MSBA Team 7 Homework 4b

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Introduction to Business Analytics

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I. Data Exploration & Model Building

1. Data Exploration

To begin with we imported all the needed library and modules for this homework.

load libraries and modules

```
[ ]  import pandas as pd
     import numpy as np
     import matplotlib.pyplot as plt
     import seaborn as sns
     import pandas as pd
     from sklearn.model_selection import train_test_split # splits arrays or matrices into random train and test subsets
```

Then we imported the excel file using the read_excel() function.

```
[ ]  df = pd.read_excel("./HW4.xlsx", sheet_name=0, header=0)
     df.head(10)
```

	sequence_number	US	source_a	source_c	source_b	source_d	source_e	source_m	source_o	source_h	...	source_x	source_w	Freq	last_update_days_ago	1st_update_days_ago	Web order	Gender=male	Address_is_res	Purchase	Spending
0	1	1	0	0	1	0	0	0	0	0	...	0	0	2	3662	3662	1	0	1	1	127.87
1	2	1	0	0	0	0	1	0	0	0	...	0	0	0	2900	2900	1	1	0	0	0.00
2	3	1	0	0	0	0	0	0	0	0	...	0	0	2	3883	3914	0	0	0	1	127.48
3	4	1	0	1	0	0	0	0	0	0	...	0	0	1	829	829	0	1	0	0	0.00
4	5	1	0	1	0	0	0	0	0	0	...	0	0	1	869	869	0	0	0	0	0.00
5	6	1	0	0	0	0	0	0	0	0	...	0	0	1	1995	2002	0	0	1	0	0.06
6	7	1	0	0	0	0	0	0	0	0	...	0	1	2	1498	1529	0	0	1	0	0.06
7	8	1	0	0	1	0	0	0	0	0	...	0	0	1	3397	3397	0	1	0	0	0.08
8	9	1	1	0	0	0	0	0	0	0	...	0	0	4	525	2914	1	1	0	1	488.50
9	10	1	1	0	0	0	0	0	0	0	...	0	0	1	3215	3215	0	0	0	1	173.50

10 rows × 25 columns

We wanted to understand the distribution of our data better so we explored the data by looking at the summary statistics to get the min/max/mean/stdv information using summary_stats. We also explored the column data types, and the target variable distribution.

```
[ ]  # Describe the data for central tendency and other statistical descriptions
     # for display/output format purpose we turn the descriptions result into a dataframe so that we can see the results for each column
     summary_stats = pd.DataFrame(df.describe())
     print(summary_stats[summary_stats.columns[:15]])
     print(summary_stats[summary_stats.columns[15:]])
```

```
       sequence_number           US     source_a     source_c     source_b  \
count      2000.000000  2000.000000  2000.000000  2000.000000  2000.000000
mean       1000.500000     0.824500     0.126500     0.056000     0.060000
std         577.494589     0.380489     0.332495     0.229979     0.237546
min           1.000000     0.000000     0.000000     0.000000     0.000000
25%         500.750000     1.000000     0.000000     0.000000     0.000000
50%        1000.500000     1.000000     0.000000     0.000000     0.000000
75%        1500.250000     1.000000     0.000000     0.000000     0.000000
max        2000.000000     1.000000     1.000000     1.000000     1.000000

          source_d     source_e     source_m     source_o     source_h  \
count  2000.000000  2000.000000  2000.00000  2000.000000  2000.000000
mean      0.041500     0.151000     0.01650     0.033500     0.052500
std       0.199493     0.358138     0.12742     0.179983     0.223089
min       0.000000     0.000000     0.00000     0.000000     0.000000
25%       0.000000     0.000000     0.00000     0.000000     0.000000
50%       0.000000     0.000000     0.00000     0.000000     0.000000
75%       0.000000     0.000000     0.00000     0.000000     0.000000
max       1.000000     1.000000     1.00000     1.000000     1.000000

          source_r     source_s     source_t     source_u     source_p  \
count  2000.000000  2000.000000  2000.00000  2000.000000  2000.000000
mean      0.068500     0.047000     0.02150     0.119000     0.006000
std       0.252665     0.211692     0.14508     0.323869     0.077246
min       0.000000     0.000000     0.00000     0.000000     0.000000
25%       0.000000     0.000000     0.00000     0.000000     0.000000
50%       0.000000     0.000000     0.00000     0.000000     0.000000
75%       0.000000     0.000000     0.00000     0.000000     0.000000
max       1.000000     1.000000     1.00000     1.000000     1.000000
          source_x     source_w         Freq  last_update_days_ago  \
count  2000.000000  2000.000000  2000.000000           2000.000000
mean      0.018000     0.137500     1.417000           2155.101000
std       0.132984     0.344461     1.405738           1141.302846
min       0.000000     0.000000     0.000000              1.000000
25%       0.000000     0.000000     1.000000           1133.000000
50%       0.000000     0.000000     1.000000           2280.000000
75%       0.000000     0.000000     2.000000           3139.250000
max       1.000000     1.000000    15.000000           4188.000000

       1st_update_days_ago    Web order  Gender=male  Address_is_res  \
count          2000.000000  2000.000000  2000.000000     2000.000000
mean           2435.601500     0.426000     0.524500        0.221000
std            1077.872233     0.494617     0.499524        0.415024
min               1.000000     0.000000     0.000000        0.000000
25%            1671.250000     0.000000     0.000000        0.000000
50%            2721.000000     0.000000     1.000000        0.000000
75%            3353.000000     1.000000     1.000000        0.000000
max            4188.000000     1.000000     1.000000        1.000000

          Purchase     Spending
count  2000.000000  2000.000000
mean      0.500000   102.560745
std       0.500125   186.749816
min       0.000000     0.000000
25%       0.000000     0.000000
50%       0.500000     1.855000
75%       1.000000   152.532500
max       1.000000  1500.060000
```

