Project_4_Part1_Regression_Analysis

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1 Project 4 - Part 1 Regression Analysis

Gorkem Camli (105709280)

Library imports

Dataset Exploration Diamonds Data

```
(53940, 10)
```

	carat	cut	color	clarity	depth	table	price	x	y	z
1	0.23	Ideal	E	SI2	61.5	55.0	330	3.95	3.98	2.43
2	0.21	Premium	E	SI1	59.8	61.0	327	3.89	3.84	2.31
3	0.23	Good	E	VS1	56.9	65.0	328	4.05	4.07	2.31
4	0.29	Premium	I	VS2	62.4	58.0	337	4.20	4.23	2.63
5	0.31	Good	J	SI2	63.3	58.0	338	4.34	4.35	2.75

```
carat      float64
cut         object
color       object
clarity     object
depth      float64
table      float64
price        int64
x          float64
y          float64
z          float64
dtype: object
```

Gas Turbine CO and NOx Emission Data

```
(36733, 12)
```

	AT	AP	AH	AFDP	GTEP	TIT	TAT	TEY	CDP	\
0	4.5878	1018.7	83.675	3.5758	23.979	1086.2	549.83	134.67	11.898	
1	4.2932	1018.3	84.235	3.5709	23.951	1086.1	550.05	134.67	11.892	
2	3.9045	1018.4	84.858	3.5828	23.990	1086.5	550.19	135.10	12.042	
3	3.7436	1018.3	85.434	3.5808	23.911	1086.5	550.17	135.03	11.990	
4	3.7516	1017.8	85.182	3.5781	23.917	1085.9	550.00	134.67	11.910	

```
        CO     NOX  year
0  0.32663  81.952  2011
1  0.44784  82.377  2011
2  0.45144  83.776  2011
3  0.23107  82.505  2011
4  0.26747  82.028  2011
```

```
                AT            AP            AH          AFDP          GTEP  \
count  36733.000000  36733.000000  36733.000000  36733.000000  36733.000000
mean      17.712726   1013.070165     77.867015      3.925518     25.563801
std        7.447451      6.463346     14.461355      0.773936      4.195957
min       -6.234800    985.850000     24.085000      2.087400     17.698000
25%       11.781000   1008.800000     68.188000      3.355600     23.129000
50%       17.801000   1012.600000     80.470000      3.937700     25.104000
75%       23.665000   1017.000000     89.376000      4.376900     29.061000
max       37.103000   1036.600000    100.200000      7.610600     40.716000

                TIT           TAT           TEY           CDP            CO  \
count  36733.000000  36733.000000  36733.000000  36733.000000  36733.000000
mean    1081.428084    546.158517    133.506404     12.060525      2.372468
std       17.536373      6.842360     15.618634      1.088795      2.262672
min     1000.800000    511.040000    100.020000      9.851800      0.000388
25%     1071.800000    544.720000    124.450000     11.435000      1.182400
50%     1085.900000    549.880000    133.730000     11.965000      1.713500
75%     1097.000000    550.040000    144.080000     12.855000      2.842900
max     1100.900000    550.610000    179.500000     15.159000     44.103000

                NOX
count  36733.000000
mean      65.293067
std       11.678357
min       25.905000
25%       57.162000
50%       63.849000
75%       71.548000
max      119.910000
```

```
         year
count   36733
unique      5
top      2012
freq     7628
```

```
       AT      AP      AH    AFDP    GTEP     TIT     TAT     TEY     CDP  \
0  4.5878  1018.7  83.675  3.5758  23.979  1086.2  549.83  134.67  11.898
1  4.2932  1018.3  84.235  3.5709  23.951  1086.1  550.05  134.67  11.892
```

```
2  3.9045  1018.4  84.858  3.5828  23.990  1086.5  550.19  135.10  12.042
3  3.7436  1018.3  85.434  3.5808  23.911  1086.5  550.17  135.03  11.990
4  3.7516  1017.8  85.182  3.5781  23.917  1085.9  550.00  134.67  11.910

      NOX  year
0  81.952  2011
1  82.377  2011
2  83.776  2011
3  82.505  2011
4  82.028  2011
```

1.1 Before Training

1.1.1 Standardization

Question 1

Diamonds Data For diamonds data, all the categorical features are quality features, therefore I used Ordinal Encoder to encode them. While encoding the given labels, I specified the ordering from low to high quality for the cut, color, clarity features. For example, for cut categories: Fair gets the lowest label number whereas Ideal got the highest. Later, for both numerical and encoded categorical features, standard scaler is applied. Target variable is kept same.

```
Index(['carat', 'depth', 'table', 'x', 'y', 'z'], dtype='object')
Index(['cut', 'color', 'clarity'], dtype='object')
```

```
Raw Diamonds Data
```

```
   carat      cut color clarity  depth  table  price     x     y     z
1   0.23    Ideal     E     SI2   61.5   55.0    330  3.95  3.98  2.43
2   0.21  Premium     E     SI1   59.8   61.0    327  3.89  3.84  2.31
3   0.23     Good     E     VS1   56.9   65.0    328  4.05  4.07  2.31
4   0.29  Premium     I     VS2   62.4   58.0    337  4.20  4.23  2.63
```

```
Diamonds Data After Standardization and Category Feature Encoding
```

```
      carat       cut     color   clarity     depth     table  price  \
1 -1.198168  0.981473  0.937163 -1.245215 -0.174092 -1.099672    330
2 -1.240361  0.085889  0.937163 -0.638095 -1.360738  1.585529    327
3 -1.198168 -1.705279  0.937163  0.576145 -3.385019  3.375663    328
4 -1.071587  0.085889 -1.414272 -0.030975  0.454133  0.242928    337

          x         y         z
1 -1.587837 -1.536196 -1.571129
2 -1.641325 -1.658774 -1.741175
3 -1.498691 -1.457395 -1.741175
4 -1.364971 -1.317305 -1.287720
```

```
Description of Diamonds data after standardization
```

```
              carat           cut         color       clarity         depth  \
count  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04
mean   2.444878e-16  1.454281e-16  1.338360e-16 -8.114467e-17 -3.996902e-15
std    1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00
min   -1.261458e+00 -2.600864e+00 -2.002131e+00 -1.852335e+00 -1.308760e+01
25%   -8.395232e-01 -8.096951e-01 -8.264134e-01 -6.380951e-01 -5.231053e-01
50%   -2.066210e-01  8.588908e-02 -2.385547e-01 -3.097505e-02  3.531678e-02
75%    5.106683e-01  9.814733e-01  9.371628e-01  5.761450e-01  5.239361e-01
max    8.886075e+00  9.814733e-01  1.525021e+00  2.397505e+00  1.204139e+01

              table         price             x             y             z
count  5.394000e+04  53940.000000  5.394000e+04  5.394000e+04  5.394000e+04
mean   9.695207e-17   3934.801557  2.782103e-16 -8.430615e-17 -2.002271e-16
std    1.000009e+00   3989.442321  1.000009e+00  1.000009e+00  1.000009e+00
min   -6.470073e+00    327.000000 -5.109120e+00 -5.020931e+00 -5.014556e+00
25%   -6.521385e-01    952.000000 -9.103248e-01 -8.882800e-01 -8.909461e-01
50%   -2.046051e-01   2403.000000 -2.777553e-02 -2.147398e-02 -1.237618e-02
75%    6.904618e-01   5327.250000  7.210542e-01  7.052421e-01  7.103184e-01
max    1.680167e+01  18823.000000  4.465203e+00  4.654965e+01  4.004758e+01
```

Gas Data For gas data, I dropped the CO column and will use NOX as the target variable. Only categorical feature is year. It is considered as an ordered feature, we could use ordinal encoder for it. It is also possible to use one-hot-encoding. I used Ordinal Encoder to encode them. While encoding, I specified the ordering from low to high. Later, for both numerical and encoded categorical features, standard scaler is applied. Target variable is kept same (NOX).

```
Index(['AT', 'AP', 'AH', 'AFDP', 'GTEP', 'TIT', 'TAT', 'TEY', 'CDP'],
dtype='object')
Index(['year'], dtype='object')

years:  ['2011' '2012' '2013' '2014' '2015']

Raw Gas Data

       AT      AP      AH    AFDP    GTEP     TIT     TAT     TEY     CDP  \
0  4.5878  1018.7  83.675  3.5758  23.979  1086.2  549.83  134.67  11.898
1  4.2932  1018.3  84.235  3.5709  23.951  1086.1  550.05  134.67  11.892
2  3.9045  1018.4  84.858  3.5828  23.990  1086.5  550.19  135.10  12.042
3  3.7436  1018.3  85.434  3.5808  23.911  1086.5  550.17  135.03  11.990

      NOX  year
0  81.952  2011
1  82.377  2011
2  83.776  2011
3  82.505  2011

Gas Data After Standardization and Category Feature Encoding
```

```
         AT        AP        AH      AFDP      GTEP       TIT       TAT  \
0 -1.762362  0.871052  0.401627 -0.451875 -0.377702  0.272119  0.536589
1 -1.801920  0.809164  0.440351 -0.458207 -0.384376  0.266417  0.568742
2 -1.854113  0.824636  0.483432 -0.442831 -0.375081  0.289227  0.589203
3 -1.875718  0.809164  0.523263 -0.445415 -0.393909  0.289227  0.586280

        TEY       CDP     NOX      year
0  0.074502 -0.149273  81.952 -1.399443
1  0.074502 -0.154783  82.377 -1.399443
2  0.102033 -0.017015  83.776 -1.399443
3  0.097551 -0.064774  82.505 -1.399443
```

Description of Gas data after standardization

```
                 AT            AP            AH          AFDP          GTEP  \
count  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04
mean  -1.176081e-16 -1.233647e-14 -5.942306e-16 -1.015144e-15  5.230467e-16
std    1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00
min   -3.215577e+00 -4.211524e+00 -3.719067e+00 -2.375059e+00 -1.874640e+00
25%   -7.964882e-01 -6.606830e-01 -6.693112e-01 -7.363991e-01 -5.802810e-01
50%    1.185304e-02 -7.274427e-02  1.799983e-01  1.574091e-02 -1.095835e-01
75%    7.992472e-01  6.080269e-01  7.958550e-01  5.832377e-01  8.334799e-01
max    2.603647e+00  3.640553e+00  1.544343e+00  4.761549e+00  3.611191e+00

                TIT           TAT           TEY           CDP           NOX  \
count  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04  36733.000000
mean   9.609823e-15 -8.300659e-15  9.888369e-16 -4.673376e-16     65.293067
std    1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00     11.678357
min   -4.597825e+00 -5.132585e+00 -2.144032e+00 -2.028623e+00     25.905000
25%   -5.490425e-01 -2.102398e-01 -5.798539e-01 -5.745191e-01     57.162000
50%    2.550115e-01  5.438962e-01  1.431620e-02 -8.773591e-02     63.849000
75%    8.879903e-01  5.672802e-01  6.769952e-01  7.296924e-01     71.548000
max    1.110388e+00  6.505859e-01  2.944830e+00  2.845821e+00    119.910000

               year
count  3.673300e+04
mean  -7.427883e-17
std    1.000014e+00
min   -1.399443e+00
25%   -6.946951e-01
50%    1.005331e-02
75%    7.148017e-01
max    1.419550e+00
```

I could have also standardized the target variables. The advantage of standardizing the target variables are especially when training models such as NN. Having very large range of target variables can make it difficult to adapt and assign weights to predict the results. This is because larger target results require larger weights.

I also tried one-hot encoding but the result but it makes more sense to use ordinal encoder due to quality nature of the variables and also for the efficiency. I tried also one-hot encoder but results seemed to be better and faster with this one, so I decided to go with ordinal encoder.

1.1.2 Profiling Results

Pandas profiling is used to explore the dataset for both diamonds and gas dataset. The results can be seen below:

1.1.3 Data Inspection

To further understand the data I did fata inspection and answered the following questions:

Question 2 Pearson Correlation Heatmap:

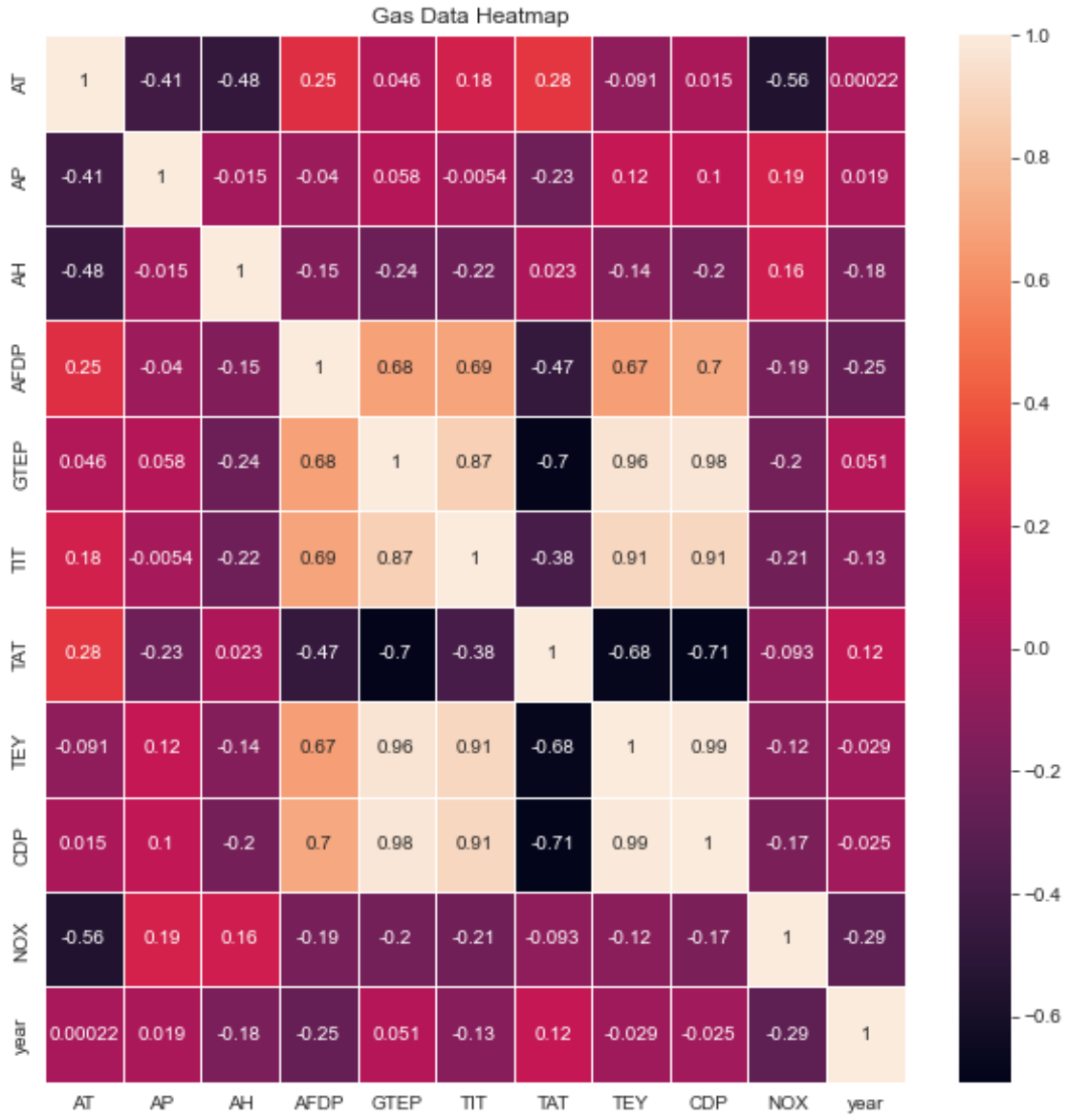
For Pearson correlation the values are between -1 to 1. Values closer -1 means strong negative correlation, values closer 1 means strong positive correlation and values closer to 0 means low correlation. High correlation means there is a strong linear relationship between two variables. If it is closer to 1, means increasing one variable we expect increase in the other. If the value is closer to -1, high negative correlation, increasing one variable will result in the decrease of the other variable. Having a value close to 0 means that there is no strong linear relation betweeen the two variables, changing one doesn't have a clear effect on the other as a direct increase or decrease. Having a pearson correlation 0 or close to 0 doesn't mean there is no relationship between the two, a nonlinear relationship may exist, it is just that we cannot tell nonlinear relationship by just looking Pearson correlation.

For both datasets heatmap with pearson correlation is plotted:

Diamonds Data:

In the diamonds data Pearson Correlation heatmap, we see high correlation on carat,x, y, z and price columns. The pearson correlation values between price and carat is 0.92, x=0.88, y=0.87 and z=0.86. Carat seems to be the most important feature to tell the diamond price. The high correlation suggest carat, x, y, z values are the most predictive features for predicting the price of a diamond. The pearson correlation for these features are positive for target variable price. This means there is a positive relationship between these variables and price, hence the increasing any of these 4 features will lead the diamond price to be higher. These makes sense in the real world as well since the bigger diamonds (dimensions x,y,z) and/or carat (weight) are generally more expensive.

Gas Data:

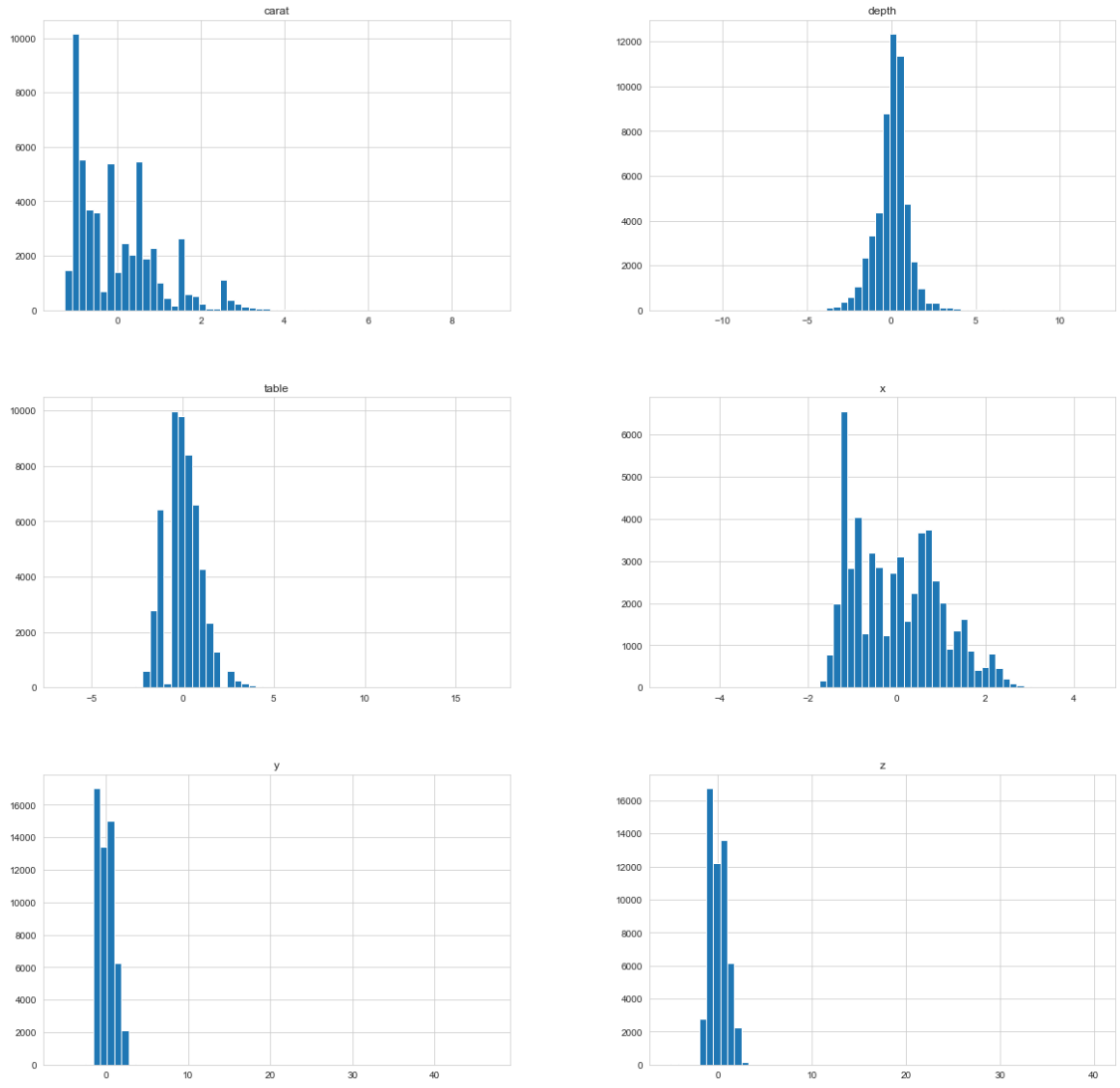


In the gas data Pearson Correlation heatmap, we see negative high correlation on AT column with our target variable NOX. This tells increasing AT tend to lowers NOX values. But rest of the variables don't seem very correlated with the NOX variable. This tells that we might have a hard time to have good results for the predictions (at least for the linear models).

What is interesting though other features seem to be correlated with each other, TAT, TEY, CDP and GTEP looks like very correlated with each other. TAT has high negative correlation with TEY, CDP and GTEP. GTEP correlation with TEY and CDP is very high and positive around 0.96, 0.98. The relations are same betweeen these 3 variables, this means we can drop 2 of them and only keep one, otherwise our models would put more emphasis on these data in order to predict the results.

Question 3 Histogram of the numerical features for each dataset can be seen below:

Diamond Dataset:



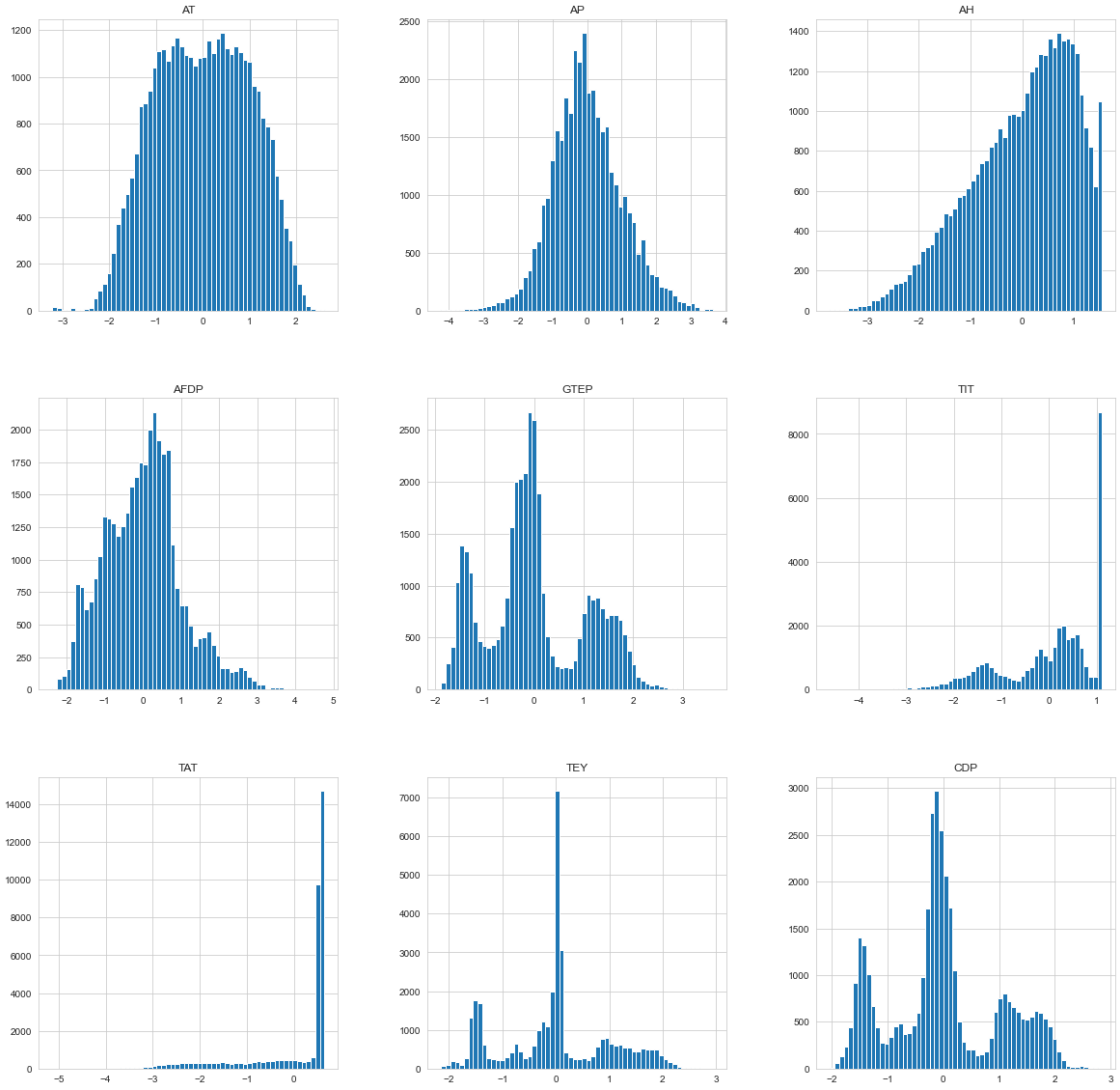
	carat	cut	color	clarity	depth	\
count	5.394000e+04	5.394000e+04	5.394000e+04	5.394000e+04	5.394000e+04	
mean	2.444878e-16	1.454281e-16	1.338360e-16	-8.114467e-17	-3.996902e-15	
std	1.000009e+00	1.000009e+00	1.000009e+00	1.000009e+00	1.000009e+00	
min	-1.261458e+00	-2.600864e+00	-2.002131e+00	-1.852335e+00	-1.308760e+01	
25%	-8.395232e-01	-8.096951e-01	-8.264134e-01	-6.380951e-01	-5.231053e-01	
50%	-2.066210e-01	8.588908e-02	-2.385547e-01	-3.097505e-02	3.531678e-02	
75%	5.106683e-01	9.814733e-01	9.371628e-01	5.761450e-01	5.239361e-01	
max	8.886075e+00	9.814733e-01	1.525021e+00	2.397505e+00	1.204139e+01	

	table	price	x	y	z
count	5.394000e+04	53940.000000	5.394000e+04	5.394000e+04	5.394000e+04
mean	9.695207e-17	3934.801557	2.782103e-16	-8.430615e-17	-2.002271e-16
std	1.000009e+00	3989.442321	1.000009e+00	1.000009e+00	1.000009e+00
min	-6.470073e+00	327.000000	-5.109120e+00	-5.020931e+00	-5.014556e+00
25%	-6.521385e-01	952.000000	-9.103248e-01	-8.882800e-01	-8.909461e-01
50%	-2.046051e-01	2403.000000	-2.777553e-02	-2.147398e-02	-1.237618e-02
75%	6.904618e-01	5327.250000	7.210542e-01	7.052421e-01	7.103184e-01
max	1.680167e+01	18823.000000	4.465203e+00	4.654965e+01	4.004758e+01

Diamond Data:

Carat and x features' histogram seems to be right skewed. Y and z plots have few outliers around 40 and they don't seem to follow gaussian distribution. Depth and table seems to be close to normal distribution.

