dist
high-Misc-18132711_dist
high-Retail-Res-310211_dist
high-Foundaries-382111_dist
high-Retail-Res-18135811_dist
high-Manufacturing-4955911_dist
high-FoodPlant-512911_dist
high-Manufacturing-3963411_dist
high-Retail-Res-7845611_dist
high-AutoRepair-195711_dist
high-WWTP-203811_dist
high-Retail-Res-10517111_dist
high-Waste-10708011_dist
high-Manufacturing-14071611_dist
high-Foundaries-405311_dist
Pressure
high-Eateries-375111_dist
high-Retail-Res-18697211_dist
high-AsphaltPlant-808611_dist
high-FoodPlant-340611_dist
high-Manufacturing-140211_dist
high-Manufacturing-14182811_dist
high-Retail-Res-15721111_dist
high-Manufacturing-445511_dist
Precip
high-AsphaltPlant-10510811_dist
Radiation
Feature


Feature selection using test data for NO2 Dataset
Importance
0.00
0.05
0.10
0.15
0.20
0.25
grouping
AsphaltPlant
AutoRepair
EGen
Eateries
FoodPlant
Foundaries
Manufacturing
Misc
Retail
Transportation
WWTP
Waste
high-Manufacturing-14267411_dist
Dist
high-FoodPlant-14318611_dist
high-EGen-10707511_dist
high-Manufacturing-773811_dist
high-Retail-Res-10460511_dist
high-Retail-Res-338911_dist
high-FoodPlant-804911_dist
high-EGen-136511_dist
high-Manufacturing-13983311_dist
high-Retail-Res-448011_dist
high-Retail-Res-18133511_dist
high-WWTP-379511_dist
high-Retail-Res-18496511_dist
high-Transportation-444911_dist
high-Misc-382911_dist
number_intersections
high-Manufacturing-10457511_dist
high-Retail-Res-127511_dist
high-Retail-Res-13825511_dist
high-Foundaries-382111_dist
high-Misc-15974511_dist
high-Retail-Res-18495611_dist
high-Eateries-771711_dist
high-Retail-Res-13761011_dist
high-Misc-13985611_dist
Maxtemp
high-FoodPlant-808811_dist
high-WWTP-203811_dist
high-Retail-Res-7845611_dist
Radiation
high-Retail-Res-310411_dist
high-Manufacturing-4955911_dist
high-Retail-Res-200611_dist
high-Retail-Res-18697911_dist
high-AutoRepair-195711_dist
high-Waste-10708011_dist
high-Retail-Res-14122011_dist
high-FoodPlant-512911_dist
high-Misc-18132711_dist
Mintemp
high-Retail-Res-15721111_dist
high-Manufacturing-14071611_dist
high-Manufacturing-140211_dist
high-Retail-Res-18697211_dist
high-Eateries-375111_dist
high-Retail-Res-18135811_dist
high-AsphaltPlant-808611_dist
high-Manufacturing-3963411_dist
high-Retail-Res-310211_dist
high-Retail-Res-15745711_dist
high-Manufacturing-14182811_dist
high-Foundaries-405311_dist
high-FoodPlant-340611_dist
Precip
high-Manufacturing-445511_dist
high-Retail-Res-10517111_dist
high-AsphaltPlant-10510811_dist
Pressure
Feature

Apply PCA And Test Performance of Several Models

We performed (results not shown here) a PCA + DecisionTree Regressor that resulted in the selection of 31 components, and the mean cross validation score for the BC test dataset was 0.60. Similarly, the NO2 dataset resulted in the selection of 50 PCs with a cross validation score of 0.78. In this case, we test whether applying PCA really improves the model performance. We test several different models on the training and test set and calculate the R2 for the model with PCA and without PCA.