This dataset contains 2000 entries and 25 variables. Our target variable for this task is Spending. There are no missing values for this task and the variables for this task are all numeric: besides spending target variable which is of float data type, all the others are of integer type.

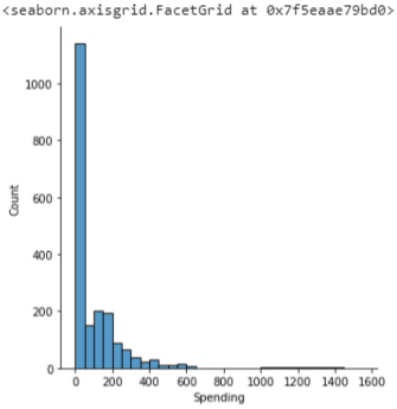
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2000 entries, 0 to 1999
Data columns (total 25 columns):
 #   Column                Non-Null Count  Dtype
---  ------                --------------  -----
 0   sequence_number       2000 non-null   int64
 1   US                    2000 non-null   int64
 2   source_a              2000 non-null   int64
 3   source_c              2000 non-null   int64
 4   source_b              2000 non-null   int64
 5   source_d              2000 non-null   int64
 6   source_e              2000 non-null   int64
 7   source_m              2000 non-null   int64
 8   source_o              2000 non-null   int64
 9   source_h              2000 non-null   int64
 10  source_r              2000 non-null   int64
 11  source_s              2000 non-null   int64
 12  source_t              2000 non-null   int64
 13  source_u              2000 non-null   int64
 14  source_p              2000 non-null   int64
 15  source_x              2000 non-null   int64
 16  source_w              2000 non-null   int64
 17  Freq                  2000 non-null   int64
 18  last_update_days_ago  2000 non-null   int64
 19  1st_update_days_ago   2000 non-null   int64
 20  Web order             2000 non-null   int64
 21  Gender=male           2000 non-null   int64
 22  Address_is_res        2000 non-null   int64
 23  Purchase              2000 non-null   int64
 24  Spending              2000 non-null   float64
dtypes: float64(1), int64(24)
memory usage: 390.8 KB
```

After visualizing the Spending target variable, we see that it is heavily skewed to the right with most of it clustering in the 0-50 bin.