Gas Dataset:



```
                AT            AP            AH          AFDP          GTEP  \
count  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04
mean  -1.176081e-16 -1.233647e-14 -5.942306e-16 -1.015144e-15  5.230467e-16
std    1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00
min   -3.215577e+00 -4.211524e+00 -3.719067e+00 -2.375059e+00 -1.874640e+00
25%   -7.964882e-01 -6.606830e-01 -6.693112e-01 -7.363991e-01 -5.802810e-01
50%    1.185304e-02 -7.274427e-02  1.799983e-01  1.574091e-02 -1.095835e-01
75%    7.992472e-01  6.080269e-01  7.958550e-01  5.832377e-01  8.334799e-01
max    2.603647e+00  3.640553e+00  1.544343e+00  4.761549e+00  3.611191e+00

                TIT           TAT           TEY           CDP           NOX  \
count  3.673300e+04  3.673300e+04  3.673300e+04  3.673300e+04  36733.000000
mean   9.609823e-15 -8.300659e-15  9.888369e-16 -4.673376e-16     65.293067
std    1.000014e+00  1.000014e+00  1.000014e+00  1.000014e+00     11.678357
min   -4.597825e+00 -5.132585e+00 -2.144032e+00 -2.028623e+00     25.905000
25%   -5.490425e-01 -2.102398e-01 -5.798539e-01 -5.745191e-01     57.162000
50%    2.550115e-01  5.438962e-01  1.431620e-02 -8.773591e-02     63.849000
75%    8.879903e-01  5.672802e-01  6.769952e-01  7.296924e-01     71.548000
max    1.110388e+00  6.505859e-01  2.944830e+00  2.845821e+00    119.910000

               year
count  3.673300e+04
mean  -7.427883e-17
std    1.000014e+00
min   -1.399443e+00
25%   -6.946951e-01
50%    1.005331e-02
75%    7.148017e-01
max    1.419550e+00
```

Gas Data:

AT, AP features seem to have close distributions to normal distributions. AH, AFDP are left skewed, CO is right skewed and features such as GTEP, TEY, CDP are tri-modal dsitributions.

What preprocessing can be done if the distribution of a feature has high skewness?

There are different ways to handle high skewed data and reduce its skewness:

1- Log Transform (natural log)
2- Square root transform
2- Box-Cox transformation

There are different transformation possibilities to address the skewness of the data, and it is difficult to determine which one needs to be applied. This generally depends highly on the current doistribution of the data. Box-Cox transformation is a family of transformations where you select λ value typically from -5 to 5. Optimal λ is chosen based on the data where its transformation is

the best approximation of a normally distributed curve. The transformation of data y is simply $y_{\text{transformed}} = y^{\lambda}$.

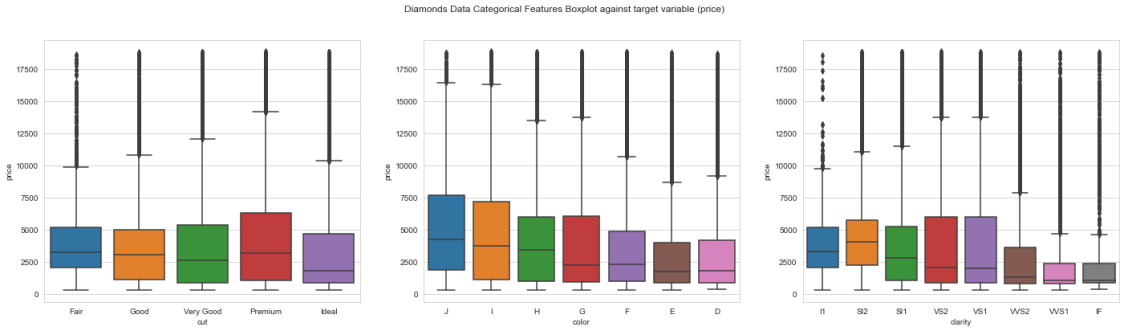
$\lambda = 0$ corresponds to the natural log of the data.
$\lambda = 0.5$ corresponds to the square root transform of the data.

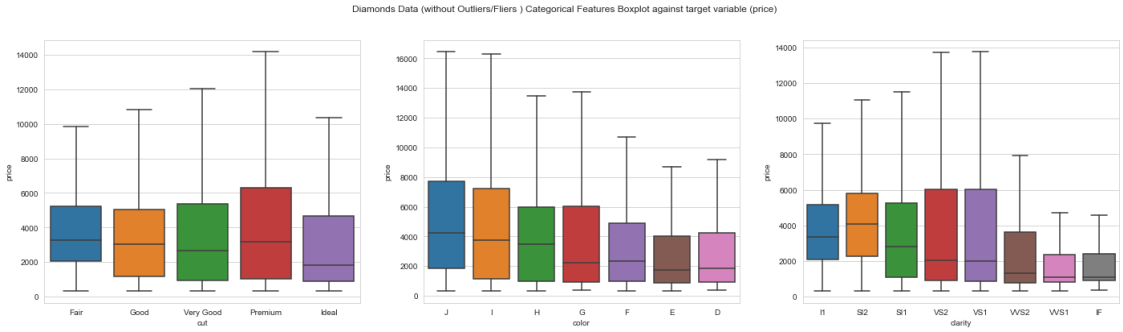
Hence, the first two approach is also contained within the Box-Cox transformation family.

By applying Box-Cox Transformation one can decrese the high skewness and make the data distribution closer to normal distribution.

Question 4 Box plot of categorical features in each dataset against target variable. For each dataset I plotted two boxplots one with fliers and the other one without fliers (showfliers=False to not show outliers). I added the plots without fliers as I noticed that there are extreme values that stretch the plots too much and makes the boxplots compact, by not showing outliers, I can zoom in the boxplot itself to visually better see the differences between category values.

Diamonds Data:





Diamond Dataset:

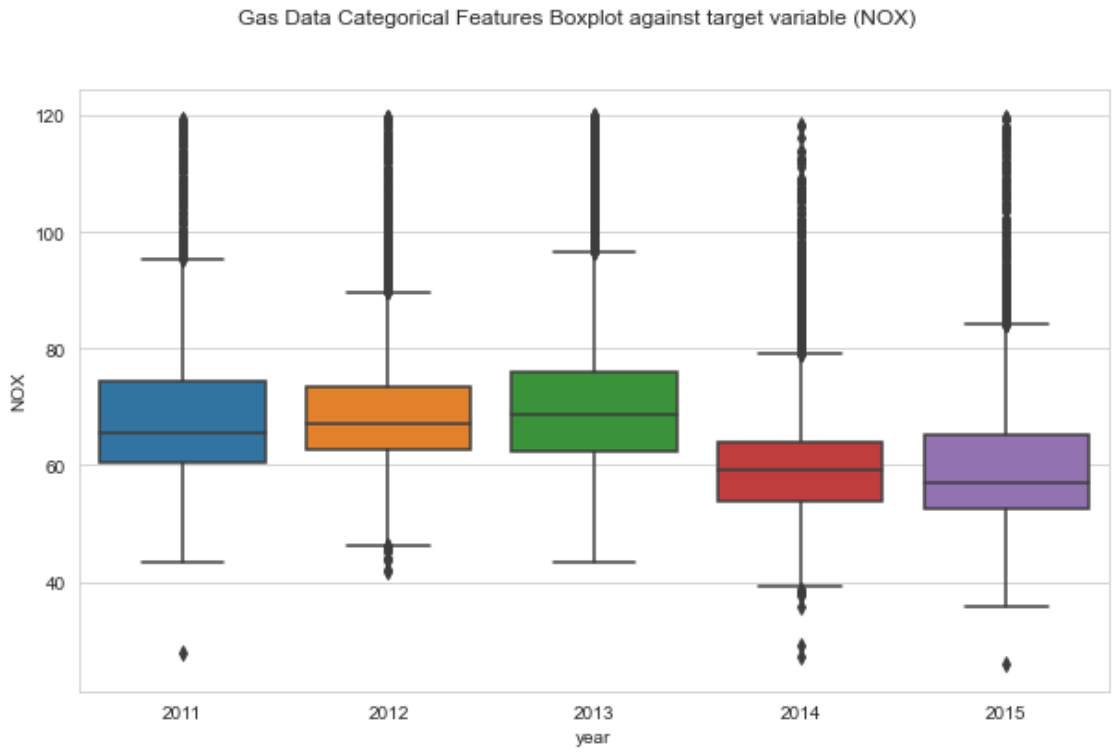
Cut boxplots: The minimum of the cut categories are all very close. The median values are close to each other except for the Ideal cut where the median price is lower compared to its counterparts. One surprising thing to see is that even though Ideal is the best quality, the median, 3rd percentile and maximum (Q3+1.5*IQR) prices are lower compared to Premium and Very Good cut categories.

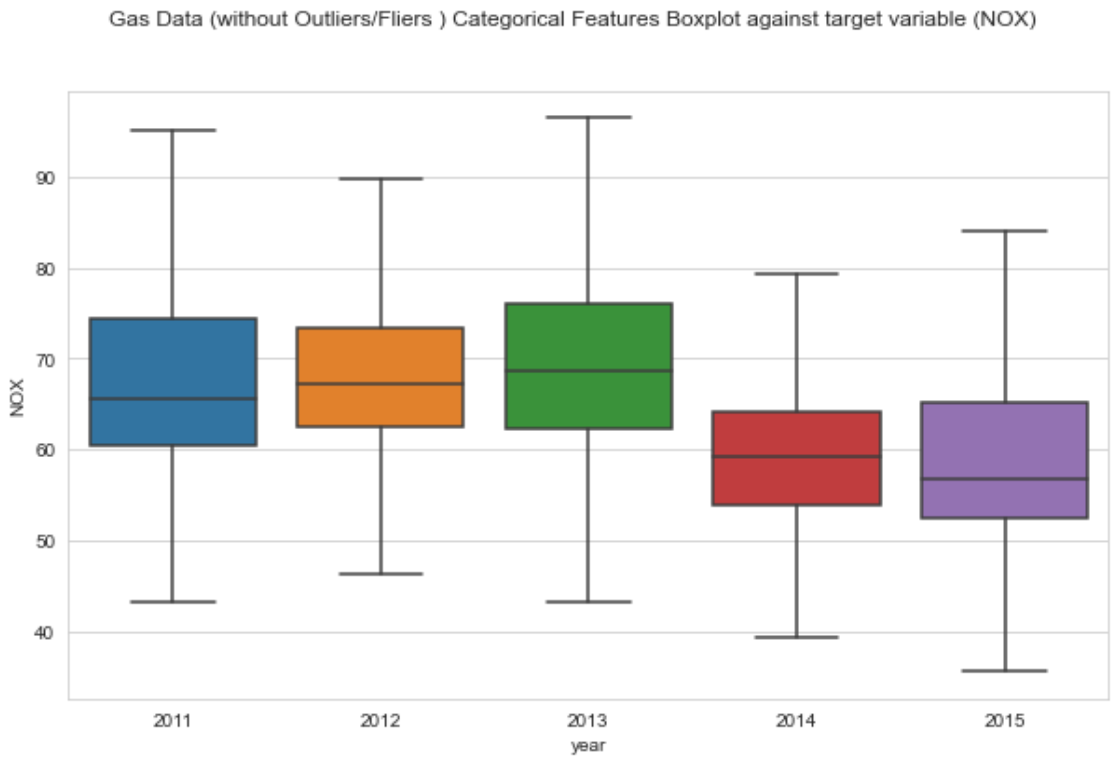
*Premium cut has a higher 3rd percentile and maximum (Q3+1.5*IQR) values compared to other categories. All cuts have outlier prices that goes as high as around 17500. From the plot, we can say that the median and minimum price ranges are similar between cut types.

Color boxplots: J color seems to have higher prices since its 1st quartile, median and 3rd quartile are higher than its counter parts. If we group colors by similar price distributions we can say that J,I pricing distribution are close to each other, with the highest price distributions and E,D is the colors where diamond prices are lower overall. Though outliers exists for all color types that has peak prices. For lower color quality the median and 3rd quartile prices are higher compared to the high quality colors.

Clarity boxplots: This is the variable that has most diverse price distributions on its categories. The highest median and minimum value price belongs to SI2. VS2 and VS1 distiributions looks like very similar, these two types of clarity seems to have a lower median but highest 3rd quartile compared to other clarity levels. Best clarity level IF, price distribution is more compact toward lower price ranges. Again all categories have many outliers.

Gas Data:

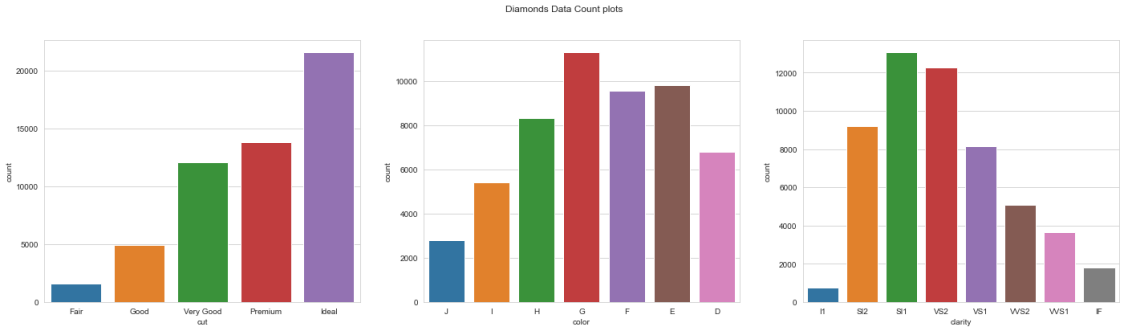




Gas Dataset:

year boxplots: The NOX distributions seem to be very similar for years 2011, 2012 and 2013. Medians are similar for these 3 years. Although 1st, 3rd and minimum, maximum values of these 3 boxplots are different ranges. When we check 2014 and 2015, on the other hand, we see that NOX ranges captures are way lower compared the previous 3 years. The median values are lower, but even the 3rd quartiles and maximum for these 2 years are considerably lower than the previous 3 years. This can help us understand how NOX levels changed in Turkey within the 5 years.

Question 5



In the diamonds data:

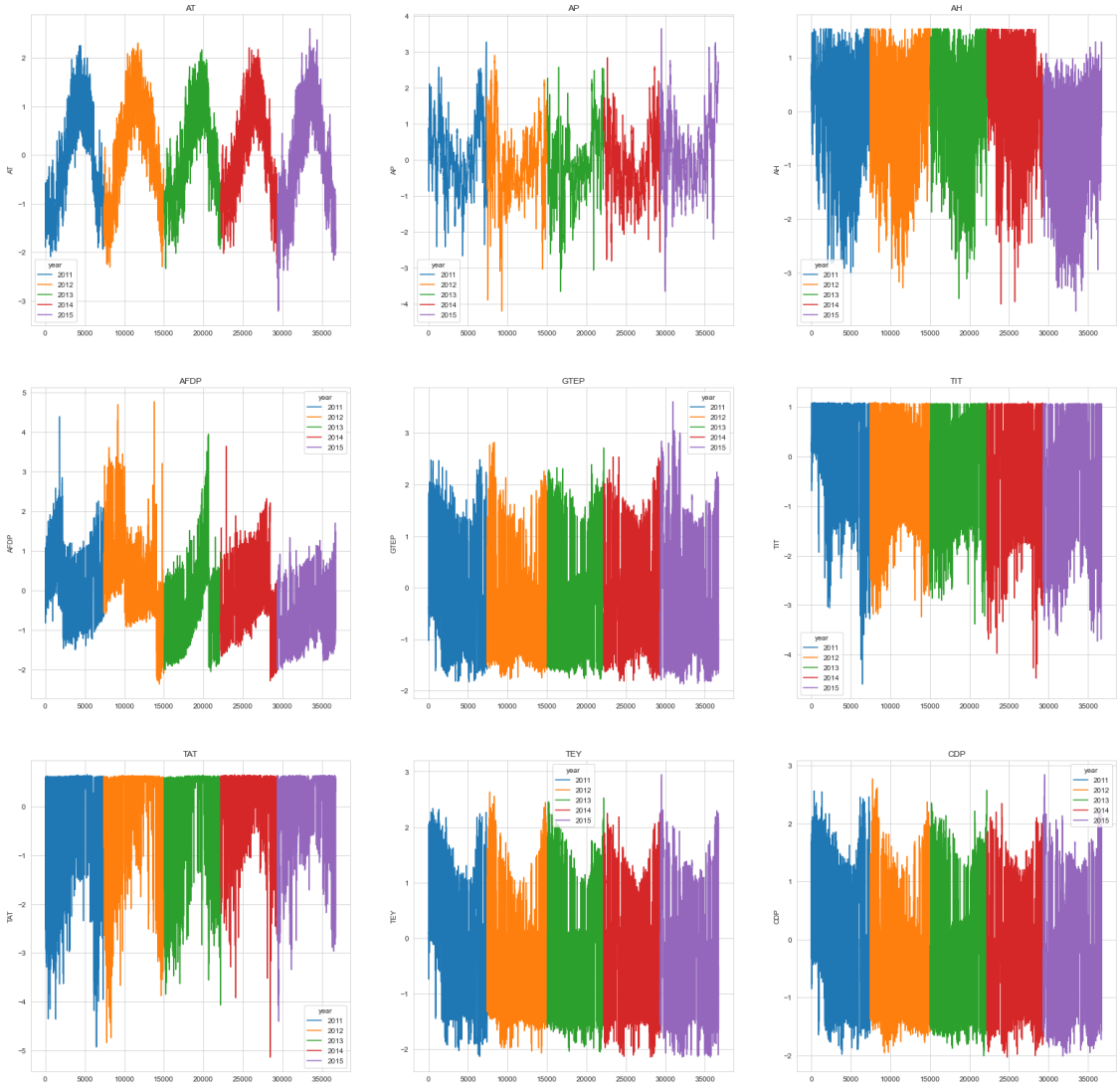
Cut categories is not equally distributed in the data, ideal cut has the largest sample size. Actually cut quality vs sample size for that cut has positive relationship. Better quality cuts have more samples in the dataset.

Color categories are better distributed in the dataset compared to cut, but still not equally distributed per se. J has the lowest sample count in the dataset whereas G has the highest. Looks like the majority of the data has medium level quality colors.

Clarity variable for the data is uneven as well. The majority of the samples in the dataset lies within SI2, SI1 and VS2 categories (low-medium quality). There are fewer samples for the worst and best clarity diamonds.

Question 6 For the Gas Emission dataset, plot the yearly trends for each feature and compare them. The data points don't have timestamps but you may assume the indices are times.

I plotted yearly trends for each feature in the Gas dataset, each year is colored to be able to see patterns more clearly. Indices used as times.



From the abov plots, we can see that there are clear yearly patterns for all of the features. This is most obvious in the AT feature where we can see the same reversed V shape for each year. Some feature results are more varied within year such as TEY and CDP where it makes harder to understand the pattern, however even for those ones we can see some patterns such as towards the middle-end of each year there are some drops for all years compared to the beginning and end og each 5 years.

Feature Selection For this part Mutual Info Regressiong and F regression is used from sklearn library for both datasets. For each preprocessed feature I computed the mutual info and f regression values against target variable.

Question 7 Mutual Info (MI) Regression calculates the dependency between two vairables and it should be a nonnegative value. 0 means two variables are independent from each other, higher MI values corresponds to higher dependency between the variables.

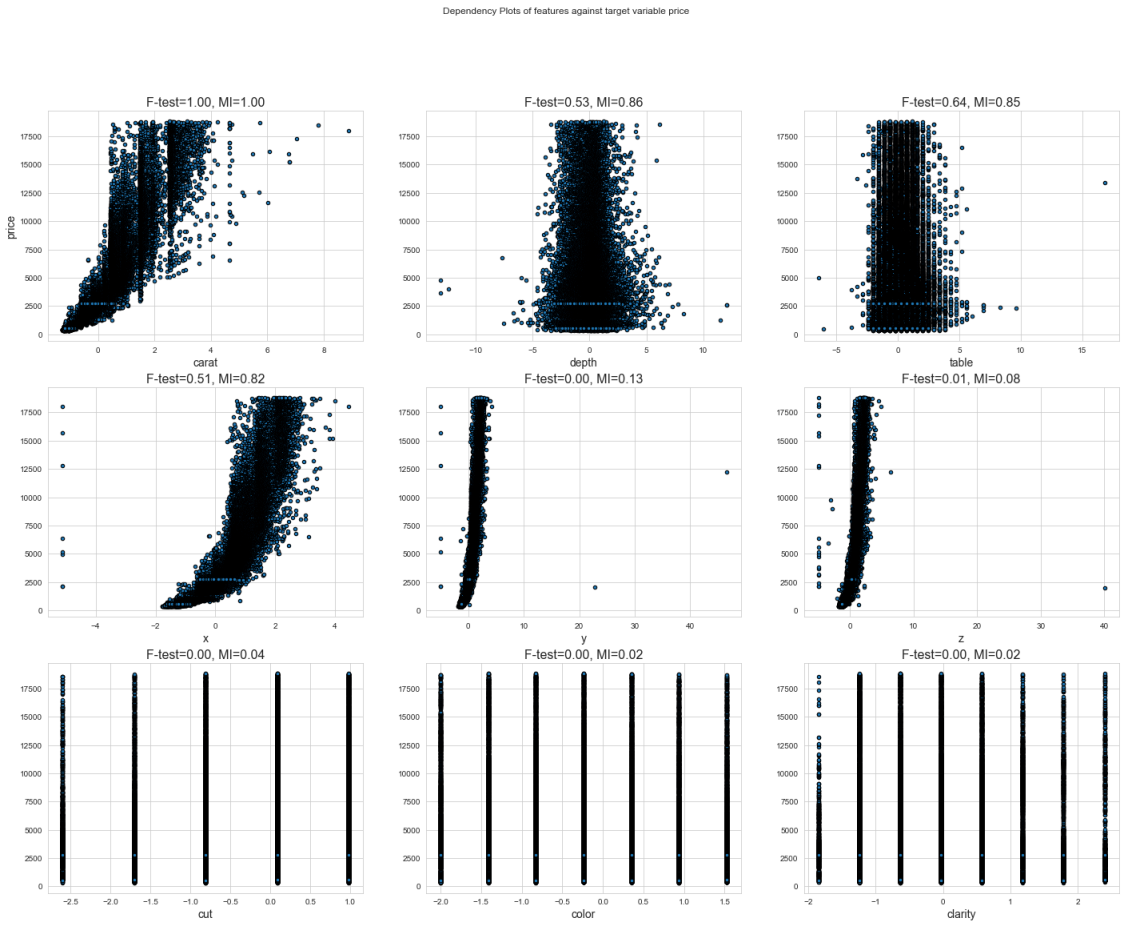
F Regreesion performs univariate linear regression tests to capture the relationship between the given variables.

Diamonds Data Diamonds Data Mutual Info Regression & F Regression

	Feature Name	Mutual Info Regression Score	Mutual Info Regression Score - Scaled	F Regression Score	F Regression Score - Scaled
0	carat	1.65247	1	304051	1
4	y	1.42218	0.860636	160916	0.529238
3	x	1.41241	0.854726	193742	0.6372
5	z	1.36035	0.823219	154923	0.50953
8	clarity	0.217059	0.131354	1188.01	0.00390726
7	color	0.137524	0.0832233	1654.4	0.00544119
6	cut	0.0600886	0.0363628	154.784	0.000509073
2	table	0.0329356	0.0199311	886.119	0.00291437
1	depth	0.0301225	0.0182287	6.11586	2.01146e-05

Table above shows the mutual info and f regression reasult for each variable against target variable price. Table is ordered by Mutual Info Regression Score - Scaled column.

Diamonds Data Scatter Plot of features vs target variable along with Scaled Mutual Info and F Regression Scores



Diamonds Data Most important Features:

Mutual Info Regression most important 4 features: carat, y, x, z.

F Regression most important 4 features: carat, x, y, z.

The order between mutual info and f regression for feature importances are slightly different.

I also experimented on different feature sets with Linear Regression model to see how their performance would change. All features in the diamond dataset seems to be helping for prediction since subset of the features perform worse with Linear Regression model. Given that diamonds dataset has very few variables, I decided to keep all of them and skip the feature selection part. In addition to this the experiments done on Q11 supports this decision, with the OLS experiment some results with other linear packages show that all features are important with p value being less than 0.05. You can refer to Q11 explanation for more details on this.

```
10-fold CV Linear Regression Experiment with All Features:
 Features:['carat', 'depth', 'table', 'x', 'y', 'z', 'cut', 'color', 'clarity']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1206.280596794617
```

```
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1205.045050850985


10-fold CV Linear Regression Experiment with Top 6 Features:
 Features:['carat', 'x', 'y', 'z', 'clarity', 'color']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1221.6042206336504
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1228.2203041711414


10-fold CV Linear Regression Experiment with Top 4 Features:
 Features:['carat', 'x', 'y', 'z']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1512.5608891324323
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1405.0166387786403


Top 5 Mutual Info Regr. features:
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1327.377219542444
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1301.0941071078018


Top 5 F Regr. features:
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1454.506944116645
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1375.540845810717
```

Gas Data Gas Data Mutual Info Regression & F Regression

	Feature Name	Mutual Info Regression Score	\
5	TIT	0.279721	
7	TEY	0.274431	
0	AT	0.268504	
4	GTEP	0.249459	
8	CDP	0.232809	
3	AFDP	0.143041	
9	year	0.141031	
6	TAT	0.120372	
1	AP	0.0960705	
2	AH	0.0430093	

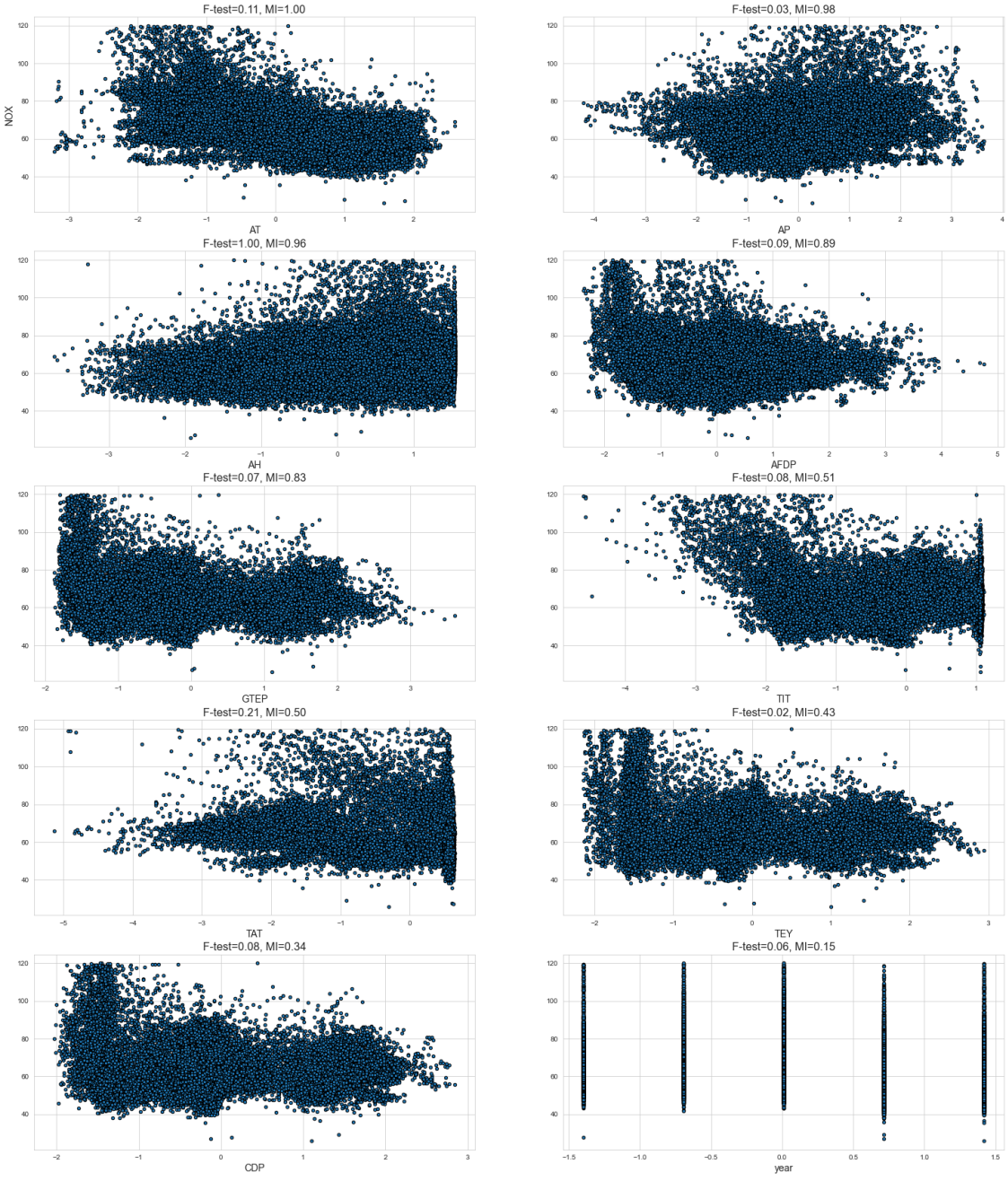
	Mutual Info Regression Score	- Scaled F Regression Score	\
5	1	1760.54	
7	0.981089	502.111	
0	0.959901	16622.8	

4	0.891814	1556.57
8	0.832292	1109.82
3	0.51137	1349.46
9	0.504185	3421.69
6	0.430329	319.01
1	0.343451	1404.93
2	0.153758	1023.09

	F Regression Score - Scaled
5	0.105911
7	0.0302062
0	1
4	0.0936405
8	0.0667649
3	0.0811813
9	0.205844
6	0.0191911
1	0.0845184
2	0.0615477

Table above shows the mutual info and f regression reasult for each variable against target variable NOX. Table is ordered by Mutual Info Regression Score - Scaled column. TIT, TEY, AT, GTEP and CDP seems to be the most important features for Mutual Info Regression. For F Regression the most important feature seems to be AT. However, it is also important to note that the unscaled values for both of the results for each feature scores are relatively low.