Methodology:

Similar to the above approach, we first scale the dataset using StandarScaler() method such that each column has a mean = 0 and variance = 1. After this, we create a PCA object and set the variance to be 0.99. Next, we test different models using 5-fold cross validation on the test dataset. The different models that were tested include:

1) Linear Regression
2) Ridge Regression
3) RidgeCV Regression
4) Huber Regression
5) Bayesian Ridge
6) Bagging
7) Random Forest

Results:

BC Dataset:

The R2 score for the training data with and without PCA for the BC dataset is shown below. The results show that applying PCA does not really improve the model performance, at least for the test data.

R2 with PCA for training data:

	R Square Score
Linear	0.588995
Ridge	0.546910
RidgeCV	0.578782
Bayesian Ridge	0.578883
Hubber	0.492165
Bagging	0.775148
RandomForest	0.790851

R2 with PCA for test data

	R Square Score
Linear	0.574383
Ridge	0.527219
RidgeCV	0.563863
Bayesian Ridge	0.562670
Hubber	0.479324
Bagging	0.714963
RandomForest	0.743671

R2 without PCA for test data:

	R Square Score
Linear	0.555311
Ridge	0.541292
RidgeCV	0.550310
Bayesian Ridge	0.545387
Hubber	0.522175
Bagging	0.696226
RandomForest	0.715134

NO2 Dataset:
The R2 score for different models are shown below:

R2 with PCA for training data:

	R Square Score
Linear	0.649465
Ridge	0.616807
RidgeCV	0.636670
Bayesian Ridge	0.635459
Hubber	0.540464
Bagging	0.884280
RandomForest	0.893266

R2 with PCA for test data:

	R Square Score
Linear	0.637097
Ridge	0.598221
RidgeCV	0.627137
Bayesian Ridge	0.624936
Hubber	0.528650
Bagging	0.863286
RandomForest	0.876086

R2 without PCA for test data:

	R Square Score
Linear	0.663888
Ridge	0.641820
RidgeCV	0.654200
Bayesian Ridge	0.643589
Hubber	0.626353
Bagging	0.878333
RandomForest	0.889857

The above results show that applying PCA does not really improve the model performance, at least for the test data.

Gridsearch different models for comparison

We adopt a gridsearch and cross validation to test the performance of different model based on the prediction score. Here, we first split the data into test train split, and then test Ridge regression, Random Forest and the XGBoost approach. For each model, we perform a gridsearch to identify the best parameters (such as optimal tree depth, number of estimators etc.) in order to find the best parameters for each model. The ridge regression is also tested with and without PCA.

Methodology:

First , split the data into test and train set. Next, we first scale the dataset using StandarScaler() method such that each column has a mean = 0 and variance = 1. Next, define grid parameters for different types of model and perform a gridsearch CV over each. The first model is a RandomforestRegressor. Grid parameters are number of estimators, max_features, and max_depth. Second model is a Ridge Regression model. Grid parameters include Alpha and fit_intercept. Third model is XGBoost, with grid parameters like max_depth, learning rate and number of estimators.

Results:

BC Dataset

Model Type	Best Parameter	Mean CV score for best estimator	Training R2	Test R2
Ridge regression with PCA	Alpha = 0	0.588	0.594	0.577
Ridge regression without PCA	Alpha = 0	0.588	0.594	0.577
Random Forest	Max depth = 15 Estimators = 300	0.782	0.921	0.769
XGBRegressor	Learning rate = 0.1 max depth = 10 estimators = 100	0.798	0.925	0.791

NO2 Dataset

Model Type	Best Parameter	Mean CV score for best estimator	Training R2	Test R2
Ridge regression with PCA	Alpha = 0	0.649	0.652	0.640
Ridge regression without PCA	Alpha = 0	0.649	0.652	0.640
Random Forest	Max depth = 50 Estimators = 400	0.888	0.985	0.898
XGBRegressor	Learning rate = 0.1	0.899	0.967	0.91

	max depth = 10 estimators = 100			

Summary:

XGBRegressor performs the best, followed by random forest