```
sns.displot(df, x="Spending", binwidth=50)
```

```
<seaborn.axisgrid.FacetGrid at 0x7f5eaae79bd0>
```



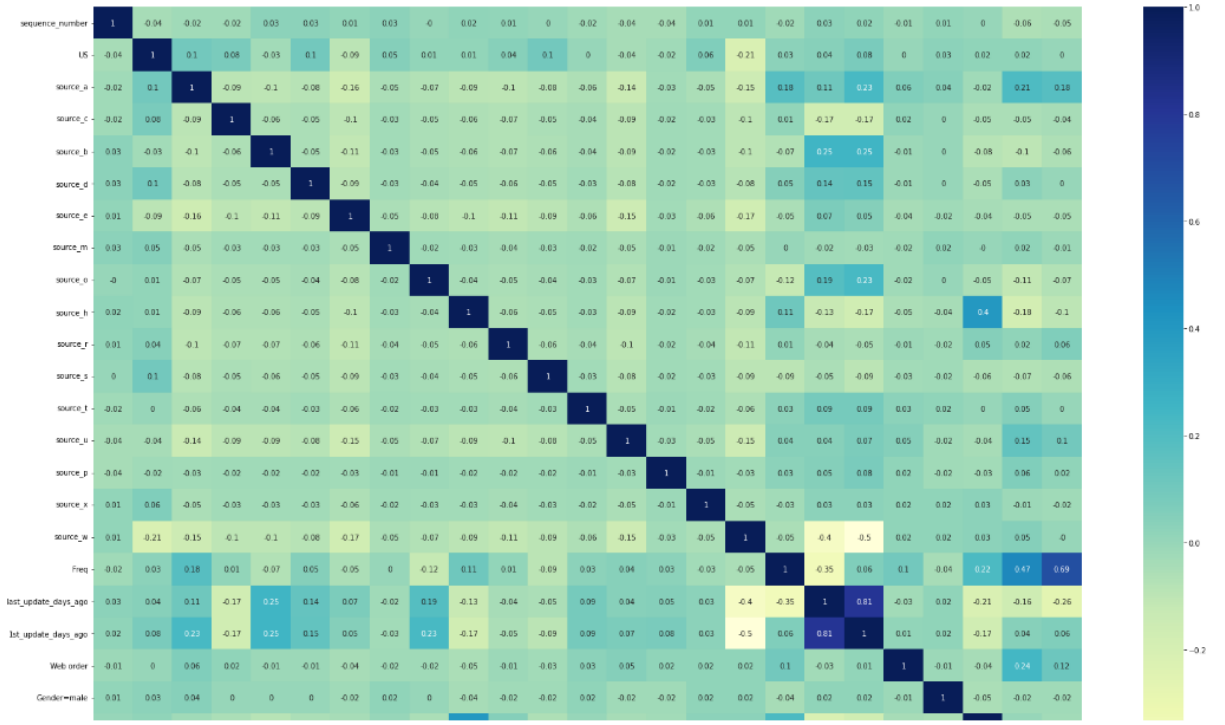
We created a correlation matrix to look at the relationship between all the features in the dataset. Seems spending has a relatively stronger correlation with Freq and Purchase. And 1st_update_days_ago and last_updated_days_ago has a strong correlation of 0.81.

```
# Correlation Matrix
plt.figure(figsize = (30,20))

p1 = round(df.corr(), 2)

sns.heatmap(p1,cmap="YlGnBu", annot=True)
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f67e7fd27d0>
```



2. Model Induction

a. Linear Regression Model

We set the attributes and target variable of 'Spending'. X is our attributes which are all the variables we use for prediction.

```
[ ]  from sklearn.model_selection import train_test_split
     X = df[df.columns[ df.columns != 'Spending']].values      # attributes
     y = df['Spending'].values                                 # target variable
```

The data is then fitted in a simple linear regression model using cross validation use a k set as 10. We use negative mean squared error to evaluate the generalization performance because the largest negative mse equals the smallest mse and that yields the best model

```
[5]  ################################## Fit Simple Linear Regression Model ##################################

     from sklearn.linear_model import LinearRegression     # ordinary least squares Linear Regression
     from sklearn.model_selection import cross_val_score, GridSearchCV   # evaluate a score by cross-validation