Gas Data Scatter Plot of features vs target variable along with Scaled Mutual Info and F Regression Scores



Gas Data Most important Features:

Mutual Info Regression most important 5 features: TIT, TEY, AT, GTEP and CDP

F Regression most important 3 features: AT, year, TIT.

Important features found by mutual info and f regression are very different.

I also experimented on different feature sets with Linear Regression model to see how their performance would change. All features in the RMSE dataset seems to be helping for prediction since subset of the features perform worse with Linear Regression model.

```
10-fold CV Linear Regression Experiment with All Features:
 Features:['AT', 'AP', 'AH', 'AFDP', 'GTEP', 'TIT', 'TAT', 'TEY', 'CDP', 'year']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.030473106723004
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
8.881846484410762


10-fold CV Linear Regression Experiment with Top MI Reg. Features:
 Features:['TIT', 'TEY', 'AT', 'GTEP', 'CDP']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  9.14421286309772
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
9.455365986158789


10-fold CV Linear Regression Experiment with Top F Reg. Features:
 Features:['AT', 'year', 'TIT']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.870111551541857
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
9.278648847152846


Top 5 Mutual Info Regr. features:
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  9.14421286309772
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
9.455365986158792


Top 5 F Regr. features:
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.836818159830631
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
9.356935850552805
```

Though one thing I realized when I was looking at the heatmap 3 of the features are very correlated with each other, and it might makes sense to drop 2 of them. Since this is the feature selection part, I will also explore this in here.

However, it is also important that the decision to drop is only based on what I saw in the heatmap, one could make better decision by knowing the meaning of each gas types and see if they are really correlated with each other. Since I am no expert in this area, I will check below to see if dropping two of them (CDP and GTEP) will help with the model performance.

```
10-fold CV Linear Regression Experiment with Top F Reg. Features:
 Features:['AT', 'AP', 'AH', 'AFDP', 'TIT', 'TAT', 'TEY', 'year']
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.036895416801087
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
8.713495424542154
```

The model performance is slightly improved, avg. 10-fold cross validation RMSE score decreased from 8.8 to 8.7, we can see that it doesn't hurt deleting these features. Given that 3 of these features (GTEP, TEY and CDP) are very correlated with each other, I considered to drop them. Though as I said I am no expert and a better decision can be made by experts in these area.

In addition to that the names of these features from the table are below: CDP: Compressor discharge pressure TEY: Turbine energy yield GTEP: Gas turbine exhaust pressure

Again this doesn't tell me too much about the data.

I found the paper published for this dataset and its benchmark. I realized that the authors of the paper also saw a correlation between these two variables, point out that it has benefits in predictive modelling and they might be dropped. However, in their experiment results and feature importances I saw that they kept these variables. Given that they are more knowledgable, experts in the field, the ones who prepared and benchmarked the dataset, and I didn't see huge changes in the above results, I finally decided to keep them and use all the features.

Paper link: https://journals.tubitak.gov.tr/elektrik/issues/elk-19-27-6/elk-27-6-54-1807-87.pdf

How does this step affect the performance of your models in terms of test RMSE?

Feature selection has different effects on the performance of the test data. If the removed features contains redundant data, noise or unrelated to the target variable, this step reduces the chances for overfitting, enhance the model generalization and improves the test RMSE score. This means if features selected precisely, test RMSE score is expected to lower and model to perform better. However, if deleted features contain important information that can be used for the prediction, the test RMSE score would increase and model performing worse. That is why, feature selection is a not a trivial step and should be performed carefully on which data we want to keep and remove. Feature selection also help decreasing both training and inference time given that we have to deal with less data.

If we think specifically for feature selection based on mutual information, it is not only limited to linear dependency but it rather quantifies the amount of information obtained from observing one variable about the other one. Whereas f regression captures only linear relationship between variables. Ideally, both feature selection methods expect to decrease redundant variables which leads less opportunity to overfit the model and better generalization. This means we expect to have good performing models with lower RMSE test scores. However, again we need to be careful, for example, with f regression we might possibly discard important nonlinear features during feature selection. This might hurt the model performance and increase the test RMSE score. To conclude, feature selection is a step to help reducing overfitting and to have generalization, improving both performance and time to train and inference of the model and leads to lower test RMSE score if performed successfully.

1.2 Linear Regression

Question 8 What is the objective function?

The Linear Regression model prediction is made:

$$\hat{y} = b + \sum_{i=1}^{p} x_i w_i = x^T w \tag{1}$$

$\hat{y}$ is predicted value, b bias (intercept term), p is the number for features, w is weights and x is the input data. (In the second part of the equation b is incorparated in the w in this case.).

Using RMSE as our error metric:

Ordinary Least Squares (Linear Regression without Regularization) Objective Function:

$$\min_w ||(Xw - Y)||_2^2 \tag{2}$$

Lasso Regression (L1 Regularization) Objective Function:

$$\min_w ||(Xw - Y)||_2^2 + \lambda ||w||_1 \tag{3}$$

Ridge Regression (L2 Regularization) Objective Function:

$$\min_w ||(Xw - Y)||_2^2 + \lambda ||w||_2^2 \tag{4}$$

X input, Y ground truth label, w parameters and λ is the regularization strength, hyperparameter to be tuned.

Explain how each regularization scheme affects the learned hypotheses.

Regularization techniques are used to avoid model overfitting and improving model generalization by adding a penalty term to the objective function. The intuition behind regularization is that by adding penalty terms related to the model weights (coefficients), the optimizer won't try to increase some weights larger and larger, so it encourages the weights to be kept small.

- **Lasso Regression:**

Lasso is also called L1 Regularization, it adds the absolute value of magnitude of coefficients (L1 norm) as penalty term to the loss function. It's advantage is it can set some coefficients to 0 (create sparse solutions), hence it might eliminate some features and can be considered as a built-in feature selection. It has unstable solution and may have multiple solutions for the optimization problem.

- **Ridge Regression:**

Ridge also called as L2 regularization since it adds squared magnitude of coefficients (squared L2 norm) as penalty term to the loss function. It forces the coefficients to be lower, close to 0 but not 0. The output is therefore non-sparse and it doesn't choose some subset of the features. It is computationally efficient since it has analytical solutions. After L2 regularization the optimal solutions are generally more stable.

Question 9 For each model I applied 10-fold cross-validation and measured average RMSE errors for training and validation sets.

How to pick optimal penalty (lambda) parameter? (alpha in sklearn)

There are several ways to select best values for choosing optimal regaularization value for linear models:

1- Via cross validation and grid search
2- Using information criterion (AIC, BIC) for Lasso Regression
3- Using model specific cross validations implemented in sklearn such as LassoCV and RidgeCV.

Lasso and Ridge models also have their own special cross validation implementations in scikit-learn to find a good value of penalty scores. They are called LassoCV and RidgeCV model, but the scores are calculated in terms of MSE rather than RMSE and only test scores are returned. Given that we are also interested on the training scores for the questions, I could't use these functions.

For Lasso Regression you can see the results of different lambda (alpha in sklearn) parameters both with Cross Validation + GridSearch and with AIC, BIC method. For Ridge Regression alpha value is only done with 10-fold cross validation over gridsearch with different lambda (alpha in sklearn) values.

Note: For cross validation results, sklearn scoring function uses negative RMSE values (neg_root_mean_squared_error) to be able to minimize the loss function. That is why the returned RMSE values are negative and we can simply get their absolute results as the RMSE value.

Diamonds Data Results Ordinary Least Squares (Linear Regression without Regularization)

```
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1206.280596794617
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1205.045050850985
```

Check RMSE results for each of the 10-fold:

```
Train RMSEs: [1246.67693953 1248.66216822 1230.78437231 1190.65068211
954.23438537
 1157.68140298 1256.25260037 1252.99820555 1264.05281144 1260.81240006]
Validation RMSEs:  [ 942.74216047  918.48055067 1112.58133725 1480.56810359
2806.51518647
 1699.75830566  815.69881421  877.61209435  670.86071043  725.63324541]
```

Lasso Regression

I tried alpha values from 1e-8 to 1e6. Results can be seen from below table:

	mean_train_score	mean_validation_score	model_name	param_model__alpha
14	1206.280597	1205.045051	Lasso	1e-08
15	1206.280597	1205.045051	Lasso	1e-07
16	1206.280597	1205.045052	Lasso	1e-06
17	1206.280597	1205.045064	Lasso	1e-05
18	1206.280597	1205.045161	Lasso	0.0001
19	1206.280597	1205.046257	Lasso	0.001

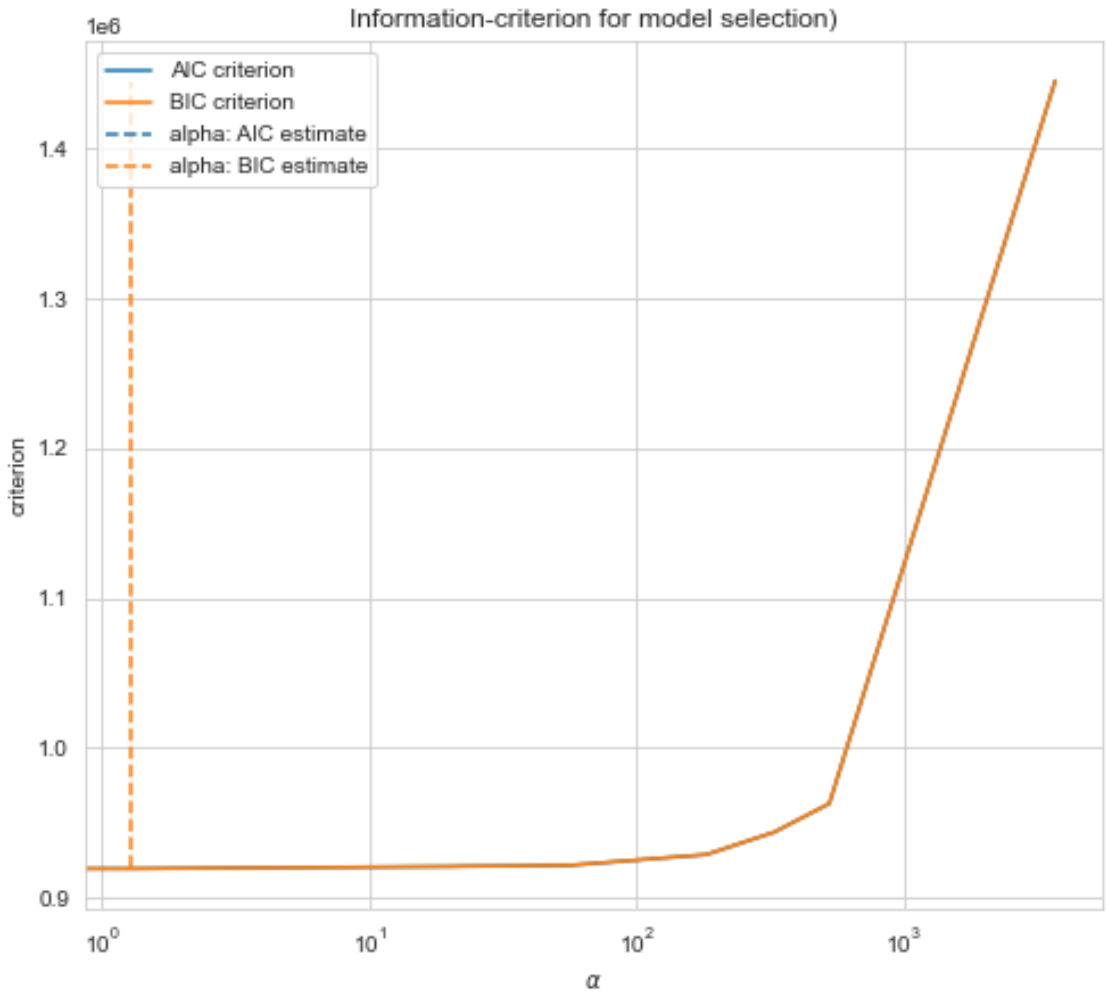
20	1206.280605	1205.057629	Lasso	0.01
21	1206.281434	1205.175550	Lasso	0.1
22	1206.357387	1206.498138	Lasso	1
23	1210.657916	1225.290602	Lasso	10
24	1251.275772	1244.896044	Lasso	100
25	1843.911711	1770.022846	Lasso	1000
26	3957.162324	3544.036398	Lasso	10000
27	3957.162324	3544.036398	Lasso	100000

The best average train and validation RMSE scores for Lasso Regression are in the 1205-1206 ranges. A good range for alpha is in this case is around 0.01 and 1. Since the RMSE doesn't change too much, we can pick 1 as the optimal penalty parameter. The reason behind is that we want to have simpler model that could achieve a good performance. Having a higher regularization helps us having simpler model and we can see that with $\alpha = 1$ we can achieve average RMSE results very close to the ones we found in the case of no regularization both in training and validation sets.

Penalty Selection based on AIC/BIC for Lasso

Lasso model fit with Lars using BIC (Bayes Information criterion) or AIC (Akaike information criterion) for model selection. These two criterion are used to select the regularization parameter. A good model should explain well the data while being simple to achieve that a trade-off between the goodness of fit and the complexity of the model is made.

```
<pandas.io.formats.style.Styler at 0x7ff049a17e10>
```



According to AIC criterion good alpha value is 0, and BIC criterion is around 1.3. This also supports the result we found above.

Ridge Regression

I tried alpha values from 1e-8 to 1e6. Results can be seen from below table:

	mean_train_score	mean_validation_score	model_name	param_model__alpha
0	1206.280597	1205.045051	Ridge	1e-08
1	1206.280597	1205.045051	Ridge	1e-07
2	1206.280597	1205.045051	Ridge	1e-06
3	1206.280597	1205.045052	Ridge	1e-05
4	1206.280597	1205.045059	Ridge	0.0001
5	1206.280597	1205.045137	Ridge	0.001
6	1206.280597	1205.045909	Ridge	0.01
7	1206.280598	1205.053637	Ridge	0.1
8	1206.280754	1205.131037	Ridge	1

9	1206.295931	1205.916546	Ridge	10
10	1207.536689	1214.414691	Ridge	100
11	1248.699264	1292.818122	Ridge	1000
12	1458.983908	1489.476610	Ridge	10000
13	2112.850610	1950.711595	Ridge	100000

In the case of Rigde regression we can increase the regularization in the range of 1-10. With the similar reasoning explained for Lasso, I will pick 10 as the optimal parameter.

Best Regularization with optimal penalty parameter

In the diamonds dataset, both Lasso and Ridge Regularization reach the same optimal results for average RMSE on training and validation sets. These results are also same for Linear Regression without regularization and lies in within 1205-1206 RMSE score. If we only look at the average optimal results, these 3 models don't really have much difference. When I checked the std of the train and validation RMSE scores for 10-fold cv(shown below) and the scores for each fold individually, again there is nothing very different for Lasso and Ridge Regression.

If I choose one, I would pick Ridge regularization since it seems to be better regularization scheme for diamonds data for the overall RMSE scores for higher regularization values. The avg. scores are way lower in Ridge then Lasso. For example Lasso when alpha=1000 avg RMSE validation score=1770 and Ridge when alpha=1000 avg RMSE validation score=1292. Therefore, Ridge regularization is best regularization scheme with optimal penalty 1.

Ridge Regression Results (test score columns are actually validation score here, crossvalidate names them as test.)

	split0_test_score	split1_test_score	split2_test_score	split3_test_score	\
8	-943.047423	-918.745592	-1112.593318	-1480.207682	
9	-945.772298	-921.113590	-1112.713075	-1476.998752	

	split4_test_score	split5_test_score	split6_test_score	split7_test_score	\
8	-2806.756166	-1700.057234	-815.570266	-877.496956	
9	-2809.011538	-1702.738090	-814.432034	-876.470311	

	split8_test_score	split9_test_score	mean_validation_score	\
8	-670.987363	-725.848366	1205.131037	
9	-672.135127	-727.780644	1205.916546	

	std_test_score	rank_test_score
8	617.997804	16
9	618.307116	18

	split0_train_score	split1_train_score	split2_train_score	\
8	-1246.677053	-1248.662286	-1230.784516	
9	-1246.688078	-1248.673713	-1230.798464	

	split3_train_score	split4_train_score	split5_train_score	\
8	-1190.650864	-954.234736	-1157.681538	
9	-1190.668558	-954.268267	-1157.694613	

```
   split6_train_score  split7_train_score  split8_train_score  \
8        -1256.252739        -1252.998340        -1264.052939
9        -1256.266196        -1253.011377        -1264.065238

   split9_train_score  mean_train_score  std_train_score
8        -1260.812526       1206.280754        90.084923
9        -1260.824805       1206.295931        90.078895
```

Lasso Regression Results (test score columns are actually validation score here, crossvalidate names them as test.)

```
    split0_test_score  split1_test_score  split2_test_score  \
22        -948.420031        -923.845640       -1113.481926
23       -1001.156908        -974.532777       -1125.583926

    split3_test_score  split4_test_score  split5_test_score  \
22       -1476.159596       -2810.451532       -1705.121582
23       -1436.060043       -2869.030266       -1761.357107

    split6_test_score  split7_test_score  split8_test_score  \
22        -812.459728        -874.713354        -671.818620
23        -788.742713        -848.425307        -684.250555

    split9_test_score  mean_validation_score  std_test_score  rank_test_score
22        -728.509373            1206.498138      618.777888               19
23        -763.766418            1225.290602      632.064742               21

    split0_train_score  split1_train_score  split2_train_score  \
22        -1246.742106        -1248.726980        -1230.852788
23        -1250.603468        -1252.591315        -1234.881322

    split3_train_score  split4_train_score  split5_train_score  \
22        -1190.696045         -954.420070        -1157.758913
23        -1194.615517         -961.823509        -1162.617515

    split6_train_score  split7_train_score  split8_train_score  \
22        -1256.316502        -1253.061068        -1264.115736
23        -1260.161182        -1256.757931        -1267.712219

    split9_train_score  mean_train_score  std_train_score
22        -1260.883657       1206.357387        90.051053
23        -1264.815178       1210.657916        88.987987
```

Best model feature importance:

From the best found linear regression model (Ridge Regression) we see the coefficients below:

```
                    carat           x     clarity      color         cut  \
Coefficients   5092.655074 -984.480857  826.612634  548.94111  134.816544
coef_absolute  5092.655074  984.480857  826.612634  548.94111  134.816544
```

	depth	table	y	z
Coefficients	-114.319163	-59.802654	49.963989	-20.679798
coef_absolute	114.319163	59.802654	49.963989	20.679798

According to coeffs, the most important feature is carat, followed by x, clarity, color and cut. x, depth, table and z has reverse relation with target variable whereas the other features have positive correlation.

Gas Data Results Ordinary Least Squares (Linear Regression without Regularization)

```
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.030473106723004
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
8.881846484410762
```

Check RMSE results for each of the 10-fold:

```
Train RMSEs: [8.20232426 8.0507639  8.1187614  8.17650722 7.74108808 7.83083707
 7.79695147 8.26129408 8.19835912 7.92784446]
Validation RMSEs:  [ 7.43536346  8.57794857  7.89249311  7.21361859 11.91720141
10.28186932
 11.55608868  6.192516    7.87080299  9.88056272]
```

Lasso Regression

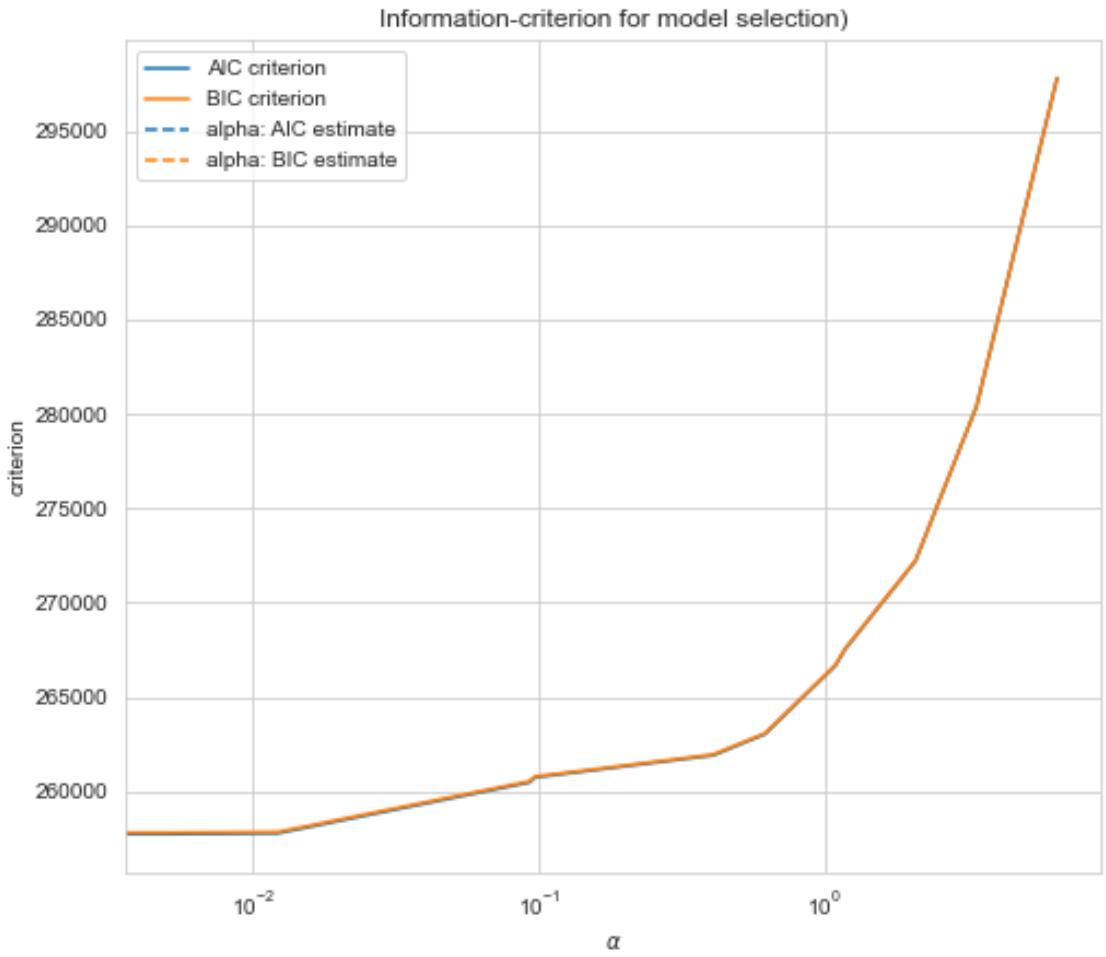
I tried alpha values from 1e-8 to 1e6. Results can be seen from below table:

	mean_train_score	mean_validation_score	model_name	param_model__alpha
14	8.030497	8.890395	Lasso	1e-08
15	8.030497	8.890394	Lasso	1e-07
16	8.030497	8.890384	Lasso	1e-06
17	8.030496	8.890279	Lasso	1e-05
18	8.030491	8.889226	Lasso	0.0001
19	8.030507	8.878864	Lasso	0.001
20	8.036236	8.802989	Lasso	0.01
21	8.343862	8.958754	Lasso	0.1
22	8.888678	9.370859	Lasso	1
23	11.656838	11.747458	Lasso	10
24	11.656838	11.747458	Lasso	100
25	11.656838	11.747458	Lasso	1000
26	11.656838	11.747458	Lasso	10000
27	11.656838	11.747458	Lasso	100000

The best average train and validation RMSE scores for Lasso Regression are in the 8.03-8.9 ranges. A good alpha value in this case is 0.01 where validation score is minimized.

Penalty Selection based on AIC/BIC for Lasso

```
<pandas.io.formats.style.Styler at 0x7ff048b51350>
```



According to AIC and BIC criterion good alpha value is 0.

Ridge Regression

I tried alpha values from 1e-8 to 1e6. Results can be seen from below table:

	mean_train_score	mean_validation_score	model_name	param_model__alpha
0	8.030473	8.881846	Ridge	1e-08
1	8.030473	8.881846	Ridge	1e-07
2	8.030473	8.881846	Ridge	1e-06
3	8.030473	8.881846	Ridge	1e-05
4	8.030473	8.881846	Ridge	0.0001
5	8.030473	8.881841	Ridge	0.001
6	8.030473	8.881795	Ridge	0.01
7	8.030473	8.881332	Ridge	0.1
8	8.030498	8.876794	Ridge	1
9	8.032520	8.839102	Ridge	10
10	8.094992	8.761643	Ridge	100

11	8.316408	8.949233	Ridge	1000
12	8.778942	9.323730	Ridge	10000
13	10.333445	10.634421	Ridge	100000

In the case of Rigde best alpha value is 100 where validation score is minimized.