     # A linear regression with multiple features
     # multiple linear regression class
     mlr = LinearRegression(fit_intercept=True,            # whether to calculate the intercept for this model (true by default, otherwise data is expec
                            n_jobs=-1)                     # speedup computations by using multiple processors; -1 means use all processors
     mlr.fit(X, y)

     #Outer CV
     scores = cross_val_score(mlr,                                          # cross-validation scores
                              X,
                              y,
                              scoring='neg_mean_squared_error', # optimizes for MSE
                              cv=10)                                        # fit model to the data

     print(f"Slopes:\n {mlr.coef_}")                  # estimated coefficients for the linear regression model
     print(f"Intercept:\n {mlr.intercept_}")            # estimated intercept for the linear regression model
     print(f"\n Cross Validation Scores(neg_mean_squared_error):\n{scores}\n")
     print("\n Statistics of Cross Validation Performance: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std()*2)) # estimate mean and variance from cross
```

Interpretation of the result:

After cross validation we can see the coefficient and the intercept for our model as the attached snippet. The negative mean suquare is -15071.61 +/- 14313.32.

```
Slopes:
 [-4.56774359e-03 -7.40483130e+00 -3.50148285e+00 -5.63762559e+01
 -1.24245505e+01 -4.38189791e+01 -2.23893219e+01 -3.85902600e+01
  1.36402367e+01 -7.66059914e+01  1.61403016e+01 -2.16583335e+01
 -4.23863004e+01 -2.45448284e+00 -5.81550406e+01 -1.58703726e+01
 -2.12615622e+01  7.73611642e+01 -1.55763782e-02  5.82365505e-03
 -3.35465991e+00 -1.58239877e+00 -6.36110845e+01  9.17879335e+01]
Intercept:
 11.843131581078296

 Cross Validation Scores(R-squares):
[-13691.3433862  -34526.53238019 -16803.58093127 -11748.19567626
 -17323.62122884 -10962.28569609  -8928.96710438  -7663.55653107
 -13396.82094557 -15671.17351217]


 Statistics of Cross Validation Performance: -15071.61 (+/- 14313.32)
```

b. K-NN Model

We trained the Knn Model with all the default parameters with a Knn neighbor of 5, minkowski metric with a power parameter of 2, all processing parallel jobs, and set it to a similarity-moderated kNN.

```
[7] ######################################### Train the Model ############################################

    from sklearn import neighbors

    # KNeighborsRegressor is a numeric predictor implementing the k-nearest neighbors average.
    # Learn more about it here https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsRegressor.html

    # Set parameters of KNeighborsClassifier
    knnReg = neighbors.KNeighborsRegressor(n_neighbors=5, # n_neighbors is the k in the kNN
                           p=2,                   # power parameter for the Minkowski metric. We used p = 2,
                           metric='minkowski',    # the default metric is minkowski, which is a generalization of the Euclidean distance
                                                  # with p=2 is equivalent to the standard Euclidean distance.
                                                  # with p=1 is equivalent to the Mahattan distance.
                           n_jobs=-1,             # the number of parallel jobs to run for neighbors search. -1 means using all processors
                           weights='distance')    # We choose 'distance' because we wanted to apply a similarity-moderated kNN
    # Train the model
    knnReg.fit(X, y)

    ############################### CROSS VALIDATION FOR KNN ##############################################
    scores = cross_val_score(knnReg,                                    # cross-validation scores
                             X,
                             y,
                             scoring='neg_mean_squared_error', # optimizes for MSE
                             cv=10)                                     # fit model to the data

    print(f"\n Cross Validation Scores(neg_mean_squared_error):\n{scores}\n")
    print("\n Statistics of Cross Validation Performance: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std() * 2))
```

Interpretation of the Result:
The MSE is 29053.46 with a std of +/- 21725.64. We will compare the final performance in the comparison session.

```
 Cross Validation Scores(neg_mean_squared_error):
[-35669.82745479 -51945.57148689 -31072.34303898 -22319.26166525
 -39948.81146301 -21973.55085935 -18969.59455752 -12205.59779847
 -26346.43090974 -30083.64831465]


 Statistics of Cross Validation Performance: -29053.46 (+/- 21725.64)
```

c. Regression Tree

We built the regression tree using DecisionTreeRegressor with a random state of 42. WE fit the model using X, y. We did not specify a maximum depth, minimum sample split or leaf.

And then the cross_val_score to generate the cross-validation scores and optimize the model using mse.