Best Regularization with optimal penalty parameter

Top 3 results from experiment:

	mean_train_score	mean_validation_score	model_name	param_model__alpha
10	8.094992	8.761643	Ridge	100
20	8.036236	8.802989	Lasso	0.01
9	8.032520	8.839102	Ridge	10

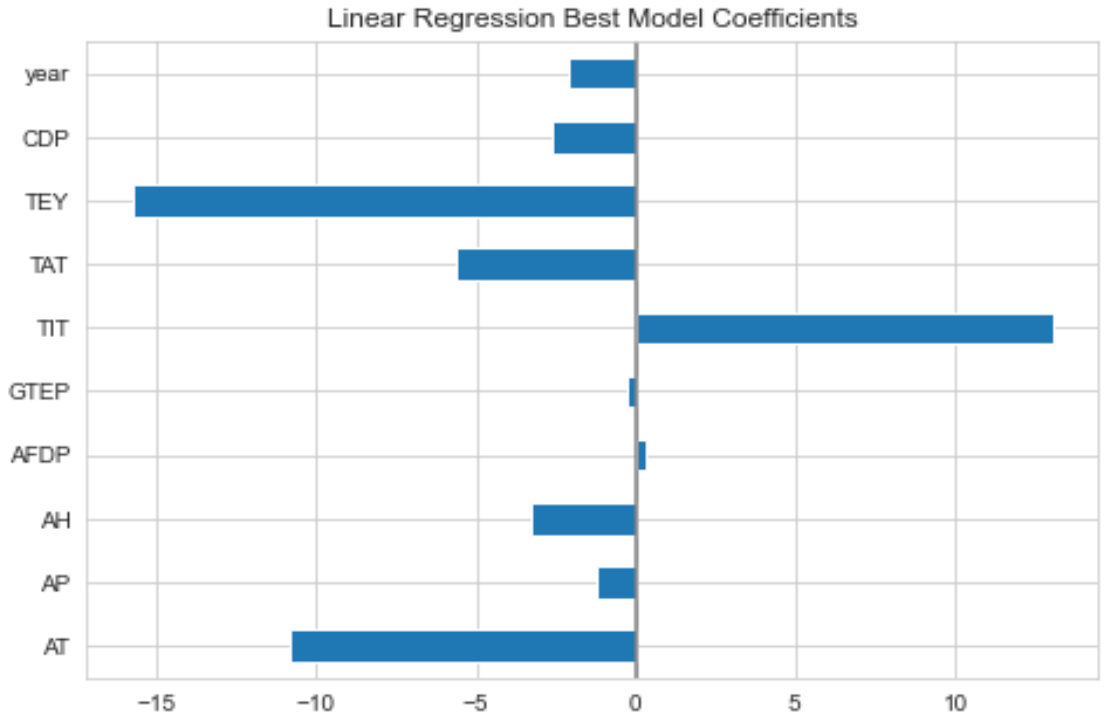
In the gas dataset, both Lasso and Ridge Regularization reach similar optimal results for average RMSE on training and validation sets. These results are also very close for Linear Regression without regularization and lies in within 8-8.8 RMSE score. Ridge regularization seem to perform slighlty better than Lasso, therefore the best regularization scheme for this dataset is Ridge with alpha 100.

Best model feature importance:

From the best found linear regression model (Ridge Regression) we see the coefficients below:

	TEY	TIT	AT	TAT	AH	CDP	\
Coefficients	-15.753769	13.057814	-10.803841	-5.660252	-3.279827	-2.640984	
coef_absolute	15.753769	13.057814	10.803841	5.660252	3.279827	2.640984	

	year	AP	AFDP	GTEP
Coefficients	-2.102134	-1.204434	0.30354	-0.263377
coef_absolute	2.102134	1.204434	0.30354	0.263377



According to coeffs, the most important 5 features are TEY, followed by TIT, then AT, TAT and AH. Only TIT is the positively correlatead feature with NOX within these 5 important features found.

Question 10 The same experiments as Q9 applied on unscaled features.

Diamond Dataset Unscaled Feature results

```
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  1206.2805967946167
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
1205.045050850984
```

Check RMSE results for each of the 10-fold:

```
Train RMSEs: [1246.67693953 1248.66216822 1230.78437231 1190.65068211
954.23438537
 1157.68140298 1256.25260037 1252.99820555 1264.05281144 1260.81240006]
Validation RMSEs:  [ 942.74216047  918.48055067 1112.58133725 1480.56810359
2806.51518647
 1699.75830566  815.69881421  877.61209435  670.86071043  725.63324541]
```

	mean_train_score	mean_validation_score	model_name	param_model__alpha
14	1206.280597	1205.045051	Lasso	1e-08
15	1206.280597	1205.045051	Lasso	1e-07
16	1206.280597	1205.045053	Lasso	1e-06

17	1206.280597	1205.045073	Lasso	1e-05
18	1206.280597	1205.045263	Lasso	0.0001
19	1206.280597	1205.047165	Lasso	0.001
20	1206.280609	1205.066857	Lasso	0.01
21	1206.281892	1205.272222	Lasso	0.1
22	1206.403372	1207.533286	Lasso	1
23	1215.137979	1238.590955	Lasso	10
24	1362.777782	1459.776195	Lasso	100
25	2049.825908	1984.620077	Lasso	1000
26	3957.162324	3544.036398	Lasso	10000
27	3957.162324	3544.036398	Lasso	100000

	mean_train_score	mean_validation_score	model_name	param_model__alpha
0	1206.280597	1205.045051	Ridge	1e-08
1	1206.280597	1205.045051	Ridge	1e-07
2	1206.280597	1205.045051	Ridge	1e-06
3	1206.280597	1205.045055	Ridge	1e-05
4	1206.280597	1205.045088	Ridge	0.0001
5	1206.280597	1205.045421	Ridge	0.001
6	1206.280597	1205.048757	Ridge	0.01
7	1206.280619	1205.082125	Ridge	0.1
8	1206.282816	1205.417296	Ridge	1
9	1206.492542	1208.905905	Ridge	10
10	1220.380991	1249.715537	Ridge	100
11	1388.872280	1472.734228	Ridge	1000
12	1597.964835	1620.737422	Ridge	10000
13	2266.684099	2074.013462	Ridge	100000

Gas Dataset Unscaled Feature results

```
Linear Regression (OLS) Train Avg RMSE accross 10-fold cv:  8.030473106723004
Linear Regression (OLS) Validation Avg RMSE accross 10-fold cv:
8.881846484410753
```

Check RMSE results for each of the 10-fold:

```
Train RMSEs: [8.20232426 8.0507639  8.1187614  8.17650722 7.74108808 7.83083707
 7.79695147 8.26129408 8.19835912 7.92784446]
Validation RMSEs:  [ 7.43536346  8.57794857  7.89249311  7.21361859 11.91720141
10.28186932
 11.55608868  6.192516    7.87080299  9.88056272]
```

	mean_train_score	mean_validation_score	model_name	param_model__alpha
14	8.030497	8.890395	Lasso	1e-08
15	8.030497	8.890395	Lasso	1e-07
16	8.030497	8.890389	Lasso	1e-06
17	8.030497	8.890334	Lasso	1e-05
18	8.030495	8.889781	Lasso	0.0001

19	8.030495	8.884250	Lasso	0.001
20	8.031513	8.841661	Lasso	0.01
21	8.036915	8.728267	Lasso	0.1
22	8.166387	8.714142	Lasso	1
23	9.562444	9.933988	Lasso	10
24	11.656838	11.747458	Lasso	100
25	11.656838	11.747458	Lasso	1000
26	11.656838	11.747458	Lasso	10000
27	11.656838	11.747458	Lasso	100000

	mean_train_score	mean_validation_score	model_name	param_model__alpha
0	8.030473	8.881846	Ridge	1e-08
1	8.030473	8.881846	Ridge	1e-07
2	8.030473	8.881846	Ridge	1e-06
3	8.030473	8.881846	Ridge	1e-05
4	8.030473	8.881846	Ridge	0.0001
5	8.030473	8.881846	Ridge	0.001
6	8.030473	8.881843	Ridge	0.01
7	8.030473	8.881816	Ridge	0.1
8	8.030473	8.881545	Ridge	1
9	8.030482	8.878971	Ridge	10
10	8.030814	8.861215	Ridge	100
11	8.032528	8.786004	Ridge	1000
12	8.056832	8.580556	Ridge	10000
13	8.412807	8.791324	Ridge	100000

Does feature scaling play any role (in the cases with and without regularization)?

For diamonds data, Ridge Regression on scaled data has lower average RMSE values for the alpha > 10 compared the same lambda values applied on unscaled data on Ridge. For Lasso, we see that for larger alpha values, we see the same trend, scaled data has either lower or very similar value compared the unscaled data. The trends are same both in train and validation sets. This experiment shows that scaling our data is a good technique, which helps us getting better avg. RMSE scores especially against higher penalty regularization parameter values (seen from above tables). It is also important to note that the best/optimal avg. RMSE values found for scaled and unscaled data are almost same for optimal Ridge and optimal Lasso alpha values lying in the 1205-1206 range. For the unscaled data, the optimal value for regularization parameters are smaller, for Ridge optimal alpha is 1 and for Lasso alpha is 0.1.

From the experiments on diamonds data above, scaling data doesn't seem to play a role on the case without regularization. For the regularization on the other hand, scaling improves the avg. RMSE scores across different lambda values. This means for unscaled data the choice of regularization parameter is more crucial since the RMSE results can explode and grow very quickly when the data is unscaled and an unoptimal lambda parameter is chosen.

`Diamonds Data Scaled Best Results`

	mean_train_score	mean_validation_score	model_name	param_model__alpha
0	1206.280597	1205.045051	Ridge	1e-08
1	1206.280597	1205.045051	Ridge	1e-07

```
14       1206.280597            1205.045051      Lasso              1e-08
```

```
Diamons Data Unscaled Best Results
```

```
    mean_train_score  mean_validation_score model_name param_model__alpha
0         1206.280597            1205.045051      Ridge              1e-08
14        1206.280597            1205.045051      Lasso              1e-08
1         1206.280597            1205.045051      Ridge              1e-07
```

For the gas data, the validation scores for scaled and unscaled data are again very similar. Unscaled results are slightly better than the scaled ones as it can be seen below. But it doesn't play a big role.

```
Gas Data Scaled Best Results
```

```
    mean_train_score  mean_validation_score model_name param_model__alpha
10          8.094992               8.761643      Ridge                100
20          8.036236               8.802989      Lasso               0.01
9           8.032520               8.839102      Ridge                 10
```

```
Gas Data Unscaled Best Results
```

```
    mean_train_score  mean_validation_score model_name param_model__alpha
12          8.056832               8.580556      Ridge              10000
22          8.166387               8.714142      Lasso                  1
21          8.036915               8.728267      Lasso                0.1
```

Question 11 Some linear regression packages return p-values for different features. What is the meaning of them and how can you infer the most significant features?

P-values for each feature tests a null hypothesis that the coefficient has no effect (equal to 0). A typical threshold for p-value is 0.05 (corresponds to 95% confidence interval. A p-value lower than threshold (< 0.05) means we should reject the null hypothesis and the feature is important for the prediction of the target variable. A p-value higher than threshold, means that the feature is statistically not significant to predict the target variable, the change in target variable is not associated with the feature. The p-values can be used to find most meaningful feature and may be used to decide which features to keep in the model and which ones we can remove.

scipy.stats.linregress and statsmodels.regression.linear_model.OLS are two library models that returns p-values for each feature where we can infer most significant features using them. I experimented with statsmodels.regression.linear_model.OLS on diamonds dataset to find important features for scaled and unscaled dataset:

Diamonds Data Diamonds Data Scaled (statsmodels.regression.linear_model.OLS) Results

```
OLS params:
 carat      5092.655074
depth      -114.319163
table       -59.802654
x          -984.480857
```

```
y            49.963989
z           -20.679798
cut         134.816544
color       548.941110
clarity     826.612634
dtype: float64
```

These are the coefficients assigned to each feature. The highest coefficient is given to carat meaning carat has the highest positive impact on the diamond price. Whereas x has the largest negative coefficient which means x also has a high impact, this time inverse relation, on the diamond price: lower the x the higher price we can assign.

OLS Summary for Scaled Diamonds Data:

```
                                OLS Regression Results
==============================================================================
=======
Dep. Variable:                   price   R-squared (uncentered):
0.460
Model:                             OLS   Adj. R-squared (uncentered):
0.460
Method:                  Least Squares   F-statistic:
5100.
Date:                 Tue, 15 Mar 2022   Prob (F-statistic):
0.00
Time:                         23:43:50   Log-Likelihood:
-5.2549e+05
No. Observations:               53940   AIC:
1.051e+06
Df Residuals:                   53931   BIC:
1.051e+06
Df Model:                           9
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
carat       5092.6551     83.184     61.222      0.000    4929.614    5255.696
depth       -114.3192     23.251     -4.917      0.000    -159.891     -68.748
table        -59.8027     22.299     -2.682      0.007    -103.510     -16.096
x           -984.4809    133.775     -7.359      0.000   -1246.681    -722.281
y             49.9640     80.234      0.623      0.533    -107.295     207.223
z            -20.6798     86.048     -0.240      0.810    -189.334     147.975
cut          134.8165     21.602      6.241      0.000      92.475     177.158
color        548.9411     18.771     29.244      0.000     512.150     585.733
clarity      826.6126     19.645     42.077      0.000     788.108     865.117
==============================================================================
Omnibus:                    12438.546   Durbin-Watson:                   0.100
Prob(Omnibus):                  0.000   Jarque-Bera (JB):           659440.386
Skew:                          -0.141   Prob(JB):                         0.00
```

```
Kurtosis:                       20.127   Cond. No.                         18.0
==============================================================================

Notes:
[1] R² is computed without centering (uncentered) since the model does not
contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
```

By looking the p-values in the above table (P >|t|), we can see that carat, depth, x, cut, color, clarity values have p-values lower than 0.05 and are the most important features. The R^2 and adjusted R^2 values for the model is 0.46 which is pretty low.

Diamonds Data Unscaled (statsmodels.regression.linear_model.OLS) Results

When we used unscaled data to apply OLS the R^2 and adjusted R^2 results are very high, 0.953 with all the diamonds features. Also all the features have p-values lower than 0.05. This means that with unscaled features OLS can fit a good linear model where all features are important for the prediction.

```
OLS params:
 carat      10587.758498
depth         -41.693458
table          -8.901253
x            -770.488938
y              60.599056
z            -121.711175
cut           144.798827
color         324.416568
clarity       506.522714
dtype: float64
                                 OLS Regression Results
==============================================================================
=======
Dep. Variable:                   price   R-squared (uncentered):
0.953
Model:                             OLS   Adj. R-squared (uncentered):
0.953
Method:                  Least Squares   F-statistic:
1.210e+05
Date:                 Tue, 15 Mar 2022   Prob (F-statistic):
0.00
Time:                         23:43:50   Log-Likelihood:
-4.5975e+05
No. Observations:               53940   AIC:
9.195e+05
Df Residuals:                   53931   BIC:
9.196e+05
Df Model:                           9
Covariance Type:            nonrobust
```

	coef	std err	t	P>|t|	[0.025	0.975]
carat	1.059e+04	48.719	217.323	0.000	1.05e+04	1.07e+04
depth	-41.6935	2.025	-20.587	0.000	-45.663	-37.724
table	-8.9013	2.132	-4.175	0.000	-13.080	-4.722
x	-770.4889	33.062	-23.304	0.000	-835.291	-705.687
y	60.5991	20.676	2.931	0.003	20.074	101.124
z	-121.7112	34.465	-3.531	0.000	-189.263	-54.159
cut	144.7988	5.016	28.865	0.000	134.967	154.631
color	324.4166	3.256	99.640	0.000	318.035	330.798
clarity	506.5227	3.485	145.344	0.000	499.692	513.353

Omnibus:	12161.268	Durbin-Watson:	1.132
Prob(Omnibus):	0.000	Jarque-Bera (JB):	614443.485
Skew:	-0.100	Prob(JB):	0.00
Kurtosis:	19.533	Cond. No.	860.

Notes:
[1] R^2 is computed without centering (uncentered) since the model does not contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Gas Data Gas Data Scaled (statsmodels.regression.linear_model.OLS) Results

```
OLS params:
 AT     -12.906630
AP      -1.493527
AH      -3.317940
AFDP     0.289539
GTEP     0.568738
TIT     19.725546
TAT     -7.755266
TEY    -28.881104
CDP      2.063782
year    -1.339015
dtype: float64
```

These are the coefficients assigned to each feature. The highest absolute coefficient is given to TEY which has the highest negative impact on the NOX. Whereas TIT has the largest positive coefficient, and second biggest absolute coefficient, which means TIT also has a high impact, this time it has positive relation, on the NOX prediction.

OLS Summary for Scaled Gas Data:

OLS Regression Results

```
=======
Dep. Variable:                      y   R-squared (uncentered):
0.016
Model:                            OLS   Adj. R-squared (uncentered):
0.016
Method:                 Least Squares   F-statistic:
60.38
Date:                Tue, 15 Mar 2022   Prob (F-statistic):
2.89e-122
Time:                        23:43:50   Log-Likelihood:
-2.0590e+05
No. Observations:               36733   AIC:
4.118e+05
Df Residuals:                   36723   BIC:
4.119e+05
Df Model:                          10
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
AT           -12.9066      0.992    -13.008      0.000     -14.851     -10.962
AP            -1.4935      0.422     -3.537      0.000      -2.321      -0.666
AH            -3.3179      0.430     -7.713      0.000      -4.161      -2.475
AFDP           0.2895      0.554      0.523      0.601      -0.796       1.375
GTEP           0.5687      1.937      0.294      0.769      -3.228       4.365
TIT           19.7255      3.137      6.289      0.000      13.577      25.874
TAT           -7.7553      1.662     -4.666      0.000     -11.013      -4.498
TEY          -28.8811      5.533     -5.219      0.000     -39.727     -18.036
CDP            2.0638      5.721      0.361      0.718      -9.150      13.278
year          -1.3390      0.619     -2.163      0.031      -2.552      -0.126
==============================================================================
Omnibus:                     7598.785   Durbin-Watson:                   0.006
Prob(Omnibus):                  0.000   Jarque-Bera (JB):            26667.084
Skew:                           1.024   Prob(JB):                         0.00
Kurtosis:                       6.637   Cond. No.                         47.7
==============================================================================

Notes:
[1] R² is computed without centering (uncentered) since the model does not
contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
```

By looking the p-values in the above table (P >|t|), we can see that all features except AFDP, GTEP and CDP are important features for NOX prediction. They añń have p-values lower than 0.05 and are the most important features. The R^2 and adjusted R^2 values for the model is 0.016 which is pretty low.

Gas Data Unscaled (statsmodels.regression.linear_model.OLS) Results

When we used unscaled data to apply OLS the R^2 and adjusted R^2 results are very high, 0.985 with all the diamonds features. Also all the features have p-values lower than 0.05 except GTEP. This means that with unscaled features OLS can fit a good linear model where all features are important (except GTEP) for the prediction.

```
OLS params:
 AT     -1.717197
AP     -0.240365
AH     -0.230917
AFDP    0.379716
GTEP    0.102995
TIT     1.105622
TAT    -1.133994
TEY    -1.793823
CDP     1.505362
year   -0.959536
dtype: float64
                                 OLS Regression Results
==============================================================================
=======
Dep. Variable:                        y   R-squared (uncentered):
0.985
Model:                              OLS   Adj. R-squared (uncentered):
0.985
Method:                   Least Squares   F-statistic:
2.441e+05
Date:                  Tue, 15 Mar 2022   Prob (F-statistic):
0.00
Time:                          23:43:50   Log-Likelihood:
-1.2885e+05
No. Observations:                36733   AIC:
2.577e+05
Df Residuals:                    36723   BIC:
2.578e+05
Df Model:                           10
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
AT            -1.7172      0.015   -115.065      0.000      -1.746      -1.688
AP            -0.2404      0.007    -34.351      0.000      -0.254      -0.227
AH            -0.2309      0.004    -64.187      0.000      -0.238      -0.224
AFDP           0.3797      0.088      4.324      0.000       0.208       0.552
GTEP           0.1030      0.055      1.874      0.061      -0.005       0.211
TIT            1.1056      0.020     54.190      0.000       1.066       1.146
TAT           -1.1340      0.030    -38.034      0.000      -1.192      -1.076
TEY           -1.7938      0.037    -48.895      0.000      -1.866      -1.722
CDP            1.5054      0.624      2.414      0.016       0.283       2.728
```

```
year          -0.9595      0.053    -18.059      0.000      -1.064      -0.855
==============================================================================
Omnibus:                     7518.162   Durbin-Watson:                   0.376
Prob(Omnibus):                  0.000   Jarque-Bera (JB):            26205.615
Skew:                           1.016   Prob(JB):                         0.00
Kurtosis:                       6.605   Cond. No.                     2.35e+04
==============================================================================

Notes:
[1] R² is computed without centering (uncentered) since the model does not
contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[3] The condition number is large, 2.35e+04. This might indicate that there are
strong multicollinearity or other numerical problems.
```

1.3 Polynomial Regression

Question 12 For each polynomial regression model I applied 10-fold cross-validation and measured average RMSE errors for training and validation sets.

For this experiment, I created a pipeline to extract polynomial features with PolynomialFeatures() in sklearn and applied Linear Regression on the compound features (I used Lasso and Ridge Regression models for regularization). Grid search over 10-fold cv is applied to tune degrees for polynomial features and alpha for the regularization. Degree range is [2, 3, 4] and alpha range is $[10^{-4}, 10^{3}]$.

Diamond Data

Polynomial Regression Experiment Results Top 10 hyperparameter combination results based on based mean validation score. From the below table, the best combinations 10-fold avg train RMSE: 921.57 avg validation RMSE: 882.22 which are way better than the Linear Regression results which were around 1205-1206 RMSE results for both metrics.

```
    mean_train_score  mean_validation_score  \
42         921.572213             882.226435
39         782.419320            1129.772967
36         763.272005            1615.358097
21         795.955216            1667.221668
24         757.769711            1777.435298
27         757.769829            1777.748836
30         757.771652            1780.882997
45        1841.870944            1790.712541
33         757.857294            1809.238839
46        2023.787034            1902.183814

                           param_model  param_model__alpha  \
42  Lasso(alpha=100, random_state=142)            100.0000
39  Lasso(alpha=100, random_state=142)             10.0000
```

36	Lasso(alpha=100, random_state=142)	1.0000
21	Ridge(random_state=142)	1000.0000
24	Lasso(alpha=100, random_state=142)	0.0001
27	Lasso(alpha=100, random_state=142)	0.0010
30	Lasso(alpha=100, random_state=142)	0.0100
45	Lasso(alpha=100, random_state=142)	1000.0000
33	Lasso(alpha=100, random_state=142)	0.1000
46	Lasso(alpha=100, random_state=142)	1000.0000

	param_poly_features__degree
42	2
39	2
36	2
21	2
24	2
27	2
30	2
45	2
33	2
46	3

Best model found from GridSearch:

The best model is Lasso with alpha 100 and PolynomialFeatures set with degree 2.

```
Best Model: Pipeline(steps=[('poly_features', PolynomialFeatures()),
                ('model', Lasso(alpha=100, random_state=142))])
Best Model Params: {'model': Lasso(alpha=100, random_state=142), 'model__alpha':
100, 'poly_features': PolynomialFeatures(), 'poly_features__degree': 2}
```

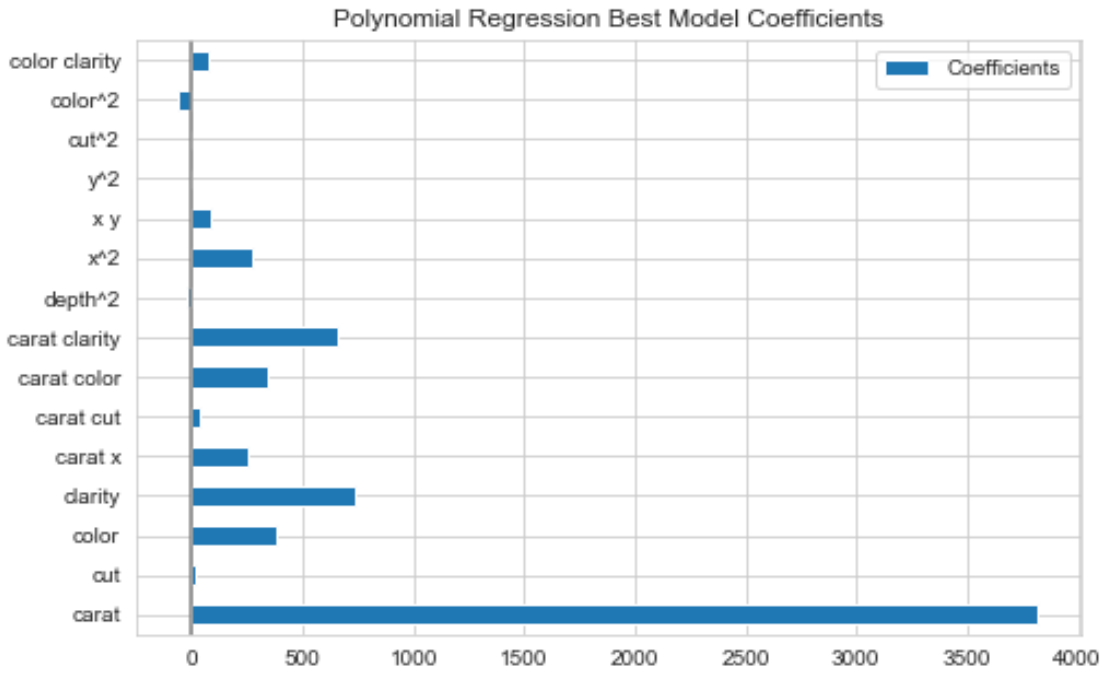
Coefficient of the best model and Most Salient Features:

Since the selected best model is with Lasso Regularization, we can see that most of the features have 0 coefficients.

	Coefficients
1	0.000000
carat	3819.165766
depth	-0.000000
table	-0.000000
x	0.000000
y	0.000000
z	0.000000
cut	19.424984
color	379.512189
clarity	736.942242
carat^2	0.000000
carat depth	-0.000000
carat table	-0.000000

```
carat x          255.502250
carat y            0.000000
carat z            0.000000
carat cut         36.487862
carat color      340.220949
carat clarity    658.568956
depth^2          -25.612413
depth table        0.000000
depth x           -0.000000
depth y           -0.000000
depth z           -0.000000
depth cut          0.000000
depth color        0.000000
depth clarity      0.000000
table^2           -0.000000
table x           -0.000000
table y           -0.000000
table z           -0.000000
table cut          0.000000
table color        0.000000
table clarity      0.000000
x^2              272.697483
x y               83.223653
x z                0.000000
x cut              0.000000
x color            0.000000
x clarity          0.000000
y^2               -0.961110
y z                0.000000
y cut              0.000000
y color            0.000000
y clarity          0.000000
z^2                0.000000
z cut              0.000000
z color            0.000000
z clarity          0.000000
cut^2             -5.943162
cut color         -0.000000
cut clarity       -0.000000
color^2          -58.635986
color clarity     79.471302
clarity^2         -0.000000
```

Lasso Regression assigns 0 values to coefficients as seen above, to understand salient features better, I plotted the non-zero coefficients only.



Non-zero Coefficients ordered from highest to lowest absolute coefficient values:

	carat	clarity	carat clarity	color	\
Coefficients	3819.165766	736.942242	658.568956	379.512189	
coef_absolute	3819.165766	736.942242	658.568956	379.512189	

	carat color	x^2	carat x	x y	color clarity	\
Coefficients	340.220949	272.697483	255.50225	83.223653	79.471302	
coef_absolute	340.220949	272.697483	255.50225	83.223653	79.471302	

	color^2	carat cut	depth^2	cut	cut^2	y^2
Coefficients	-58.635986	36.487862	-25.612413	19.424984	-5.943162	-0.96111
coef_absolute	58.635986	36.487862	25.612413	19.424984	5.943162	0.96111

From the coefficients, we can see that Lasso assigns 0 to many of the features and only small number of them have non-zero coefficients. Within the most salient features, the most important one is carat with the biggest coefficient 3819.17. This means the increase in price is positively correlated with the carat coefficient. Clarity is the second most important feature followed by compound carat clarit feature, color, carat color, x^2 and carat x. Color^2, depth^2, cut^2 and y^2 also has negative correlation with diamond price. Decreasing either one of them leads to increase the price. The coefficient values also matter, the bigger the absolute coefficient value means the bigger impact it has on the target variable (pricing the diamond), the more important the feature in terms of predicting the target variable.

Gas Data

Polynomial Regression Experiment Results Top 10 hyperparameter combination results based on based mean validation score. From the below table, the best combinations 10-fold avg train RMSE: 5.72 avg validation RMSE: 7.15 which are way better than the Linear Regression results which were around 8.1-8.76 RMSE results for both metrics.

```
    mean_train_score  mean_validation_score  \
35          5.719778               7.155798
34          5.827271               7.171435
22          5.508430               7.226445
23          5.273528               7.369680
33          6.246073               7.436532
18          5.682998               7.459753
21          6.055840               7.464865
19          5.119546               7.514624
20          4.895412               7.588859
31          5.156848               7.655462

                          param_model  param_model__alpha  \
35  Lasso(alpha=0.1, random_state=142)                0.10
34  Lasso(alpha=0.1, random_state=142)                0.10
22             Ridge(random_state=142)             1000.00
23             Ridge(random_state=142)             1000.00
33  Lasso(alpha=0.1, random_state=142)                0.10
18             Ridge(random_state=142)              100.00
21             Ridge(random_state=142)             1000.00
19             Ridge(random_state=142)              100.00
20             Ridge(random_state=142)              100.00
31  Lasso(alpha=0.1, random_state=142)                0.01

    param_poly_features__degree
35                            4
34                            3
22                            3
23                            4
33                            2
18                            2
21                            2
19                            3
20                            4
31                            3
```

Best model found from GridSearch:

The best model is Lasso with alpha 0.1 and PolynomialFeatures set with degree 4. alpha 0.1 with degree 3 is also the second best result where the validation scores of both options are very close to each other.

```
Best Model: Pipeline(steps=[('poly_features',
                PolynomialFeatures(degree=4, interaction_only='False')),
```

```
                ('model', Lasso(alpha=0.1, random_state=142))])
Best Model Params: {'model': Lasso(alpha=0.1, random_state=142), 'model__alpha':
0.1, 'poly_features': PolynomialFeatures(degree=4, interaction_only='False'),
'poly_features__degree': 4}
```

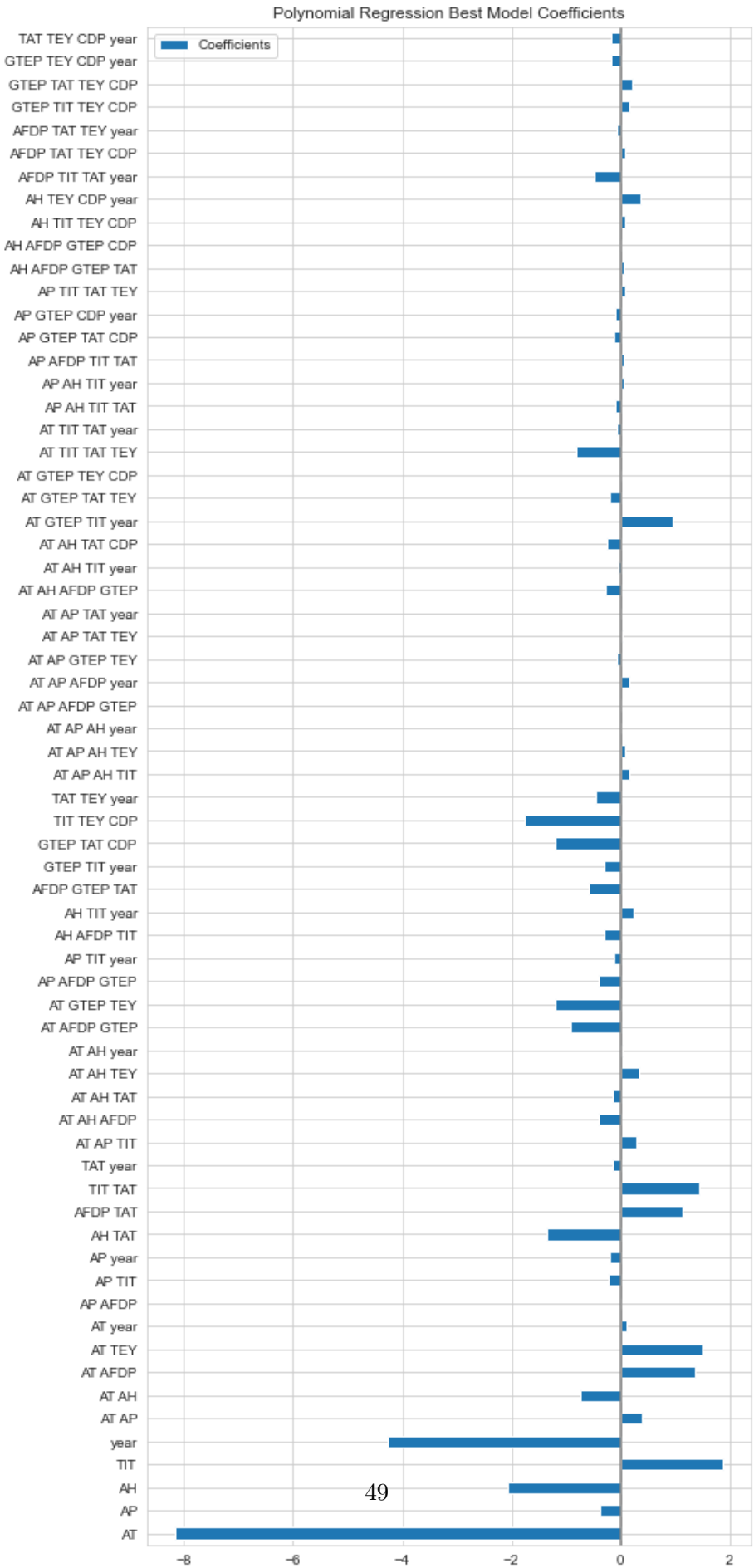
Coefficient of the best model and Most Salient Features:

Since the selected best model is with Lasso Regularization, we can see that most of the features have 0 coefficients.

```
                   Coefficients
1                      0.000000
AT                    -8.175731
AP                    -0.380350
AH                    -2.069612
AFDP                   0.000000
…                         …
TIT TAT TEY CDP        0.000000
TIT TAT TEY year      -0.000000
TIT TAT CDP year      -0.000000
TIT TEY CDP year       0.000000
TAT TEY CDP year      -0.168597

[386 rows x 1 columns]
```

Lasso Regression assigns 0 values to coefficients as seen above, to understand salient features better, I plotted the non-zero coefficients only.


Polynomial Regression Best Model Coefficients
Coefficients
TAT TEY CDP year
GTEP TEY CDP year
GTEP TAT TEY CDP
GTEP TIT TEY CDP
AFDP TAT TEY year
AFDP TAT TEY CDP
AFDP TIT TAT year
AH TEY CDP year
AH TIT TEY CDP
AH AFDP GTEP CDP
AH AFDP GTEP TAT
AP TIT TAT TEY
AP GTEP CDP year
AP GTEP TAT CDP
AP AFDP TIT TAT
AP AH TIT year
AP AH TIT TAT
AT TIT TAT year
AT TIT TAT TEY
AT GTEP TEY CDP
AT GTEP TAT TEY
AT GTEP TIT year
AT AH TAT CDP
AT AH TIT year
AT AH AFDP GTEP
AT AP TAT year
AT AP TAT TEY
AT AP GTEP TEY
AT AP AFDP year
AT AP AFDP GTEP
AT AP AH year
AT AP AH TEY
AT AP AH TIT
TAT TEY year
TIT TEY CDP
GTEP TAT CDP
GTEP TIT year
AFDP GTEP TAT
AH TIT year
AH AFDP TIT
AP TIT year
AP AFDP GTEP
AT GTEP TEY
AT AFDP GTEP
AT AH year
AT AH TEY
AT AH TAT
AT AH AFDP
AT AP TIT
TAT year
TIT TAT
AFDP TAT
AH TAT
AP year
AP TIT
AP AFDP
AT year
AT TEY
AT AFDP
AT AH
AT AP
year
TIT
AH
AP
AT
−8
−6
−4
−2
0
2

Non-zero Coefficients ordered from highest to lowest absolute coefficient values:

```
                      AT      year        AH       TIT  TIT TEY CDP    AT TEY  \
Coefficients  -8.175731 -4.280409 -2.069612  1.888307    -1.751613  1.498123
coef_absolute  8.175731  4.280409  2.069612  1.888307     1.751613  1.498123

                TIT TAT   AT AFDP    AH TAT  GTEP TAT CDP  …  \
Coefficients   1.444971  1.357626 -1.338949     -1.195913  …
coef_absolute  1.444971  1.357626  1.338949      1.195913  …

               AH AFDP GTEP TAT  AT AH TIT year  AT AH year  AT AP TAT TEY  \
Coefficients           0.048713       -0.047831     0.03267       0.030092
coef_absolute          0.048713        0.047831     0.03267       0.030092

               AH AFDP GTEP CDP  AT AP AFDP GTEP  AT AP AH year  \
Coefficients          -0.023979           0.0165        0.01368
coef_absolute          0.023979           0.0165        0.01368

               AT GTEP TEY CDP   AP AFDP  AT AP TAT year
Coefficients          0.008394  0.005628        0.002765
coef_absolute         0.008394  0.005628        0.002765

[2 rows x 66 columns]

Total coefficient counts: 386
Zero coefficient counts: 320
```

From the coefficients, we can see that Lasso assigns 0 to many of the features and only small number of them have non-zero coefficients. 320 out of 386 possible coefficients assigned 0 values.

Within the most salient features, the most important one is AT with -8.17, showcasing negative correlation. This is followed by year and AH with smaller negative correlations. TIT has positive correlation. The first 4 highest correlation values given to non-compounda features and then the most of the remaining non-zero coefficients (the biggest absolute ones) seem to be given to the compound features.

Question 13 The experiment is done for degrees 2, 3, and 4. Given that degree=1 would be just linear results, and we want to see the results for polynomial features, I omitted degree=1 in the experiment. I also didn't include degrees higher than 4 because given the dataset, the amount of compound features created would be too much with degrees higher than 5. Another reason is that both dataset are relatively small 30-50k samples, very high degrees would more likely to cause overfit rather then help generalizing the model.

Diamonds Data What degree of polynomial is best? From experiment results we can see that the best degree is 2. The first 9 of the top 10 combinations of our experiment shows that 2 is the best degree values anf Lasso is a better regularization for this dataset.

Best model parameters:

```
{'model': Lasso(alpha=100, random_state=142),
 'model__alpha': 100,
 'poly_features': PolynomialFeatures(),
 'poly_features__degree': 2}
```

Top 10 combinations from gridsearch results sorted with lowest RMSE validation scores:

```
    mean_train_score  mean_validation_score  \
42        921.572213             882.226435
39        782.419320            1129.772967
36        763.272005            1615.358097
21        795.955216            1667.221668
24        757.769711            1777.435298
27        757.769829            1777.748836
30        757.771652            1780.882997
45       1841.870944            1790.712541
33        757.857294            1809.238839
46       2023.787034            1902.183814

                           param_model  param_model__alpha  \
42  Lasso(alpha=100, random_state=142)            100.0000
39  Lasso(alpha=100, random_state=142)             10.0000
36  Lasso(alpha=100, random_state=142)              1.0000
21            Ridge(random_state=142)           1000.0000
24  Lasso(alpha=100, random_state=142)              0.0001
27  Lasso(alpha=100, random_state=142)              0.0010
30  Lasso(alpha=100, random_state=142)              0.0100
45  Lasso(alpha=100, random_state=142)           1000.0000
33  Lasso(alpha=100, random_state=142)              0.1000
46  Lasso(alpha=100, random_state=142)           1000.0000

    param_poly_features__degree
42                            2
39                            2
36                            2
21                            2
24                            2
27                            2
30                            2
45                            2
33                            2
46                            3
```

Gas Data What degree of polynomial is best? From experiment results we can see that best degree chosen by gridsearch is 4. If we look at the top 10 combinations of best results from grid search in the below table, we can see that degree 3 is also a good choice, given that the mean

validation score has only very little difference in the second significant digits. So, one can select degree 3 as the best parameter value as well.

Best model parameters:

```
{'model': Lasso(alpha=0.1, random_state=142),
 'model__alpha': 0.1,
 'poly_features': PolynomialFeatures(degree=4, interaction_only='False'),
 'poly_features__degree': 4}
```

Top 10 combinations from gridsearch results sorted with lowest RMSE validation scores:

```
    mean_train_score  mean_validation_score  \
35          5.719778               7.155798
34          5.827271               7.171435
22          5.508430               7.226445
23          5.273528               7.369680
33          6.246073               7.436532
18          5.682998               7.459753
21          6.055840               7.464865
19          5.119546               7.514624
20          4.895412               7.588859
31          5.156848               7.655462

                          param_model  param_model__alpha  \
35  Lasso(alpha=0.1, random_state=142)                0.10
34  Lasso(alpha=0.1, random_state=142)                0.10
22            Ridge(random_state=142)             1000.00
23            Ridge(random_state=142)             1000.00
33  Lasso(alpha=0.1, random_state=142)                0.10
18            Ridge(random_state=142)              100.00
21            Ridge(random_state=142)             1000.00
19            Ridge(random_state=142)              100.00
20            Ridge(random_state=142)              100.00
31  Lasso(alpha=0.1, random_state=142)                0.01

    param_poly_features__degree
35                            4
34                            3
22                            3
23                            4
33                            2
18                            2
21                            2
19                            3
20                            4
31                            3
```

What does a very high-order polynomial imply about the fit on the training data? How do you choose this parameter? With a higher-order polynomial, we can create more complex models that covers larger hypothesis spaces. With increasing model complexity, it means we can fit the data better, however, if the degree of polynomial is higher than the optimal degree that data lies, then model may overfit the data. In case of overfitting, the fitted curve will start to memorize the training data rather then learn to generalize and find patterns. When model overfits, the training error would be low and test/validation errors would be high since it perform badly on the unseen data. We can see this from the experiment results in the above table as well. For higher degrees we see that training errors (avg RMSEs) are very low but the avg. validation scores are very high compared to the training score.

On the other hand, if the degree order is too small, the model cannot learn enough from the data and model can underfit resulting in high training and validation errors. In order to avoid overfitting or underfitting, and have a model that generalizes well, we need to choose a degree that matches with the true structure of the data. This happens when the the model has a good training score and the gap between the training and validation scores are lowest. One way to choosee optimal degree parameter, is to run cross validation with different degree values and compare the avg. training and validation results. Then choose a degree where model has low trainining RMSE and low test RMSE. The optimal point is generally when the model has low training RMSE and the gap beetween train and validation score is also lowest.

Question 14 For the diamond dataset it might make sense to craft new features such as z = x1 × x2, etc. Explain why this might make sense and check if doing so will boost accuracy.

Depending on some dataset a compound feature might make sense on predicting the target variable. For example, for the diamonds dataset the diamond price might be correlated with the diamond volume, and diamond volume can be represented by xyz. Using compounding features (combination of different features) might be more helpful in predicting target variable rather than individual columns by itself. There could be cases where individual feature might not contribute as much as a compound feature to the prediction.

I tried 2 approaches to craft new features such as z= x1 x x2.

Approach 1: Use interaction_only=True in Polynomial Features and run only for the combinations of different features. In this approach I created all possible interacted features and checked whether any of them are important features.

Approach 2: Create craft features by hand for the combinations that makes sense and could be helpful for prediction of target variable:

For diamonds dataset new hand crafted features:

```
- volume of diamond: x * y * z
- table * depth
- density of diamond: carat / (x*y*z)
```

In the results below saw that approach 1 helped us improve the accuracy. Approach 2 by adding only few selected hand-crafted features, instead of the regular features worsen the accuracy.

Approach 1: Polynomial Feature on Interactions only

I applied a randomized search with 12 samples (n_iter) with the same parameter range on q12, but this time I only used the compound features to feed in the linear model. I did 10-fold cv and Lasso, Ridge Regularizations.

Polynomial Feature Interaction Only features experiment results on top 10 combination:

```
    mean_train_score  mean_validation_score  \
39        805.512807             813.970583
40        679.765887             825.384492
42        927.309710             873.199024
21        811.508988             874.116912
41        647.222578             883.514943
43        874.565986             900.154033
44        859.818400             937.391952
22        683.784705            1067.001516
23        647.120971            1101.171040
18        789.987240            1108.538274

                          param_model  param_model__alpha  \
39  Lasso(alpha=10, random_state=142)                10.0
40  Lasso(alpha=10, random_state=142)                10.0
42  Lasso(alpha=10, random_state=142)               100.0
21           Ridge(random_state=142)              1000.0
41  Lasso(alpha=10, random_state=142)                10.0
43  Lasso(alpha=10, random_state=142)               100.0
44  Lasso(alpha=10, random_state=142)               100.0
22           Ridge(random_state=142)              1000.0
23           Ridge(random_state=142)              1000.0
18           Ridge(random_state=142)               100.0

    param_poly_features__degree
39                            2
40                            3
42                            2
21                            2
41                            4
43                            3
44                            4
22                            3
23                            4
18                            2
```

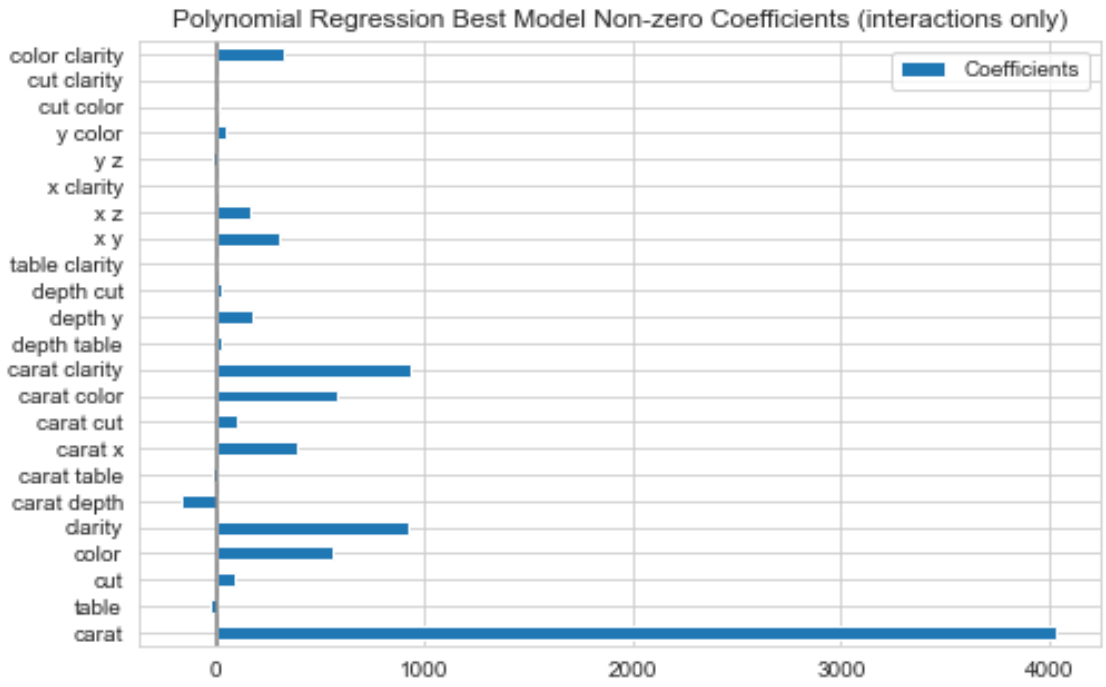
The avg 10-fold CV Train RMSE:805.51 and Validation RMSE=813.97 with interaction only features are much better then the Q12-13 results. This results the performances of the models.

```
Best model:
 Pipeline(steps=[('poly_features', PolynomialFeatures(interaction_only=True)),
                 ('model', Lasso(alpha=10, random_state=142))])
Best model parameters:
```

```
 {'model': Lasso(alpha=10, random_state=142), 'model__alpha': 10,
'poly_features': PolynomialFeatures(interaction_only=True),
'poly_features__degree': 2}
```

The coefficients of the best found model with polynomial interactions only features (non-zero coeffs only):

	Coefficients
carat	4034.341806
table	-32.671368
cut	93.303139
color	557.804933
clarity	918.785316
carat depth	-163.438333
carat table	-19.371410
carat x	384.641881
carat cut	101.794631
carat color	582.467856
carat clarity	937.881468
depth table	23.574794
depth y	173.265004
depth cut	29.052115
table clarity	-6.953471
x y	298.472237
x z	164.424270
x clarity	-3.652150
y z	-22.220218
y color	44.728856
cut color	12.634970
cut clarity	4.550465
color clarity	321.181135



Non-zero Coefficients ordered from highest to lowest absolute coefficient values:

	carat	carat clarity	clarity	carat color	\
Coefficients	4034.341806	937.881468	918.785316	582.467856	
coef_absolute	4034.341806	937.881468	918.785316	582.467856	

	color	carat x	color clarity	x y	depth y	\
Coefficients	557.804933	384.641881	321.181135	298.472237	173.265004	
coef_absolute	557.804933	384.641881	321.181135	298.472237	173.265004	

	x z	…	y color	table	depth cut	depth table	\
Coefficients	164.42427	…	44.728856	-32.671368	29.052115	23.574794	
coef_absolute	164.42427	…	44.728856	32.671368	29.052115	23.574794	

	y z	carat table	cut color	table clarity	cut clarity	\
Coefficients	-22.220218	-19.37141	12.63497	-6.953471	4.550465	
coef_absolute	22.220218	19.37141	12.63497	6.953471	4.550465	

	x clarity
Coefficients	-3.65215
coef_absolute	3.65215

[2 rows x 23 columns]

We can see that the most important features are very similar as in Q12-Q13, however the model is

only using the compounds of different features now.

Approach 2.1: Hand-crafted features - Option 1- create compound features from raw data and then scale

In this approach I only hand crafted new feature set. The process is I created the features from raw data and then scaled the. Then I checked the results on best found model and its parameters in Question 12 to see if the model performance is improved. Lasso Regression with 100 alpha is used:

```
      carat       cut     color   clarity     depth     table  price  \
1 -1.198168  0.981473  0.937163 -1.245215 -0.174092 -1.099672    330
2 -1.240361  0.085889  0.937163 -0.638095 -1.360738  1.585529    327
3 -1.198168 -1.705279  0.937163  0.576145 -3.385019  3.375663    328
4 -1.071587  0.085889 -1.414272 -0.030975  0.454133  0.242928    337
5 -1.029394 -1.705279 -2.002131 -1.245215  1.082358  0.242928    338

          x         y         z     x*y*z  table*depth   density
1 -1.587837 -1.536196 -1.571129 -1.171294    -1.188533 -0.489328
2 -1.641325 -1.658774 -1.741175 -1.218533     0.728291 -0.183160
3 -1.498691 -1.457395 -1.741175 -1.172894     1.094605 -0.396553
4 -1.364971 -1.317305 -1.287720 -1.062372     0.521653  0.382562
5 -1.240167 -1.212238 -1.117674 -0.996008     0.898804 -0.721797

              carat           cut         color       clarity         depth  \
count  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04
mean   2.444878e-16  1.454281e-16  1.338360e-16 -8.114467e-17 -3.996902e-15
std    1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00
min   -1.261458e+00 -2.600864e+00 -2.002131e+00 -1.852335e+00 -1.308760e+01
25%   -8.395232e-01 -8.096951e-01 -8.264134e-01 -6.380951e-01 -5.231053e-01
50%   -2.066210e-01  8.588908e-02 -2.385547e-01 -3.097505e-02  3.531678e-02
75%    5.106683e-01  9.814733e-01  9.371628e-01  5.761450e-01  5.239361e-01
max    8.886075e+00  9.814733e-01  1.525021e+00  2.397505e+00  1.204139e+01

              table         price             x             y             z  \
count  5.394000e+04  53940.000000  5.394000e+04  5.394000e+04  5.394000e+04
mean   9.695207e-17   3934.801557  2.782103e-16 -8.430615e-17 -2.002271e-16
std    1.000009e+00   3989.442321  1.000009e+00  1.000009e+00  1.000009e+00
min   -6.470073e+00    327.000000 -5.109120e+00 -5.020931e+00 -5.014556e+00
25%   -6.521385e-01    952.000000 -9.103248e-01 -8.882800e-01 -8.909461e-01
50%   -2.046051e-01   2403.000000 -2.777553e-02 -2.147398e-02 -1.237618e-02
75%    6.904618e-01   5327.250000  7.210542e-01  7.052421e-01  7.103184e-01
max    1.680167e+01  18823.000000  4.465203e+00  4.654965e+01  4.004758e+01

              x*y*z   table*depth       density
count  5.394000e+04  5.394000e+04  5.394000e+04
mean   3.161480e-16 -1.559664e-16 -5.342639e-15
std    1.000009e+00  1.000009e+00  1.000009e+00
min   -1.659533e+00 -8.850773e+00 -2.871741e+01
```

```
25%   -8.270555e-01 -7.116750e-01 -3.601900e-01
50%   -1.922285e-01 -9.681727e-02 -3.771660e-02
75%    5.239094e-01  6.054644e-01  3.051422e-01
max    4.742502e+01  1.603977e+01  7.746588e+01
```

```
Results for features:  ['carat', 'x', 'y', 'z', 'table*depth', 'cut', 'color',
'clarity']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.257425103957
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.9244651005379
```

```
Results for features:  ['carat', 'x*y*z', 'table', 'depth', 'cut', 'color',
'clarity']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1250.9522429042684
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.883579227349
```

```
Results for features:  ['carat', 'x', 'y', 'z', 'table', 'depth', 'cut',
'color', 'clarity', 'density']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.2749901090597
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.8990105660093
```

```
Results for features:  ['carat', 'x', 'y', 'z', 'table', 'depth', 'cut',
'color', 'clarity', 'x*y*z', 'table*depth', 'density']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.0241173671452
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.790262782626
```

By only using these 3 crafted features doesn't really help with the model performance, it rather detoriates.

Approach 2.2: Hand-crafted features - Option 2- create compound features from scaled data

In this approach I only hand crafted new feature set. The process is I created the features from scaled data directly. Then I checked the results on best found model and its parameters in Question 12 to see if the model performance is improved. Lasso Regression with 100 alpha is used:

```
      carat       cut     color   clarity     depth     table  price  \
1 -1.198168  0.981473  0.937163 -1.245215 -0.174092 -1.099672    330
2 -1.240361  0.085889  0.937163 -0.638095 -1.360738  1.585529    327
3 -1.198168 -1.705279  0.937163  0.576145 -3.385019  3.375663    328
4 -1.071587  0.085889 -1.414272 -0.030975  0.454133  0.242928    337
5 -1.029394 -1.705279 -2.002131 -1.245215  1.082358  0.242928    338
```

```
          x         y         z     x*y*z  table*depth
1 -1.587837 -1.536196 -1.571129 -1.011985     0.331656
2 -1.641325 -1.658774 -1.741175 -1.231300    -1.267281
3 -1.498691 -1.457395 -1.741175 -1.004910    -7.576892
4 -1.364971 -1.317305 -1.287720 -0.645658     0.276436
5 -1.240167 -1.212238 -1.117674 -0.492275     0.380321

              carat           cut         color       clarity         depth  \
count  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04  5.394000e+04
mean   2.444878e-16  1.454281e-16  1.338360e-16 -8.114467e-17 -3.996902e-15
std    1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00  1.000009e+00
min   -1.261458e+00 -2.600864e+00 -2.002131e+00 -1.852335e+00 -1.308760e+01
25%   -8.395232e-01 -8.096951e-01 -8.264134e-01 -6.380951e-01 -5.231053e-01
50%   -2.066210e-01  8.588908e-02 -2.385547e-01 -3.097505e-02  3.531678e-02
75%    5.106683e-01  9.814733e-01  9.371628e-01  5.761450e-01  5.239361e-01
max    8.886075e+00  9.814733e-01  1.525021e+00  2.397505e+00  1.204139e+01

              table         price             x             y             z  \
count  5.394000e+04  53940.000000  5.394000e+04  5.394000e+04  5.394000e+04
mean   9.695207e-17   3934.801557  2.782103e-16 -8.430615e-17 -2.002271e-16
std    1.000009e+00   3989.442321  1.000009e+00  1.000009e+00  1.000009e+00
min   -6.470073e+00    327.000000 -5.109120e+00 -5.020931e+00 -5.014556e+00
25%   -6.521385e-01    952.000000 -9.103248e-01 -8.882800e-01 -8.909461e-01
50%   -2.046051e-01   2403.000000 -2.777553e-02 -2.147398e-02 -1.237618e-02
75%    6.904618e-01   5327.250000  7.210542e-01  7.052421e-01  7.103184e-01
max    1.680167e+01  18823.000000  4.465203e+00  4.654965e+01  4.004758e+01

              x*y*z   table*depth
count  5.394000e+04  5.394000e+04
mean   4.215307e-18 -2.357938e-17
std    1.000009e+00  1.000009e+00
min   -3.115138e+01 -2.494149e+01
25%   -2.538809e-01 -9.321787e-02
50%   -8.649803e-02  1.546745e-01
75%   -7.972652e-03  3.096073e-01
max    1.513640e+02  5.721680e+01



Results for features:  ['carat', 'x*y*z', 'table*depth', 'cut', 'color',
'clarity']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.2751638566913
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.8986831815869


Results for features:  ['carat', 'x', 'y', 'z', 'table*depth', 'cut', 'color',
```

```
'clarity']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.2751638566913
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.8986831815869


Results for features:  ['carat', 'x*y*z', 'table', 'depth', 'cut', 'color',
'clarity']
Lasso with new features Train Avg RMSE accross 10-fold cv:  1251.2749901090597
Lasso with new features Validation Avg RMSE accross 10-fold cv:
1244.8990105660093
```

The result of this approach is also similar to Approach 2.1. and it doesn't really help model improve.

1.4 Neural Network

Question 15 For question 15, I ran a MLP model with the default parameters in sklearn (MLPRegressor). The default MLP model has 1 hidden layer with 100 neurons and activation function as relu, solver as adam.

Diamond Data From the below results we can see that Neural Network is performed much better.

To compare the best result for linear model avg Train and Validation RMSE were around 1205-1206 and for polynomial regression was avg Train RMSE: 921.572213and Avg. Validation RMSE was: 882.226435.

```
Neural Network Train Avg RMSE accross 10-fold cv:  777.6786147628094
Neural Network Validation Avg RMSE accross 10-fold cv:  747.3036406022716

Train RMSEs: [820.08474187 809.08852109 788.44200593 726.8316636  614.1550364
 728.2570057  813.74382945 823.98262994 818.55573404 833.64497961]
Validation RMSEs:  [ 643.18346529  618.63124327  823.05710113 1144.74096698
1702.28150625
 1161.93618763  166.91549116  234.49500132  531.01778216  446.77766084]
```

Gas Data From the below results we can see that Neural Network is performed much better.

To compare the best result for linear model avg Train and Validation RMSE were around 8.1-8.76 and for polynomial regression was avg Train RMSE: 5.71 and Avg. Validation RMSE was: 7.15.

```
Neural Network Train Avg RMSE accross 10-fold cv:  4.403767325900161
Neural Network Validation Avg RMSE accross 10-fold cv:  7.151286634532899

Train RMSEs: [4.47615828 4.5742852  4.48336537 4.5141129  4.21791965 4.17030782
 4.22640164 4.45268037 4.48474852 4.43769352]
Validation RMSEs:  [ 5.38507075  4.59652659  6.32313728  5.57556881 10.56163598
8.31752303
  9.66792933  6.62430684  6.91606435  7.54510338]
```

Why does it do much better than linear regression?

Neural networks can capture non-linear dependencies (with the help of activation functions such as relu) whereas linear models cannot. This means that neural network models have a larger hypothesis space to choose from including non-linear spaces and the complexity of the model is higher. Neural networks working better than linear regression suggest that for both of our dataset, its data has non-linear dependencies that help predicting the target variable.

Question 16 Adjust your network size (number of hidden neurons and depth), and weight decay as regularization. Find a good hyper-parameter set systematically.

There are different possibilities to systematically tune hyperparameters. To name a few we can use GridSearch, Randomized Search or HalvingGridSearchCV or HalvingRandomSearchCV from sklearn library. GridSearch is an exhaustive search of all parameter combinations, whereas Randomized Search sample from the all parameter combinations based on the sample number given by the user and conducts the search from that random sample. With many parameters and many candidates for each parameter, GridSearch takes a very long time to run. RandomizedSearch in that sense can be a good candidate to avoid long run times.

HalvingSearch strategies is similar to GridSearch and RandomizedSearch but it applies succesive halving after every iteration and continues parameter search by halving the candidates after each iteration. The halving strategy is much faster but doesn't support for multiple scoring in sklearn, and for the next chapters, Random Forest part we are required to calculate multiple scores for the search results. In order to stay consistent on the parameter tuning techniques, I decided to go with Randomized Search with a good sample number, I can cover wider range of parameter combinations.

The hyperparameters tuned in this question are number of hidden neurons, number of hidden layers, and weight decay (alpha) parameters in the MLPRegressor object from sklearn.

- Number of hidden layers: 1, 2, 3, 4
- Number of hidden neurons: 30, 50, 100, 120
- The specific hidden_layer_sizes parameters used in the search: [(30,),(50,),(100,), (120,), (30,30), (50, 50), (50, 50, 50), (50,50,50,50)]
- Alpha values used in the range of $[10^{-5}, 10^{3}]$; with every 10 power range from -5 to 3 included.

I used Randomized Search with 100 samples and 10-fold cross validation due to the time it takes to train each combination. The same search space is kept for both datasets.

Diamonds Data Neural Network Experiment Results

After the parameter tuning, the model performed better than the default neural network parameters. 10-fold Mean Train RMSE is now 595.01 anf 10-fold validation RMSE is 637.48 for the best model parameter combination.

These RMSE metrics were around 750-780 with the default NN results in Q15.

Top 10 best combination results:

	mean_train_score	mean_validation_score	param_model__alpha	\
53	595.010078	637.488677	10.00000	
45	601.467299	641.372646	1.00000	

```
29        616.363558             642.977524             0.01000
61        593.316732             644.878249           100.00000
21        620.648627             650.541119             0.00100
5         626.699392             658.240621             0.00001
37        603.151681             661.902062             0.10000
69        598.967497             664.097029          1000.00000
13        625.323358             667.144400             0.00010
54        568.869844             684.246047            10.00000

   param_model__hidden_layer_sizes
53                         (50, 50)
45                         (50, 50)
29                         (50, 50)
61                         (50, 50)
21                         (50, 50)
5                          (50, 50)
37                         (50, 50)
69                         (50, 50)
13                         (50, 50)
54                   (50, 50, 50)

Best Model:
 Pipeline(steps=[('model',
                 MLPRegressor(alpha=10, early_stopping=True,
                              hidden_layer_sizes=(50, 50), random_state=142))])
Best Model Params:
 {'model__hidden_layer_sizes': (50, 50), 'model__alpha': 10, 'model':
MLPRegressor(alpha=10, early_stopping=True, hidden_layer_sizes=(50, 50),
             random_state=142)}
```

Using 2 hidden layers each with 50 neurons, with alpha 10 further improved the performance of the Neural Network model results.

Gas Data Neural Network Experiment Results

After the parameter tuning, the model performed better than the default neural network parameters. 10-fold Mean Train RMSE is now 5.03 and 10-fold validation RMSE is 6.33 for the best model parameter combination.

Top 10 best combination results:

```
    mean_train_score  mean_validation_score  param_model__alpha  \
50          5.034472               6.334995                10.0
48          5.075886               6.339038                10.0
51          4.979858               6.381388                10.0
62          5.112718               6.396729               100.0
61          5.437319               6.439728               100.0
49          5.056675               6.479673                10.0
63          4.915925               6.642107               100.0
```

```
40          4.828005               6.730642                1.0
52          4.541026               6.769982               10.0
53          4.509395               6.782365               10.0

   param_model__hidden_layer_sizes
50                        (100,)
48                         (30,)
51                        (120,)
62                  (50, 50, 50)
61                      (50, 50)
49                         (50,)
63              (50, 50, 50, 50)
40                         (30,)
52                      (30, 30)
53                      (50, 50)
```

The best model parameter is 1 hidden layer with 100 neurons and alpha 10. Notice that the model can also found almost same 10-fold mean validation score with 1 hidden layer with 30 neuron size.

```
Best Model:
 Pipeline(steps=[('model',
                  MLPRegressor(alpha=10, early_stopping=True,
                               random_state=142))])
Best Model Params:
 {'model__hidden_layer_sizes': (100,), 'model__alpha': 10, 'model':
MLPRegressor(alpha=10, early_stopping=True, random_state=142)}
```

Question 17 What activation function should be used for the output?

We want our output to be a numerical value as it is a regression task. The activation function could be identity (linear activation function), in this case the output will be linear output and the predicted result range will be from $-\infty$ to ∞. Another possible activation function could be ReLu, this will also return a numerical value but the range would be from 0 to ∞.

For diamonds data set since we are predicting price, therefore, it may be better to not allow negative range for the results and make it either zero or positive value. That is why we can use ReLU as activation. On another note, the price values on our data is all positive values with a minimum price 327. Therefore, using both linear output (no activation) and Relu would be possible in these two datasets.

For gas dataset as well, the target variable is again seems to be positive valued results, again we could use either of the activation functions.

sklearn MLPRegressor uses identity activation function as default, I kept using this in my experiments.

```
NN model output activation: identity
```

Question 18 What is the risk of increasing the depth of the network too far?

Two possible things can happen if we increase the depth of network too far: 1. With the increase of depth, hidden layers, model complexity increases and the **model can overfit** as wider hypothesis space is available to fit the train data. When model overfits, the train performance would be good, ie. low RMSe score however the validation and test scores would be bad since model cannot generalize well and predicts the unseen data badly.

2. Another possibility is the direct opposite, when the model layers increases, during back propagation the gradients of the loss function might approach to zero causing vanishing gradient problem. With vanishing gradient it gets harder for model to learn and train which leads to **model underfit**. When model underfits both train and validation performances would be bad, ie. very high RMSE scores.

We can check both training and testing loss curves during training to spot either of these problems is occuring. We can also check the cross validation results of train and test scores.

Below two tables show the results for 1,2,3,4 hidden layers with each 50 neurons. The first table shows the mean_train_score values on different model alpha and hidden layer size. The second plot shows the mean_validation_scores.

For diamonds dataset, we can see that when we increase the number of hidden layers, depth of the model, the training RMSE decrease but validation RMSE increases, which shows the models start to overfit.

```
                              mean_train_score                          \
param_model__alpha                 0.00001     0.00010     0.00100
param_model__hidden_layer_sizes
(50,)                         860.387372  860.387160  860.386317
(50, 50)                      626.699392  625.323358  620.648627
(50, 50, 50)                  566.731348  566.014459  564.883705
(50, 50, 50, 50)              549.086232  545.684920  548.163076

                                                          \
param_model__alpha                0.01000     0.10000     1.00000
param_model__hidden_layer_sizes
(50,)                         860.392727  860.609681  862.323489
(50, 50)                      616.363558  603.151681  601.467299
(50, 50, 50)                  563.522269  566.650971  566.704099
(50, 50, 50, 50)              549.841766  551.695817  547.207621


param_model__alpha               10.00000    100.00000   1000.00000
param_model__hidden_layer_sizes
(50,)                         868.732516  875.627936  885.655224
(50, 50)                      595.010078  593.316732  598.967497
(50, 50, 50)                  568.869844  570.243132  567.576103
(50, 50, 50, 50)              544.183427  549.337372  551.231189

                              mean_validation_score                       \
param_model__alpha                      0.00001     0.00010     0.00100
```

```
param_model__hidden_layer_sizes
(50,)                                860.478273  860.475928  860.470553
(50, 50)                             658.240621  667.144400  650.541119
(50, 50, 50)                         752.885226  740.185870  725.238640
(50, 50, 50, 50)                     723.286306  748.312344  722.771248

                                                                      \
param_model__alpha                    0.01000     0.10000     1.00000
param_model__hidden_layer_sizes
(50,)                                860.489272  859.995527  863.376201
(50, 50)                             642.977524  661.902062  641.372646
(50, 50, 50)                         723.608246  736.513553  701.309009
(50, 50, 50, 50)                     725.818526  725.074987  718.449520


param_model__alpha                    10.00000    100.00000   1000.00000
param_model__hidden_layer_sizes
(50,)                                855.726821  863.994765  873.184344
(50, 50)                             637.488677  644.878249  664.097029
(50, 50, 50)                         684.246047  699.210512  719.523413
(50, 50, 50, 50)                     732.374139  704.885216  718.318497
```

For gas dataset, we can see that when we increase the number of hidden layers, depth of the model, the training RMSE decrease but validation RMSE increases for mos tof the cases as well.

```
                              mean_train_score                        \
param_model__alpha                 0.00001    0.00010    0.00100
param_model__hidden_layer_sizes
(50,)                                4.637899   4.639643   4.636757
(50, 50)                             4.090331   4.084285   4.100788
(50, 50, 50)                         4.035329   4.009868   4.064147
(50, 50, 50, 50)                     3.884436   3.972271   3.945383

                                                                    \
param_model__alpha                  0.01000    0.10000    1.00000    10.00000
param_model__hidden_layer_sizes
(50,)                                4.639676   4.648805   4.730151   5.056675
(50, 50)                             4.131832   4.111577   4.100098   4.509395
(50, 50, 50)                         4.057370   4.077180   4.136366   4.260865
(50, 50, 50, 50)                     3.820922   3.899991   3.929041   4.118325


param_model__alpha                  100.00000  1000.00000
param_model__hidden_layer_sizes
(50,)                                6.481601   8.306890
(50, 50)                             5.437319   7.097664
(50, 50, 50)                         5.112718   6.680367
```

```
(50, 50, 50, 50)                  4.915925   6.524656

                                mean_validation_score                        \
param_model__alpha                        0.00001    0.00010    0.00100
param_model__hidden_layer_sizes
(50,)                                    6.901441   6.913977   6.891217
(50, 50)                                 7.407305   7.326312   7.372348
(50, 50, 50)                             7.185461   7.107952   7.181652
(50, 50, 50, 50)                         7.324528   7.220236   7.190370

                                                                          \
param_model__alpha              0.01000    0.10000    1.00000    10.00000
param_model__hidden_layer_sizes
(50,)                            6.978835   6.891648   6.902512   6.479673
(50, 50)                         7.296752   7.328153   7.298903   6.782365
(50, 50, 50)                     7.120696   7.045864   7.335931   7.047754
(50, 50, 50, 50)                 8.076287   7.410987   6.966002   6.986474


param_model__alpha              100.00000  1000.00000
param_model__hidden_layer_sizes
(50,)                            7.384260   8.889102
(50, 50)                         6.439728   7.945318
(50, 50, 50)                     6.396729   7.607922
(50, 50, 50, 50)                 6.642107   7.507126
```

1.5 Random Forest

Question 19

Diamond Data Random Forest with default Parameters

10-fold CV results with default random forest parameters:

```
RF Train Avg RMSE accross 10-fold cv:  196.18467228232933
RF Validation Avg RMSE accross 10-fold cv:  752.9655008100951
```

Random Forest Parameter Tuning

I applied 10-fold cross validation to tune parameters on randomized search with 200 samples on the following parameters:

- Maximum number of Features: [‘auto’, ‘sqrt’, ‘log2’, None, 2, 3, 4, 6]
- Number of Trees: [20, 40, 60, 80, 100, 120, 140, 160, 180, 200]
- Depth of each tree: [2, 4, 6, 8, 10, None]

RF Parameter tuning Top 10 Results:

The best 10-fold avg train RMSE is 197 and avg validation RMSE is 715 which is much better than the values we found from default Random Forest parameter results.

The avg. validation RMSE is also better than linear and polynomial regression but worse than the Neural Network results.

The R^2 value for 10-fold avg train score is 0.9975 which is very high. The R^2 mean validation value is 0.644 which is on the lower side.

	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2	\
93	197.555441	715.111659	0.997510	0.644635	
35	197.555441	715.111659	0.997510	0.644635	
123	196.395238	715.684125	0.997539	0.644486	
146	196.395238	715.684125	0.997539	0.644486	
57	196.904756	715.867991	0.997526	0.644543	
143	198.482136	717.630609	0.997487	0.643213	
103	192.697889	719.262639	0.997632	0.645301	
21	202.270267	722.666892	0.997388	0.637716	
62	195.142830	723.777170	0.997571	0.642623	
25	208.128003	725.638959	0.997235	0.634496	
154	198.470291	727.487375	0.997487	0.637597	
3	195.289479	728.713337	0.997567	0.630759	
12	203.501264	730.830309	0.997358	0.633556	
136	201.883748	732.347631	0.997400	0.626449	
63	222.139587	735.982273	0.996851	0.620411	
79	222.139587	735.982273	0.996851	0.620411	
137	206.970988	737.030626	0.997264	0.623099	
164	208.162236	738.318300	0.997233	0.622015	
161	210.184932	740.602514	0.997179	0.619552	
92	212.762585	740.806831	0.997112	0.618646	
4	198.310065	741.598278	0.997492	0.618845	
72	196.059868	741.929111	0.997548	0.618026	
17	192.924766	743.101227	0.997626	0.619783	
174	202.470320	743.577195	0.997386	0.618325	
13	221.672778	746.838461	0.996864	0.609541	
124	213.398920	751.473701	0.997096	0.611386	
31	195.540911	752.749529	0.997561	0.610399	
74	196.184672	752.965501	0.997545	0.610654	
152	197.143996	753.936606	0.997521	0.608289	
50	197.143996	753.936606	0.997521	0.608289	
192	199.413138	754.992440	0.997463	0.607944	
33	238.962719	762.538946	0.996351	0.590568	
148	482.615022	776.672457	0.985139	0.541213	
94	482.461957	776.815674	0.985148	0.541342	
116	482.677973	777.751737	0.985135	0.540532	
34	482.917018	778.300251	0.985121	0.541143	
133	477.472593	785.170909	0.985451	0.527955	
29	488.145099	785.563694	0.984795	0.525774	
47	477.527549	785.701828	0.985448	0.528062	
37	477.495799	785.895313	0.985450	0.528765	
46	477.587613	786.567099	0.985444	0.527561	

19	479.758903	790.185583	0.985310	0.525314
122	507.568005	791.514223	0.983555	0.519987
90	507.982728	793.133943	0.983524	0.519088
127	508.548770	794.761791	0.983485	0.515453
130	508.698932	795.059990	0.983478	0.512507
163	477.861470	795.730562	0.985425	0.513149
182	477.999611	795.984716	0.985416	0.513514
112	477.999611	795.984716	0.985416	0.513514
30	477.656420	795.997041	0.985437	0.513704

	param_model__max_features	param_model__n_estimators	param_model__max_depth
93	log2	120	None
35	sqrt	120	None
123	sqrt	160	None
146	log2	160	None
57	3	140	None
143	sqrt	100	None
103	4	180	None
21	log2	60	None
62	4	100	None
25	sqrt	40	None
154	4	60	None
3	6	80	None
12	4	40	None
136	6	40	None
63	sqrt	20	None
79	log2	20	None
137	2	180	None
164	2	140	None
161	2	100	None
92	6	20	None
4	8	60	None
72	8	80	None
17	8	180	None
174	8	40	None
13	2	40	None
124	8	20	None
31	auto	120	None
74	auto	100	None
152	auto	80	None
50	None	80	None
192	None	60	None
33	2	20	None
148	6	160	10
94	6	180	10
116	6	140	10
34	6	120	10

133	8	160	10
29	6	20	10
47	8	120	10
37	8	100	10
46	8	80	10
19	8	40	10
122	4	180	10
90	4	120	10
127	4	100	10
130	4	80	10
163	auto	160	10
182	auto	140	10
112	None	140	10
30	None	180	10

The best parameter combination is max_features: 'sqrt', n_estimators=120, max_depth=None

```
Best Model:
 Pipeline(steps=[('model',
                 RandomForestRegressor(max_features='sqrt', n_estimators=120,
                                       n_jobs=-1, oob_score=True,
                                       random_state=142))])
Best Model Params:
 {'model__n_estimators': 120, 'model__max_features': 'sqrt', 'model__max_depth':
None, 'model': RandomForestRegressor(max_features='sqrt', n_estimators=120,
n_jobs=-1,
                      oob_score=True, random_state=142)}

Best Model OOB score:
 0.981448128437458
```

We can also decrease the number of trees as we can substantially improve computation time without loosing too much from performance as it can be seen from the above table.

It is also important to note that when we have max_depth=None we don't really put a regularization effect on trees, the depth of the trees could grow unlimited. Similarly, having max_features None has unlimited effect as well. I also checked the best parameter results when these values are not equal to None. The best 10 results when we put limited on these parameters can be seen below table:

	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2	\
148	482.615022	776.672457	0.985139	0.541213	
94	482.461957	776.815674	0.985148	0.541342	
116	482.677973	777.751737	0.985135	0.540532	
34	482.917018	778.300251	0.985121	0.541143	
133	477.472593	785.170909	0.985451	0.527955	
29	488.145099	785.563694	0.984795	0.525774	
47	477.527549	785.701828	0.985448	0.528062	
37	477.495799	785.895313	0.985450	0.528765	

46	477.587613	786.567099	0.985444	0.527561
19	479.758903	790.185583	0.985310	0.525314

	param_model__max_features	param_model__n_estimators	param_model__max_depth
148	6	160	10
94	6	180	10
116	6	140	10
34	6	120	10
133	8	160	10
29	6	20	10
47	8	120	10
37	8	100	10
46	8	80	10
19	8	40	10

By looking these results we can say that the validation RMSE is much bigger and validation R^2 is worse compared to the previous results, however the RMSE gap between train and validation scores are considerably lower. Given the data doesn't have too much samples, it makes more sense to choose a parameter with lower depth and number of trees in order to avoid overfitting, if there is no marginal change in the mean_validation RMSE. However, I beleive that this data doesn't have too much predictive power over price of diamonds given that even the best tuning results can only reach mean_validation_R^2 of 0.644 only.

Gas Data Random Forest with default Parameters

10-fold CV results with default random forest parameters:

```
RF Train Avg RMSE accross 10-fold cv:  1.3334385377542095
RF Validation Avg RMSE accross 10-fold cv:  7.033552307420598
```

Random Forest Parameter Tuning

I applied 10-fold cross validation to tune parameters on randomized search with 200 samples on the following parameters:

- Maximum number of Features: ['auto', 'sqrt', 'log2', None, 2, 3, 4, 6]
- Number of Trees: [20, 40, 60, 80, 100, 120, 140, 160, 180, 200]
- Depth of each tree: [2, 4, 6, 8, 10, None]

RF Parameter tuning Top 10 Results:

The best 10-fold avg train RMSE is 1.34 and avg validation RMSE is 6.76 which is better than the values we found from default Random Forest parameter results.

The R^2 value for 10-fold avg train score is 0.987 which is very high. The R^2 mean validation value is 0.49 which is very low.

	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2	\
164	1.342304	6.762084	0.986713	0.496042	
7	1.348743	6.762958	0.986585	0.495604	
181	1.386028	6.762969	0.985832	0.496487	

```
125         1.344213             6.763069       0.986675            0.495475
49          1.344213             6.763069       0.986675            0.495475
24          1.344213             6.763069       0.986675            0.495475
196         1.368713             6.764241       0.986183            0.496209
69          1.321832             6.781538       0.987116            0.491896
116         1.323780             6.783613       0.987079            0.491444
75          1.364797             6.796053       0.986264            0.490157

    param_model__max_features param_model__n_estimators param_model__max_depth
164                      sqrt                       180                    None
7                        sqrt                       140                    None
181                      sqrt                        60                    None
125                         3                       160                    None
49                       log2                       160                    None
24                       sqrt                       160                    None
196                         3                        80                    None
69                          4                       180                    None
116                         4                       160                    None
75                          4                        60                    None
```

The best parameter combination is max_features: 'sqrt', n_estimators=180, max_depth=None

```
Best Model:
 Pipeline(steps=[('model',
                  RandomForestRegressor(max_features='sqrt', n_estimators=180,
                                        n_jobs=-1, oob_score=True,
                                        random_state=142))])
Best Model Params:
 {'model__n_estimators': 180, 'model__max_features': 'sqrt', 'model__max_depth':
None, 'model': RandomForestRegressor(max_features='sqrt', n_estimators=180,
n_jobs=-1,
                      oob_score=True, random_state=142)}

Best Model OOB score:
 0.9024957564053923
```

However, if we check the mean validation scores we can considerably lower the n_estimators and limit the max_dept instead of None to have a better regularization for our dataset.

Decreasing the number of trees would substantially improve computation time without loosing too much from performance as it can be seen from the above table.

It is also important to note that when we have max_depth=None we don't really put a regularization effect on trees, the depth of the trees could grow unlimited. Similarly, having max_features None has unlimited effect as well. I also checked the best parameter results when these values are not equal to None. The best 10 results when we put limited on these parameters can be seen below table:

```
     mean_train_RMSE  mean_validation_RMSE  mean_train_R2  mean_validation_R2  \
30          3.775723              6.798711       0.894827            0.494492
```

119	3.610713	6.802990	0.903815	0.495103
176	3.610805	6.809854	0.903809	0.494213
66	3.610107	6.815662	0.903847	0.493449
185	3.776789	6.818777	0.894767	0.491180
27	3.781066	6.827195	0.894523	0.490624
4	3.606747	6.833424	0.904028	0.491379
95	3.559517	6.843458	0.906544	0.490892
173	3.959350	6.849650	0.884343	0.487073
143	3.525061	6.851873	0.908327	0.489752
3	3.965165	6.858520	0.883993	0.486477
31	3.628738	6.859863	0.902855	0.487493
53	3.530787	6.864812	0.908032	0.488247
73	3.964615	6.868910	0.884006	0.484301
63	3.533441	6.871307	0.907893	0.487545
161	4.389201	6.900573	0.857839	0.483253
167	4.318155	6.912368	0.862423	0.484139
101	4.318558	6.912621	0.862400	0.483288
54	3.976980	6.932200	0.883312	0.475565
129	4.586106	6.941971	0.844839	0.476915

	param_model__max_features	param_model__n_estimators	param_model__max_depth
30	4	180	10
119	6	180	10
176	6	140	10
66	6	120	10
185	4	120	10
27	4	60	10
4	6	80	10
95	8	20	10
173	3	140	10
143	8	180	10
3	log2	60	10
31	6	40	10
53	8	120	10
73	sqrt	40	10
63	8	80	10
161	6	140	8
167	8	80	8
101	8	140	8
54	log2	20	10
129	4	60	8

By looking these results we can say that the validation RMSE is bigger by only 0.05 point and validation R^2 is 0.006 worse compared to the previous results. So without hurting our results too much we can decrease our selected parameter range to max_depth 10 with even around 40-60 n_estimators.

Given the data doesn't have too much samples, it makes more sense to choose a parameter with

lower depth and number of trees in order to avoid overfitting, if there is no marginal change in the mean_validation RMSE. However, I beleive that this data doesn't have too much predictive power over NOX given that even the best tuning results can only reach mean_validation_R^2 of around 0.49 only.

Explain how these hyper-parameters affect the overall performance? Do some of them have regularization effect?

Maximum number of features: (max_features) Initially, increasing maximum number of features will help increasing the model performance. However, having too big max_features would lead the test/validation error to increase, even though training error keeps decreasing. This means model become prone to overfit with a high value of max_features. This value can be used to have regularization effect to avoid overfitting.

Number of trees: (n_estimators) Increasing number of trees at first will help with the model performance, from 1 to optimal number of trees we can see a sharp increase on both training, validation and test scores (increase in cases like accuracy, or decrease in case of RMSE error). After certain number of points however, the scores will start to stabilize and plateaus and won't change much. Having more than optimal number of trees will increase the computation time but wouldn't degrade model performance much.

Depth of each tree: (max_depth), is the longest path from root to leaf. If we increase the max depth too much, the trees can grow bigger and the training data would start to overfit after certain point, this will keep decreasing the training score. However, due to overfit, the model cannot generalize well on unseen test data and test score would increase. Hence, if we have too big maximum depth values, the model performance would start to degrade. Having very small max_depth on the other hand might cause underfitting, with low test and training score, again resulting in low performance. So we need to find an optimal value and fine tune this parameter carefully. We can create a regularization effect by decreasing the max_depth and avoid overfitting.

Question 20 Why does random forest perform well?

Random forest is an ensemble model using bagging method, this means we have multiple decision trees working as a group and final prediction is based on a majority vote instead of a decision of an individual tree. Having multiple trees help having a more robust, accurate model and reduce the variance of the model. Giving that the final predictions based on a majority vote, the final prediction result doesn't get affected from a wrong prediction of an (few) individual models because decisions is lead by the most common results. This helps Random Forest to use the power of multiple classifiers, reduce the prone to overfit and performs well.

Question 21

Diamond Data: For this question I created a model with max_depth 4, and the choose the remaining best parameters from the tuning results: when max_depth is 4, n_Estimators 60 and max_features='sqrt' have a good performance. Using higher n_estimators as it can be seen from the below table, doesn't effect the validation RMSE score too much, therefore it is a good tradeoff to have a lower n_estimators since it doesn't really hurt mean_validation RMSE. Although we can see that wiht max depth 4 results the RMSE results are much higher.

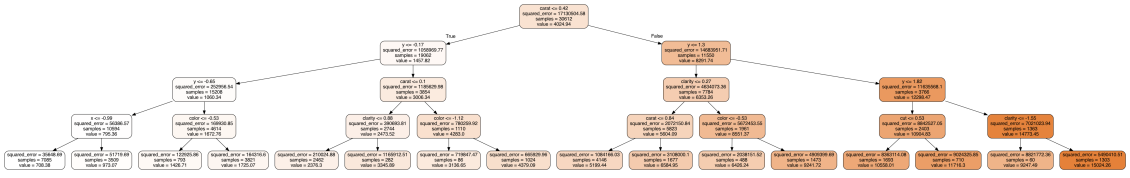
	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2	\
180	1072.816136	1279.916800	0.925749	-0.368551	
55	1078.585941	1281.970239	0.924969	-0.359162	
115	1079.506688	1283.387420	0.924840	-0.389649	
117	1035.392273	1290.707883	0.930787	-0.356440	
56	1052.997882	1299.489566	0.928445	-0.365391	
44	1112.695094	1301.492883	0.920427	-0.346200	
109	1112.695094	1301.492883	0.920427	-0.346200	
106	1110.161096	1302.317549	0.920779	-0.330555	
24	1118.652925	1302.485928	0.919572	-0.346775	
171	1118.107021	1302.533351	0.919667	-0.333305	

	param_model__max_features	param_model__n_estimators	param_model__max_depth
180	4	40	4
55	4	160	4
115	4	20	4
117	6	120	4
56	6	20	4
44	3	80	4
109	log2	80	4
106	sqrt	60	4
24	log2	140	4
171	sqrt	180	4

```
RF Train Avg RMSE accross 10-fold cv:  1055.1147964059605
RF Validation Avg RMSE accross 10-fold cv:  1283.5570855502583
```

Then I select a tree with max depth 4 and plot it.

```
Selected tree
: DecisionTreeRegressor(max_depth=4, max_features=5, random_state=1726841109)
```



Which feature is selected for branching at the root node?

Carat feature is selected as root node. This makes sense since until now, we kept finding carat is the most important feature to predicting price in the previous questions.

What can you infer about the importance of features?

For the splits of the branches: carat, x, y, clarity, color, cut features are selected, hence the features that are found to be important for this decision tree. The first split is made using carat feature and the standardized carat features lower than 0.42 goes to the left node and the rest goes to the right node, we can see that from almost 31K samples this decision splits the samples almost 2/3 to 1/3

for the next nodes, which means the feature is very imformative in terms of the being best split to separate samples. The most important feature is carat since it is used on the root node, then the the features used closer to the root are more informative, hence important features compared to the ones closer to leaf nodes. The decision rules created by this tree can be clearly seen for each node and its corresponding feature. The split decisions are made based on the feature and its corresponding threshold where mean squared error is the most reduced.

We can also observe that some features are used in several nodes and splits and chosen for new decision splits, such as carat, y, color this shows that these 3 features play more critical role for the final prediction of this specific tree.

Do the important features match what you got in part 3.2.1?

In the best model found after Linear Regression experiments, 3.2.1, the most important features were carat, x, clarity, color cut and depth in order. According to the above decision tree, we can as well see that the important features found are very similar, the only difference y and depth and the rest of the most important features are same.

Gas Data: For this question I created a model with max_depth 4, and the choose the remaining best parameters from the tuning results: when max_depth is 4, n_Estimators 40 and max_features='sqrt' have a good performance. Using higher n_estimators as it can be seen from the below table, doesn't effect the validation RMSE score too much, therefore it is a good tradeoff to have a lower n_estimators since it doesn't really hurt mean_validation RMSE. Although we can see that wiht max depth 4 results the RMSE results are higher.

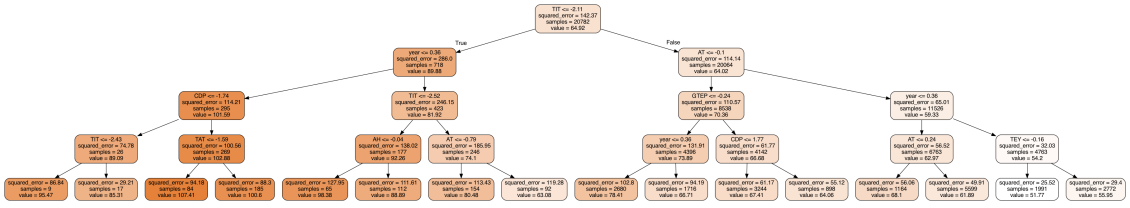
	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2	\
112	6.534284	7.699417	0.685086	0.373734	
39	6.607870	7.711528	0.677974	0.371504	
25	6.540665	7.714026	0.684467	0.372889	
92	6.611545	7.741212	0.677633	0.368894	
123	6.605133	7.745834	0.678264	0.370643	
152	6.809102	7.907231	0.658098	0.347655	
98	6.808216	7.909413	0.658200	0.347542	
11	6.811357	7.913407	0.657878	0.347506	
130	6.817238	7.917554	0.657273	0.345691	
99	6.815196	7.926607	0.657503	0.345906	

	param_model__max_features	param_model__n_estimators	param_model__max_depth
112	6	80	4
39	6	20	4
25	6	120	4
92	4	100	4
123	4	160	4
152	log2	100	4
98	sqrt	120	4
11	sqrt	140	4
130	3	60	4
99	log2	160	4

```
RF Train Avg RMSE accross 10-fold cv:  6.535650579623966
RF Validation Avg RMSE accross 10-fold cv:  7.683507321594336
```

Then I select a tree with max depth 4 and plot it.

```
Selected tree
: DecisionTreeRegressor(max_depth=4, max_features=5, random_state=1726841109)
```



Which feature is selected for branching at the root node?

TIT feature is selected as root node. The split rule is checked TIT <=-2.11.

What can you infer about the importance of features?

For the splits of the branches: TIT, year, CDP, TAT, AH, AT, GTEP, TEY are used. These features are the features found to be the most important ones that is used to split samples. The most important feature is TIT since it is used on the root node, then the the features used closer to the root are more informative, hence important features compared to the ones closer to leaf nodes. We can also observe that some features are used in several nodes and splits and chosen for new decision splits, this shows that these features play more critical role for the final prediction of this specific tree.

Do the important features match what you got in part 3.2.1?

In the best model found after Linear Regression experiments, 3.2.1, the most important features were TEY, TIT, AT, TAT and AH in order. According to the above decision tree, we can as well see that the important features found are very similar, in this case though TIT found to be more important than TEY since TIT is used as the root node.

1.6 LightGBM, CatBoost and Bayesian Optimization

I picked the Diamonds dataset for this section:

Question 22

LightGBM Parameters to tune LightGBM uses leaf-wise tree growth algorithm whereas many other tree algorithms use dept-wiswe tree growth. Leaf-wise algorithms have an advantage of converging faster but also more prone to overfitting if not used appropriatee parameters.

Parameters to tune: - num_leaves: the parameter is the main one to control complexity of the model according to the documentation. It should be smaller than 2^(max_depth) to avoid overfittting.
- min_data_in_leaf: this parameter helps prevent overfitting as well. The optimal value depends number of training samples and num_leaves. If it is large, it avoids growing too deep tree but

also may cause underfitting. According to the documentation setting it in hundreds or thousands is enough for a large dataset. Since our datasets are smaller I will try values starting from 10 to 1000. - max_depth: This parameter also limit tree depth, hence helps avoid overfitting.

There are also other parameters to use for better performance results suggested in the documentation: use large max_bin (may be slower), use small learning_rate with large num_iterations, use large num_leaves (may cause overfitting) and try dart as boosting_type.

My final set of parameters and the search space for LightGBM is:

- num_leaves = [2**(x) for x in range(4,8)]
- min_data_in_leaf = [10, 20, 50, 75, 100, 250, 500, 750, 1000]
- max_depth = [-1, 3, 4, 5, 6, 7, 8, 10, 20]
- boosting_type = ['gbdt', 'dart']
- n_estimators = [30, 50, 100, 150]
- num_iterations = list(range(100, 301, 50))
- learning_rate = [0.1, 0.05, 0.01]

I decided the above search space range based on the documentation recommendations, further research on the internet and by taking into account my dataset and the samples in there (the number of samples are not big so I tried to keep some parameters smaller, or added smaller numbers as well to try to avoid overfitting).

Reference: https://lightgbm.readthedocs.io/en/latest/Parameters-Tuning.html

CatBoost Parameters to tune For catboost the important parameters to tune for this questions are: - iterations: maximum number of trees that can be built - learning_rate - depth: Depth of the tree - l2-leaf-reg: L2 regularization coefficient which is used for leaf value calculation. - od-pval is threshold for overfitting detector, it is set to the recommended range in the documentation. - random_strength: amount of randomness to use for scoring splits , it helps avoid overfitting, - bagging_temperature: defines the settings of the Bayesian bootsrap,the higher the value the most aggressive bagging is. - border_count: number of splits for the numerical features (its alias is max_bin)

I decided on these parameters after reading catboost documentation for parameter tuning part: https://catboost.ai/en/docs/concepts/parameter-tuning For the search space for each parameter, I decided either based on the recommendation range in documenation or based on the dataset and number of samples I have in the diamonds dataset.

My final set of parameters and the search space for CatBoost is:

- iterations: Integer(50, 300)
- learning_rate: Real(0.01, 1.0, 'log-uniform')
- depth: Integer(4, 10)
- od-pval: Real(10e-10, 10e-2, 'log-uniform'), (is set to the recommended range in the documentation.)
- l2_leaf_reg': Integer(2, 20),
- random_strength': Real(1e-9, 10, 'log-uniform'),

- bagging_temperature': Real(0.0, 1.0),
- border_count': Integer(1, 255),

Question 23 Apply Bayesian optimization using skopt.BayesSearchCV from scikit-optmize to search good hyperparameter combinations in your search space. Report the best hyperparameter found and the corresponding RMSE, for both algorithms.

In this question I used the parameters and search spaces I defined for each of them to tune my parameters for LightGBM and CatBoost models. I applied Bayesian optimization with BayesSearchCV for 10-folds for both models.

LightGBM Results To be able to understand how much results are improved with parameter tuning, I also ran a 10-fold cross validation LightGBM with its default parameters. The results are below, we can see that LightGBM is already performing way better than all the other models with its default values.

```
LightGBM Train Avg RMSE accross 10-fold cv:  466.01792200127346
LightGBM Validation Avg RMSE accross 10-fold cv:  657.5308021388921
```

LightGBM Parameter Tuning Results

For LightGBM 200 samples (n_iter=200) are choosen during BayesSearchCV and 10-fold cv is applied, the parameters tuned can be seen from Q22. The top 10 best mean_validation_score score results are shown in the below table:

	mean_train_score	mean_validation_score	param_model__num_iterations	\
199	500.356272	599.345728	300	
122	500.356272	599.345728	300	
120	500.356272	599.345728	300	
118	500.356272	599.345728	300	
117	500.356272	599.345728	300	
116	500.356272	599.345728	300	
115	500.356272	599.345728	300	
114	500.356272	599.345728	300	
113	500.356272	599.345728	300	
112	500.356272	599.345728	300	

	param_model__learning_rate	param_model__n_estimators	\
199	0.1	50	
122	0.1	50	
120	0.1	150	
118	0.1	50	
117	0.1	50	
116	0.1	30	
115	0.1	100	
114	0.1	50	
113	0.1	50	
112	0.1	50	

```
     param_model__num_leaves  param_model__min_data_in_leaf  \
199                       64                             75
122                       64                             75
120                       32                             75
118                       16                             75
117                       32                             75
116                       32                             75
115                       64                             75
114                       32                             75
113                       32                             75
112                       64                             75

     param_model__max_depth param_model__boosting_type
199                       4                       gbdt
122                       4                       gbdt
120                       4                       gbdt
118                       4                       gbdt
117                       4                       gbdt
116                       4                       gbdt
115                       4                       gbdt
114                       4                       gbdt
113                       4                       gbdt
112                       4                       gbdt
```

With parameter tuning we can see that we reached even better results than the default parameter values. The mean train RMSE is around 500.35 and mean validation RMSE is around 599.34. These results are also way better than the models trained on diamonds dataset on the previous questions.

The best parameters found are:

- max depth = 4,
- min_data_in_leaf=75,
- num_iterations=300,
- num_leaves=16,
- learning_rate=0.1,
- n_estimators = 100

The best parameters and estimator chosen by BayesSearchCV is shown below:

```
Best model:
 Pipeline(steps=[('model',
                  LGBMRegressor(max_depth=4, min_data_in_leaf=75, n_jobs=1,
                                num_iterations=300, num_leaves=16,
                                random_state=142))])
Best model parameters:
 OrderedDict([('model', LGBMRegressor(max_depth=4, min_data_in_leaf=75,
n_jobs=1, num_iterations=300,
               num_leaves=16, random_state=142)), ('model__boosting_type',
'gbdt'), ('model__learning_rate', 0.1), ('model__max_depth', 4),
```

```
('model__min_data_in_leaf', 75), ('model__n_estimators', 100),
('model__num_iterations', 300), ('model__num_leaves', 16)])
```

One thing we can notice is that we actually get same scores for different combinations in the top 10 best results. When I further explored I saw that this is the case for the best 100 experiment combination results. We can explain this as: after some the mean_validation_score starts to saturate and the model cannot learn more from the data. In this case it is better to choose the best parameter combinations by minimizing the computation time and/or by choosing some of the parameters that has better regularization effects.

Below table describes the parameter tuning that has thee best training and validation mean scores. For example, we can choose a best parameter combination wheren n_estimators could be as low as 30 and still can get same results or where param_model___num_leaves is as low as 16.

	mean_train_score	mean_validation_score	param_model__num_iterations	\
count	1.010000e+02	1.010000e+02	101.0	
mean	5.003563e+02	5.993457e+02	300.0	
std	1.142539e-13	2.285077e-13	0.0	
min	5.003563e+02	5.993457e+02	300.0	
25%	5.003563e+02	5.993457e+02	300.0	
50%	5.003563e+02	5.993457e+02	300.0	
75%	5.003563e+02	5.993457e+02	300.0	
max	5.003563e+02	5.993457e+02	300.0	

	param_model__learning_rate	param_model__n_estimators	\
count	1.010000e+02	101.000000	
mean	1.000000e-01	78.910891	
std	2.789401e-17	43.379742	
min	1.000000e-01	30.000000	
25%	1.000000e-01	50.000000	
50%	1.000000e-01	50.000000	
75%	1.000000e-01	100.000000	
max	1.000000e-01	150.000000	

	param_model__num_leaves	param_model__min_data_in_leaf	\
count	101.000000	101.0	
mean	36.910891	75.0	
std	20.457810	0.0	
min	16.000000	75.0	
25%	16.000000	75.0	
50%	32.000000	75.0	
75%	64.000000	75.0	
max	64.000000	75.0	

	param_model__max_depth
count	101.0
mean	4.0
std	0.0

```
min                     4.0
25%                     4.0
50%                     4.0
75%                     4.0
max                     4.0
```

CatBoost Results To be able to understand how much results are improved with parameter tuning, I also ran a 10-fold cross validation CatBoost with its default parameters. The results are below, we can see that CatBoost is now the best model for diamonds dataset compared to the all models we performed in this project even with its default values.

```
CatBoost Train Avg RMSE accross 10-fold cv:  427.7612680829581
CatBoost Validation Avg RMSE accross 10-fold cv:  551.9742619473776
```

CatBoost Parameter Tuning Results

For CatBoost 300 samples (n_iter=300) are choosen during BayesSearchCV and 10-fold cv is applied, the parameters tuned can be seen from Q22. The top 10 best mean_validation_score score results are shown in the below table:

The best results 10-fold mean train score is 475 and mean validation score is 556.

```
     mean_train_score  mean_validation_score  param_bagging_temperature  \
279         475.666327             556.067794                   0.418524
246         466.669808             557.182539                   0.997217
288         472.834587             557.381485                   1.000000
269         479.240343             557.608886                   0.664465
267         464.279413             557.778176                   1.000000
272         462.116113             558.255516                   0.316298
265         453.928966             558.339972                   1.000000
194         459.041886             558.491466                   0.353427
275         474.309467             558.716024                   0.314705
242         466.021585             559.242403                   0.489464

     param_border_count  param_depth  param_iterations  param_l2_leaf_reg  \
279                 214            6               300                  2
246                 216            7               300                  2
288                 214            6               300                  2
269                 213            6               290                  2
267                 212            7               289                  2
272                 212            7               286                  2
265                 212            7               286                  2
194                 240            7               300                  2
275                 215            6               300                  2
242                 214            7               282                  2

     param_learning_rate  param_od_pval  param_random_strength
279             0.123266   8.715984e-09                   10.0
246             0.102324   9.829911e-02                   10.0
```

```
288             0.130456   1.000000e-01                  10.0
269             0.121453   1.000000e-01                  10.0
267             0.111908   1.000000e-01                  10.0
272             0.118755   3.518941e-02                  10.0
265             0.134351   1.000000e-01                  10.0
194             0.117091   1.000000e-01                  10.0
275             0.129174   1.000000e-01                  10.0
242             0.111860   7.063009e-09                  10.0
```

The best parameters found:

```
     mean_train_score  mean_validation_score  param_bagging_temperature  \
279        475.666327             556.067794                   0.418524

     param_border_count  param_depth  param_iterations  param_l2_leaf_reg  \
279                 214            6               300                  2

     param_learning_rate  param_od_pval  param_random_strength
279             0.123266   8.715984e-09                  10.0
```

```
Best model parameters:
 OrderedDict([('bagging_temperature', 0.4185244058413902), ('border_count',
214), ('depth', 6), ('iterations', 300), ('l2_leaf_reg', 2), ('learning_rate',
0.12326552106335201), ('od_pval', 8.715984046007978e-09), ('random_strength',
10.0)])
```

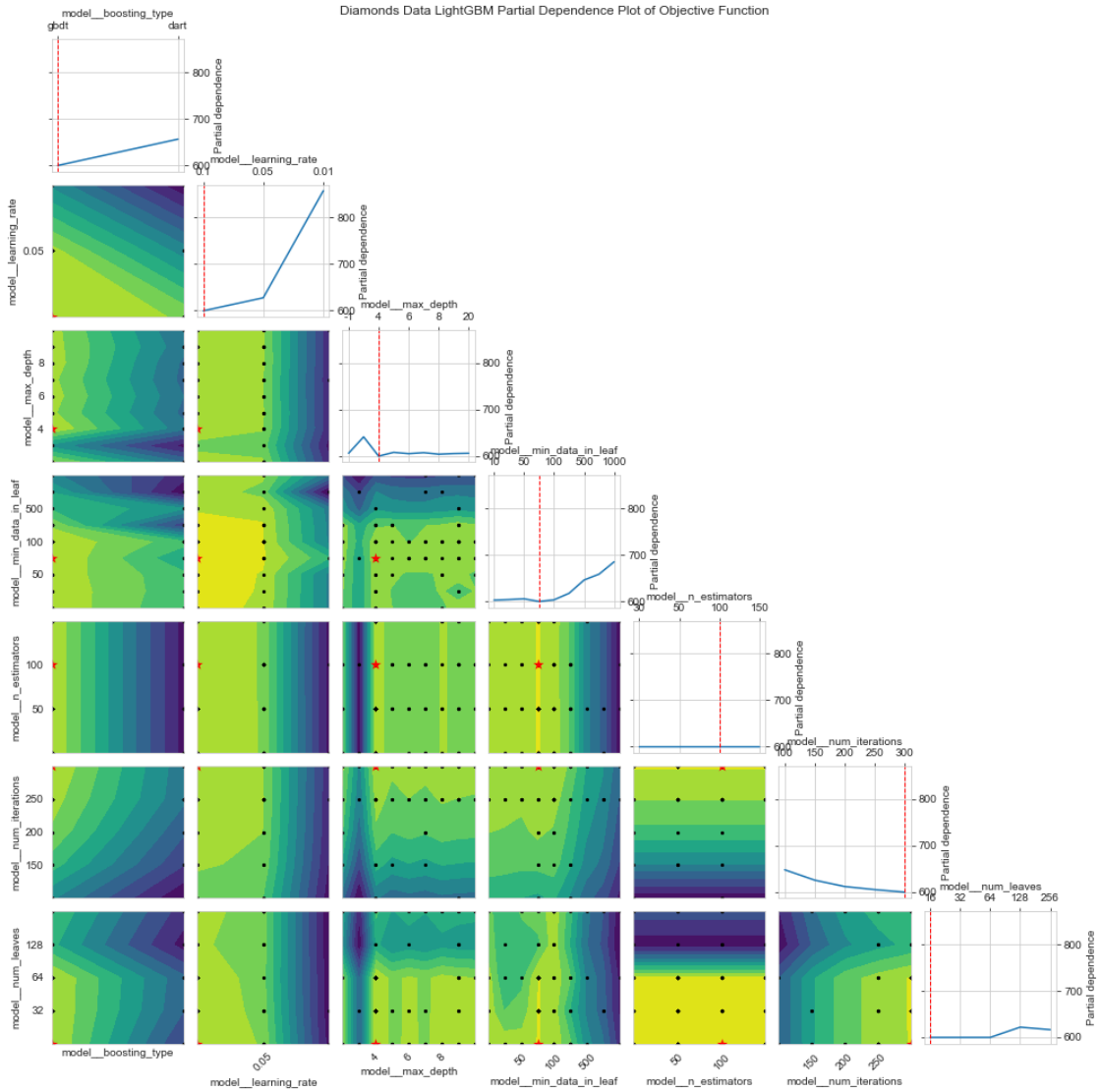
Again the validation results are very close and there isn't marginally very big difference for the first 5-6 combinations so one can choose the best combination based the resources and needs they have.

Question 24 Plot_objective plot showd the influence of each search space dimension on the objective function of BayesSearch results. The diagonal shows the effect of a single dimension on objective function and the other subplots show the effect on objective function warying two dimensions. The black dots corresponds to the samples used during optimization, red start indicates the best observed minimum.

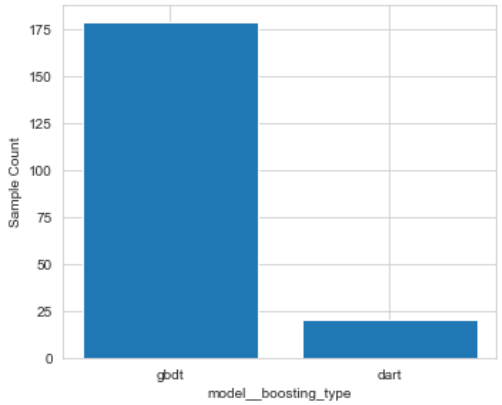
Interpret the effect of the hyperparameters using the Bayesian optimization results:

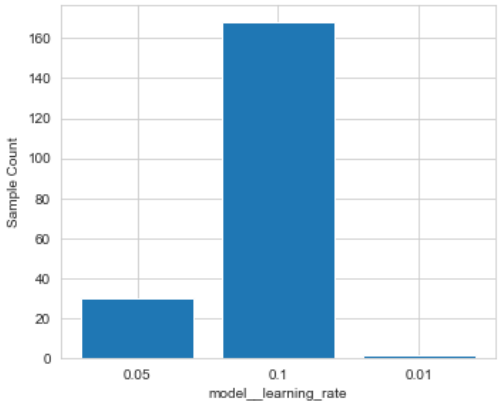
- **Which of them helps with performance? Which helps with regularization (shrinks the generalization gap)?**
- **Which affects the fitting efficiency?**
- **Endorse your interpretation with numbers and visualizations.**

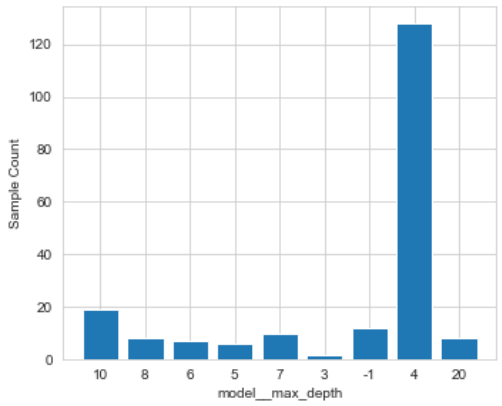
LightGBM I first plotted the Partial Dependence plot and histogram of the samples used in BayesSearch to better understand the parameters and its values used in the search and bayesian optimization:

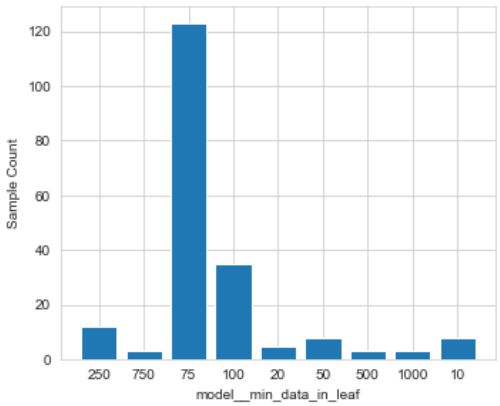

Diamonds Data LightGBM Partial Dependence Plot of Objective Function
model__boosting_type
gbdt
dart
model__learning_rate
0.1
0.05
0.01
model__max_depth
model__min_data_in_leaf
model__n_estimators
model__num_iterations
model__num_leaves
Partial dependence
600
700
800

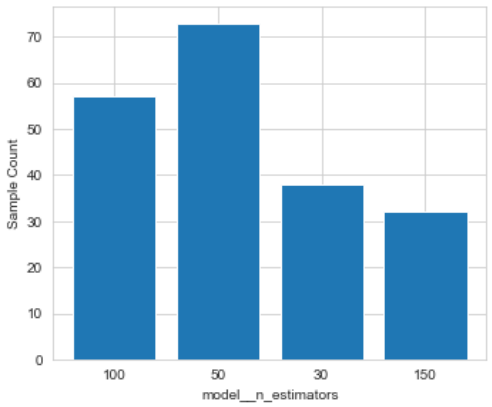
Diamonds Data LightGBM Sample Count Histogram for tuned features

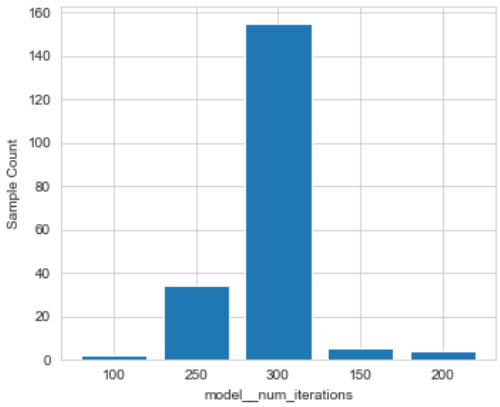


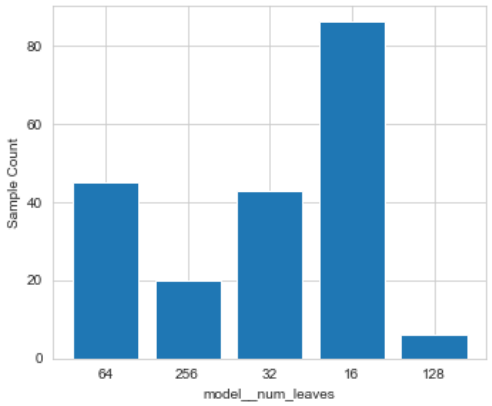


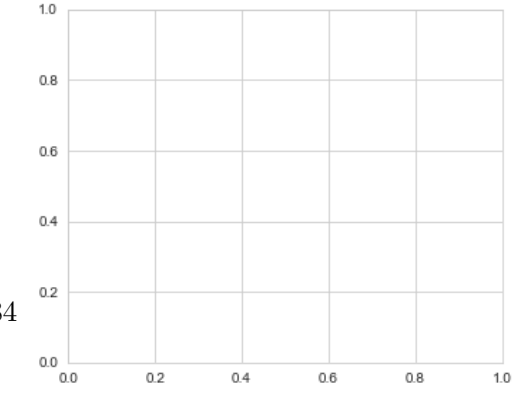












Below tables for each tuned feature shows the mean fit time, mean validation score, mean training score and the RMSE gap between mean train and validation scores:

param_model__boosting_type	dart	gbdt
mean_validation_score	732.384601	611.090529
mean_train_score	660.391542	497.698208
RMSE_gap	71.993059	113.392321
mean_fit_time	9.015170	0.574902

param_model__learning_rate	0.01	0.05	0.10
mean_validation_score	1313.382406	660.143379	609.132233
mean_train_score	1473.259320	524.846458	501.573150
RMSE_gap	-159.876914	135.296921	107.559083
mean_fit_time	4.552230	1.253376	1.461431

param_model__max_depth	-1	3	4	5	\
mean_validation_score	619.903682	702.371362	604.561980	678.761426	
mean_train_score	446.765218	613.193459	504.542860	585.237979	
RMSE_gap	173.138464	89.177903	100.019121	93.523447	
mean_fit_time	3.806712	0.405473	0.659794	0.826093	

param_model__max_depth	6	7	8	10	\
mean_validation_score	618.857126	782.929403	630.309871	632.892752	
mean_train_score	484.653455	736.480454	509.251233	495.497381	
RMSE_gap	134.203671	46.448949	121.058637	137.395371	
mean_fit_time	0.555397	2.633360	2.092659	4.347865	

param_model__max_depth	20
mean_validation_score	654.557147
mean_train_score	503.734921
RMSE_gap	150.822226
mean_fit_time	3.344031

param_model__min_data_in_leaf	10	20	50	75	\
mean_validation_score	625.887256	631.032231	626.692511	607.232678	
mean_train_score	457.509027	459.093484	474.658738	502.773876	
RMSE_gap	168.378229	171.938746	152.033773	104.458802	
mean_fit_time	1.207867	1.543826	3.418163	0.552696	

param_model__min_data_in_leaf	100	250	500	\
mean_validation_score	618.406182	662.477765	653.891559	
mean_train_score	492.621715	571.793104	564.410250	
RMSE_gap	125.784467	90.684661	89.481309	
mean_fit_time	3.721999	0.973568	5.694160	

param_model__min_data_in_leaf	750	1000
mean_validation_score	1070.571722	710.841080

```
mean_train_score               1191.445502  663.786936
RMSE_gap                       -120.873780   47.054144
mean_fit_time                     3.101194    3.726084

param_model__n_estimators          30          50          100         150
mean_validation_score      649.184105  619.245019  619.466426  611.931646
mean_train_score           555.880731  509.105813  497.169168  510.292717
RMSE_gap                    93.303374  110.139206  122.297257  101.638929
mean_fit_time                1.723009    1.594337    1.052512    1.574125

param_model__num_iterations         100         150         200         250  \
mean_validation_score        661.997451  715.500251  685.856882  671.042687
mean_train_score             545.298755  622.184556  577.071667  567.586741
RMSE_gap                     116.698696   93.315695  108.785216  103.455946
mean_fit_time                  0.292926    1.286618    3.212991    4.631984

param_model__num_iterations         300
mean_validation_score        608.418750
mean_train_score             497.731906
RMSE_gap                     110.686844
mean_fit_time                  0.741082

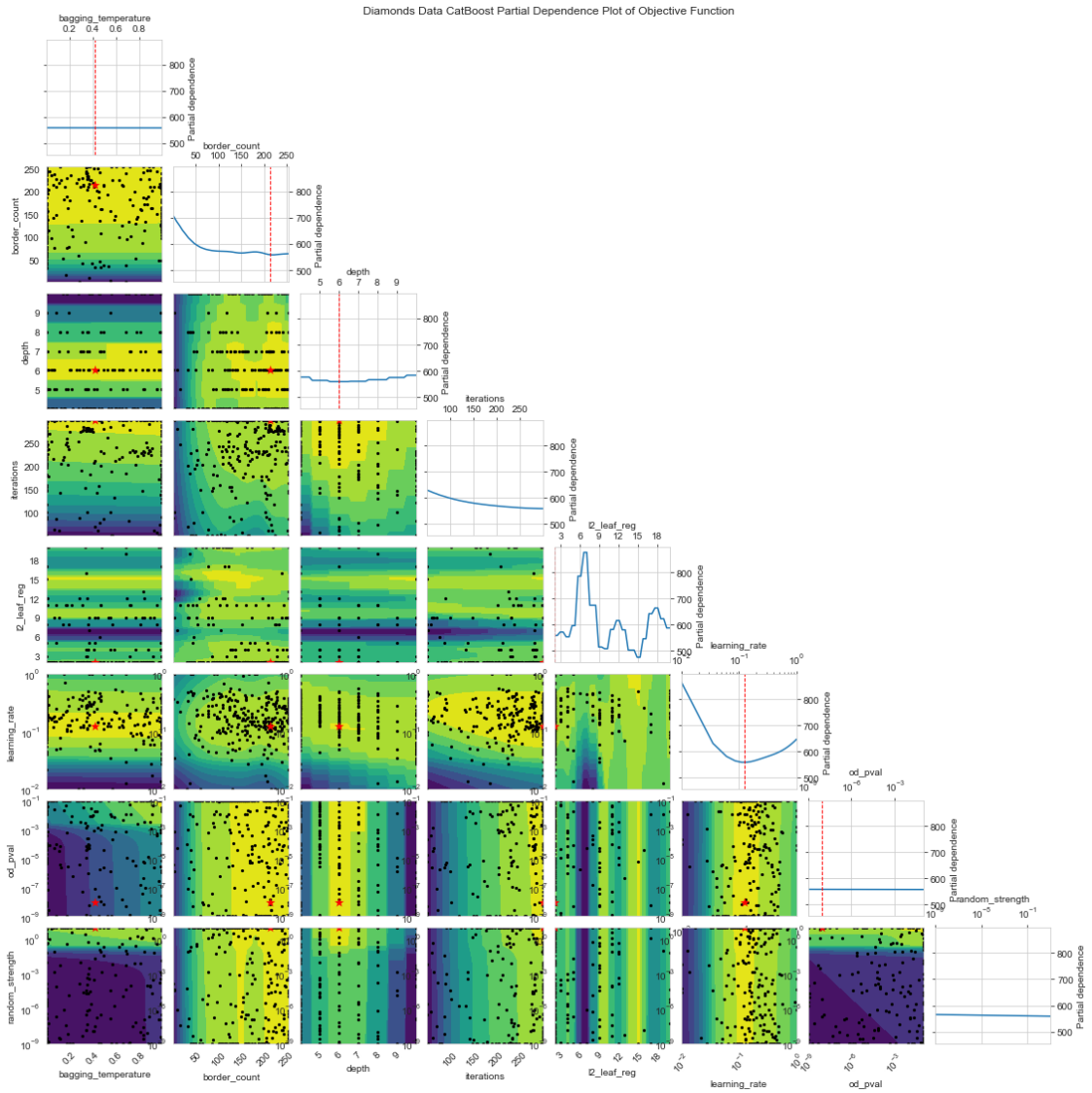
param_model__num_leaves          16          32          64          128  \
mean_validation_score    620.299137  642.961006  609.813652  626.046208
mean_train_score         513.496141  553.977861  503.870603  460.903003
RMSE_gap                 106.802996   88.983146  105.943049  165.143205
mean_fit_time              0.926784    0.851639    1.665036    2.708304

param_model__num_leaves          256
mean_validation_score    628.717030
mean_train_score         476.744514
RMSE_gap                 151.972516
mean_fit_time              4.236288
```

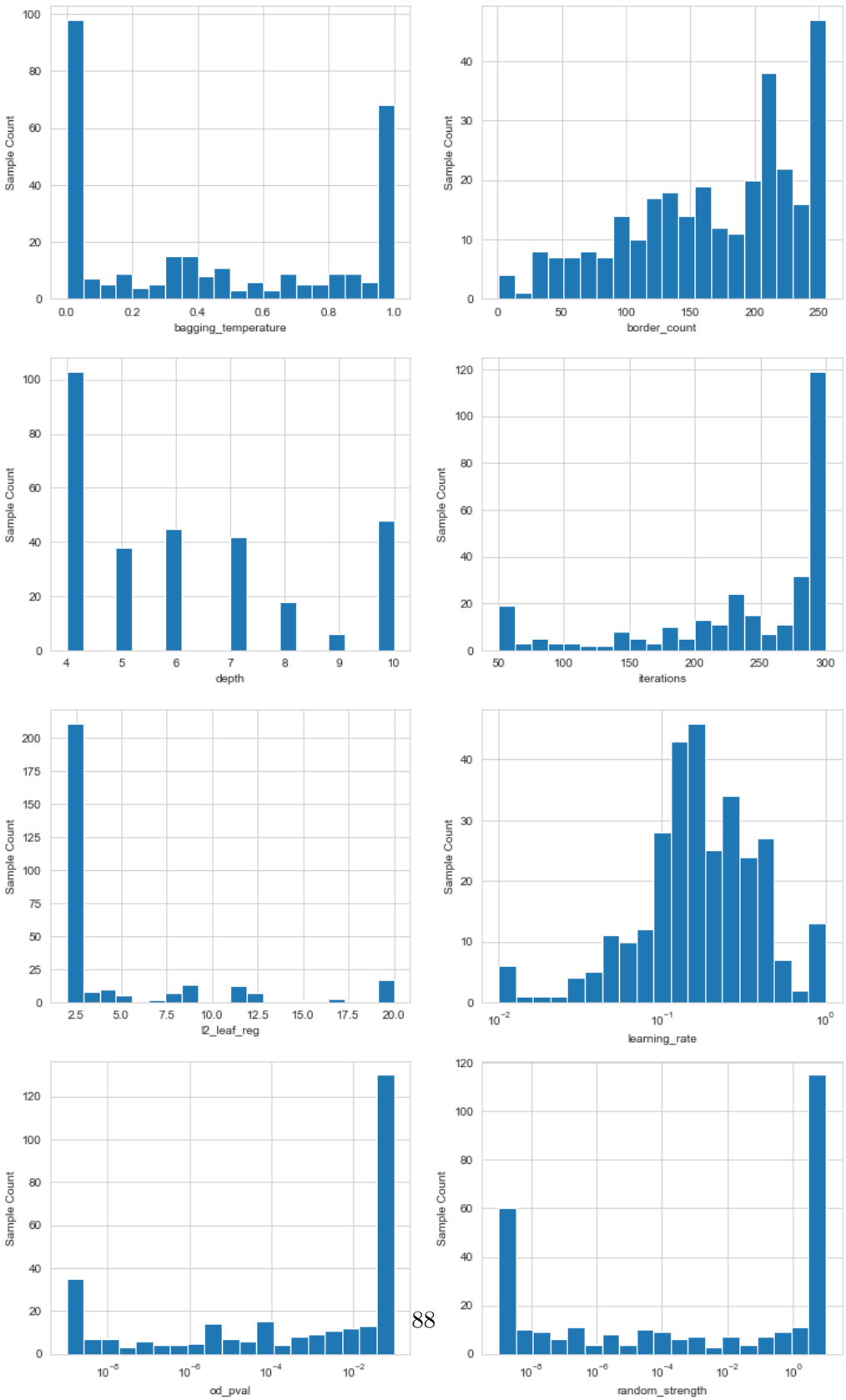
From the above plots and tables, we can interpret find hyperparameters that effect the results most, helps/hurts the fitting efficiency and the ones helps with the regularization.

For the LightGBM, according to the Partial Dependence Plot and above tables, Learning rate, boosting_type, min_data_in_leaf, num_iterations helps with the performance of the model. Num_leaves, min_data_in_leaf, max_depth seems to help with regularization. Learning rate, num_iterations and max_depth again does effect the fitting efficiency, small learning rate combined with high number of iterations and big max_depth value increase the fitting time of the model (mean fit time in the above tables). The boosting_type dart is also have way bigger fitting time compared to gbdt.

CatBoost


Diamonds Data CatBoost Partial Dependence Plot of Objective Function
bagging_temperature
border_count
depth
iterations
l2_leaf_reg
learning_rate
od_pval
random_strength
Partial dependence

Diamonds Data CatBoost Sample Count Histogram for tuned features



Below tables for each tuned feature shows the mean fit time, mean validation score, mean training score and the RMSE gap between mean train and validation scores:

param_bagging_temperature	0.000000	0.002968	0.004518	0.006950	\
mean_validation_score	596.420554	576.911417	574.596597	567.890303	
mean_train_score	490.671380	499.741331	443.984078	496.749494	
RMSE_gap	105.749175	77.170087	130.612520	71.140808	
mean_fit_time	1.467983	1.183442	1.809631	1.119211	

param_bagging_temperature	0.016229	0.016264	0.026538	0.039710	\
mean_validation_score	575.371422	578.230057	568.175920	575.617139	
mean_train_score	449.212034	496.844748	473.947187	507.465929	
RMSE_gap	126.159388	81.385309	94.228733	68.151210	
mean_fit_time	1.092802	0.680561	4.381694	0.915352	

param_bagging_temperature	0.042568	0.053071
mean_validation_score	561.070924	559.642755
mean_train_score	470.670895	476.460018
RMSE_gap	90.400029	83.182736
mean_fit_time	1.169266	1.181843

param_border_count	1	2	3	9	\
mean_validation_score	2437.885042	2155.604170	2050.695108	1113.351649	
mean_train_score	2705.875540	2030.159951	1882.821540	774.600469	
RMSE_gap	-267.990498	125.444219	167.873567	338.751180	
mean_fit_time	0.302329	1.518940	0.804732	1.016317	

param_border_count	16	31	32	34	\
mean_validation_score	868.945692	983.486290	683.633660	674.054715	
mean_train_score	684.835780	919.517794	515.289167	514.836671	
RMSE_gap	184.109911	63.968496	168.344492	159.218044	
mean_fit_time	0.843478	0.858223	1.159559	2.658881	

param_border_count	35	37
mean_validation_score	654.210713	874.935538
mean_train_score	569.609654	827.448298
RMSE_gap	84.601059	47.487241
mean_fit_time	0.928517	1.262819

param_depth	4	5	6	7	\
mean_validation_score	619.482407	581.061688	677.234097	577.630664	
mean_train_score	526.896674	485.809802	590.801220	459.122405	
RMSE_gap	92.585733	95.251886	86.432877	118.508259	
mean_fit_time	0.881004	1.270390	1.123163	1.384647	

param_depth	8	9	10
mean_validation_score	621.180552	891.826006	621.733797

mean_train_score	466.948582	760.145866	475.404196		
RMSE_gap	154.231970	131.680140	146.329601		
mean_fit_time	1.486894	2.351749	3.048691		

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param_iterations	50	52	57	60	
mean_validation_score	784.127465	628.354904	636.942447	739.782186	
mean_train_score	662.170635	552.337812	565.288087	662.767540	
RMSE_gap	121.956830	76.017092	71.654360	77.014646	
mean_fit_time	0.415664	0.160174	0.201277	0.247884	

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param_iterations	61	62	64	69	
mean_validation_score	611.386375	632.731844	615.897542	682.088667	
mean_train_score	522.973640	551.300124	541.200627	551.531170	
RMSE_gap	88.412735	81.431720	74.696915	130.557497	
mean_fit_time	0.311200	0.649670	0.250633	0.798380	

param_iterations	73	77
mean_validation_score	602.712813	635.231990
mean_train_score	491.348203	496.475672
RMSE_gap	111.364610	138.756318
mean_fit_time	0.503462	0.659570

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param_l2_leaf_reg	2	3	4	5	
mean_validation_score	592.521556	593.212444	587.557544	698.806326	
mean_train_score	482.540399	483.580004	474.519385	609.794996	
RMSE_gap	109.981157	109.632440	113.038159	89.011330	
mean_fit_time	1.552190	0.922385	0.829635	0.620922	

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param_l2_leaf_reg	6	7	8	9	
mean_validation_score	635.231990	870.853276	850.717300	738.727187	
mean_train_score	496.475672	663.469141	747.746240	610.681058	
RMSE_gap	138.756318	207.384136	102.971060	128.046130	
mean_fit_time	0.659570	0.588245	1.234575	1.877911	

param_l2_leaf_reg	11	12
mean_validation_score	620.824965	851.370087
mean_train_score	486.455947	805.707700
RMSE_gap	134.369017	45.662387
mean_fit_time	1.480590	1.482583

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param_learning_rate	0.010000	0.012573	0.013914	0.017566	
mean_validation_score	1172.742308	874.935538	929.489008	632.663857	
mean_train_score	1174.963365	827.448298	903.911986	570.690434	
RMSE_gap	-2.221056	47.487241	25.577022	61.973424	
mean_fit_time	1.634913	1.262819	1.031312	5.734875	

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param_learning_rate	0.022048	0.027387	0.027934	0.030159	
mean_validation_score	731.142892	629.020778	735.845770	609.701538	
mean_train_score	633.231155	521.534205	643.380068	500.774356	

RMSE_gap	97.911737	107.486573	92.465702	108.927182	
mean_fit_time	1.501995	4.283874	0.795100	6.437489	

param_learning_rate	0.032528	0.035221
mean_validation_score	654.259492	594.356834
mean_train_score	595.037900	534.476773
RMSE_gap	59.221592	59.880061
mean_fit_time	1.446941	2.928060

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param_od_pval	1.000000e-09	1.116487e-09	1.170697e-09	1.185287e-09	\
mean_validation_score	584.903536	567.806218	576.528644	570.639234	
mean_train_score	481.655064	484.138349	465.930763	473.850629	
RMSE_gap	103.248472	83.667870	110.597881	96.788605	
mean_fit_time	1.926178	1.005269	2.044189	0.829658	

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param_od_pval	1.281338e-09	1.847439e-09	2.654482e-09	2.655925e-09	\
mean_validation_score	569.995140	622.150930	573.167168	602.712813	
mean_train_score	463.015873	471.792595	499.362146	491.348203	
RMSE_gap	106.979267	150.358334	73.805022	111.364610	
mean_fit_time	1.397618	0.701155	5.784815	0.503462	

param_od_pval	2.805438e-09	4.801575e-09
mean_validation_score	578.230057	671.803006
mean_train_score	496.844748	581.522814
RMSE_gap	81.385309	90.280192
mean_fit_time	0.680561	0.181508

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param_random_strength	1.000000e-09	1.179524e-09	1.337562e-09	1.948190e-09	\
mean_validation_score	607.071588	568.576941	575.371422	620.678094	
mean_train_score	474.953623	454.479939	449.212034	445.365418	
RMSE_gap	132.117965	114.097002	126.159388	175.312676	
mean_fit_time	1.547080	1.115034	1.092802	1.742592	

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param_random_strength	1.970483e-09	2.317262e-09	2.657184e-09	2.911235e-09	\
mean_validation_score	576.543032	571.148219	605.680737	731.142892	
mean_train_score	476.682028	490.567075	513.124624	633.231155	
RMSE_gap	99.861004	80.581144	92.556113	97.911737	
mean_fit_time	0.963859	0.908414	0.997489	1.501995	

param_random_strength	3.064276e-09	3.137981e-09
mean_validation_score	582.312354	611.386375
mean_train_score	470.518416	522.973640
RMSE_gap	111.793937	88.412735
mean_fit_time	0.786395	0.311200

From the above plots and tables, we can interpret find hyperparameters that effect the results most, helps/hurts the fitting efficiency and the ones helps with the regularization.

For CatBoost model, according to the Partial Dependence Plot and above tables, border count, depth, iterations, l2_leaf_reg, learning_rate are thehyperparameters that has the highest effects

on model performance. The ones that has most effect is l2_leaf_reg and learning rate. You can observe the changes of RMSE score with the change of these features by looking the diagonal subplots of Partial Dependence plot. Depth, l2_leaf_reg, random_strength all seems to help with regularization. Depth parameter effects the fitting time inversely. Learning rate, iterations again effect the fitting efficiency, small learning rate combined with high number of iterations increase the fitting time of the model.

1.7 Evaluation

Question 25 The two tables below shows the 10-fold avg training and validation RMSE scores for best found model results for each algorithms.

Diamonds Best Results for Each Model

	model	mean_train_score	mean_validation_score	\
0	Lasso	1206.280597	1205.045051	
1	Ridge	1206.280597	1205.045051	
2	Polynomial Regression	921.572213	882.226435	
3	Neural Network	595.010078	637.488677	
4	Random Forest	197.555441	715.111659	
5	LightGBM	500.356272	599.345728	
6	CatBoost	475.666327	556.067794	

	abs_RMSE_gap
0	1.235546
1	1.235546
2	39.345778
3	42.478598
4	517.556217
5	98.989456
6	80.401467

Gas Best Results for Each Model

	model	mean_train_score	mean_validation_score	\
0	Lasso	8.036236	8.802989	
1	Ridge	8.094992	8.761643	
2	Polynomial Regression	5.719778	7.155798	
3	Neural Network	5.034472	6.334995	
4	Random Forest	1.342304	6.762084	

	abs_RMSE_gap
0	0.766753
1	0.666650
2	1.436020
3	1.300523
4	5.419779

Why is the training RMSE different from that of validation set?

Having a higher train validation gap, when train error is low and validation error is high, generally refers to overfitting (model starts to memorize/fitt training data very well that it cannot perform well/generalize on unseen test data).
When both train and validation errors are high and gap is small, this would mean the model underfits the data, which is model cannot learn enough from data to generalize.

Diamonds Data: For the Linear Reg. without Regularization, Lasso and Ridge Regression the train and validation scores are very similar but very high, this might suggest that they are underfitting the dataset we have. The training RMSE and validation RMSE gap is the biggest in Random Forest part, training error is very low and validation is high, suggesting overfitting. As stated in the previous sections, for Random Forest we may pick a better parameter results manually that doesn't overfit, with low gap between the train and test RMSE and low RMSE result (details on RF section). For LightGBM and CatBoost are the model types that have higher RMSE gaps, after Random Forest. Again, we can see that train score are lower and the validation scores are bit higher. This shows that the model fit better to the training data and not as much to the test data. For Polynomial Regression we see that the training score is higher than validation, this is generally not an expected behavior but might be because the regularization value chosen is big on the best model. Neural Network gap is also low, which shows model fit well to both train and validation sets. The best validation results found in all model belongs to CatBoost with 556 RMSE score and the RMSe gap is 80.4, which is acceptable.

Gas Data:

We see similar results on gas data as well, Lasso and Ridge have high train and validation scores, with little gap, referring to underfit. The models cannot fit the data very well and hypothesis space used is not enough to capture the variability in the data. Random Forest looks like overfitting again with very high gap and low train, high validation result, better parameters may bee picked manually. Polynomiald Regression and Neural Network train and validation scores are lower and the gap between them is not much, showing these models are well fit and generalizing well in the unseen test data. The best model found for gas data is neural network.

Question 26 Explain what OOB error and R^2 score means.

OOB Error: Out of bag error, measures the prediction error of Random Forest. In Random Forest we use bootsrap samples for training the trees. Then the out of bag samples are the samples that are not selected, left out ones from bootstrap samples. The out of bag samples won't be used in training and therefore can be used as unseen samples and measure model performance for the trees where they are not used as training samples. OOB score is than computed as the number of correctly predicted samples from the out of bag sample, in regression case the oob score is computed using the R^2 score between true values and predicted values for OOB samples. The OOB error is calculated as the average error for predictions from the trees that do not contain in their respective bootstrap sample (oob samples are used).

R^2 score: indicates whether the model is a good fit for the data by measuring the proportion of the variance for target variable explained by the feature variables. $R^2 = 1 - (RSS/TSS)$ RSS: sum of squares of residuals, and TSS is total sum of squares. The R^2 value is between 0 and 1, 1 means the model fit data perfectly and 100% of the variance in the target variable explained by the features used in the model.

Diamonds Data

```
Best RF Model OOB Score: 0.981448128437458
[ 473.22222222  388.26666667  430.97368421 … 2643.73809524 2940.55263158
 2779.66666667]

Best RF Model Feature Importances:
carat feature importance:0.30199465230227157
depth feature importance:0.005615268543312274
table feature importance:0.004346108749685826
x feature importance:0.19090287772735992
y feature importance:0.2554629994561144
z feature importance:0.14922971129722173
cut feature importance:0.003289634910874443
color feature importance:0.031206885821142057
clarity feature importance:0.057951861192017756
```

Best RF Model Mean Test and Train RMSE and R2 scores after 10-fold CV:

	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2
93	197.555441	715.111659	0.99751	0.644635

For best RF model diamond data, OOB score for 0.98. In Regression case R^2 scores are used to calculate OOB score. 0.98 OOB score is a good result. Avg. validation R^2 is 0.644 which is not very good.

Gas Data

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Best RF Model OOB Score: 0.9024957564053923
[82.41471831 82.39423288 81.85991228 … 89.10917722 65.38696364
 70.00585   ]

Best RF Model Feature Importances:
AT feature importance:0.3010705060339823
AP feature importance:0.04480777238527264
AH feature importance:0.0405105496218159
AFDP feature importance:0.0819215110852701
GTEP feature importance:0.0800383875929842
TIT feature importance:0.12693861634272424
TAT feature importance:0.07691051650405482
TEY feature importance:0.06028978245172857
CDP feature importance:0.048490805350535224
year feature importance:0.13902155263163204
```

Best RF Model Mean Test and Train RMSE and R2 scores after 10-fold CV:

	mean_train_RMSE	mean_validation_RMSE	mean_train_R2	mean_validation_R2
164	1.342304	6.762084	0.986713	0.496042

For best RF model gas data, OOB score for 0.90 is a good result. Avg. validation R^2 is 0.49 is not very good.