```
[8] from sklearn.model_selection import cross_val_score, GridSearchCV
    from sklearn.tree import DecisionTreeRegressor

    # Instantiate the  decision tree regressor model
    regTree = DecisionTreeRegressor(random_state=42)

    # Train the model
    regTree.fit(X, y)

    scores = cross_val_score(regTree,                                    # cross-validation scores
                             X,
                             y,
                             scoring='neg_mean_squared_error', # optimizes for MSE
                             cv=10)                                      # fit model to the data

    print(f"\n Cross Validation Scores(neg_mean_squared_error):\n{scores}\n")
    print("\n Statistics of Cross Validation Performance: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std() * 2)) # estimate mean and variance from cross validation metrics
```

Interpretation of the Result:

Below are the 10 cross validation scores for each folds. The negative mean square is -26249.26 with a std of +/- 21266.94.

```
 Cross Validation Scores(neg_mean_squared_error):
[-25982.3305495 -40767.9388455 -20780.2035985 -20354.4770155
 -19551.0335405 -47667.9100685 -21663.130696   -9141.429277
 -32132.81665   -24451.302715 ]


 Statistics of Cross Validation Performance: -26249.26 (+/- 21266.94)
```

d. Comparison

We are comparing using the cross validation generalization performance using the negative mse. We want to find the largest negative value which means the lowest mse.

```
Statistics of Cross Validation Performance: -15071.61 (+/- 14313.32)
```

KNN regressor had a cross-validation performance of -29053.46 (+/-) 21725.64

```
 Statistics of Cross Validation Performance: -29053.46 (+/- 21725.64)
```

Regression tree had a cross-validation performance of -26249.26 (+/-) 21266.94

```
 Statistics of Cross Validation Performance: -26249.26 (+/- 21266.94)
```

The multivariate regression had the best performance for cross validation with the smallest absolute MSE value with the test data. It had a cross validation performance of -15071.61 (+/-) 14313.32.

II. IMPROVING THE MODELS' PERFORMANCE WITH FEATURE ENGINEERING

We looked closely at the dataset and we have decided to create some new features and remove irrelevant features. First, we have removed the sequence number because it is an index column presented as a feature. Second, we created new features from the last_update_days_ago and 1st_update_days_ago and the feature will be the difference between these two. We don't need to square it or apply the absolute because the feature can contain non-negative values.

```
[14] import numpy as np
     new_df = df
     new_df['days_until_update'] = np.log(df['1st_update_days_ago'] - df['last_update_days_ago']+1/3)
     new_df['last_update_days_ago'] = np.log(new_df['last_update_days_ago'])
     new_df = new_df.drop(['sequence_number', '1st_update_days_ago'], axis='columns')
     new_df.columns

     Index(['US', 'source_a', 'source_c', 'source_b', 'source_d', 'source_e',
            'source_m', 'source_o', 'source_h', 'source_r', 'source_s', 'source_t',
            'source_u', 'source_p', 'source_x', 'source_w', 'Freq',
            'last_update_days_ago', 'Web order', 'Gender=male', 'Address_is_res',
            'Purchase', 'Spending', 'days_until_update'],
           dtype='object')
```

We also realized that the target variable is right-skewed and we have log-transformed it. Below is the snippet of the code that does the feature engineering. We did the train test split because in the following we may need to use the test set again just to compare the generalization performance to the original scale. But we generated our main performance metrics negative MSE using cross validation.

```
[15] from sklearn.model_selection import train_test_split
     X = new_df[new_df.columns[ new_df.columns != 'Spending']].values      # attributes
     y = new_df['Spending'].values                                  # target variable.

     X_train, X_test, y_train, y_test = train_test_split(X,
                                                         y,
                                                         test_size = 0.3,
                                                         random_state=42)
```

```
y_log = np.log(y + 1/3)
```

1. Linear Regression built with the engineered features:

We optimated the performance first only with the updated log-transformed y. We used cross-validation method to build another model this time using y_log instead of y, below are the codes we wrote to fit the data and use cross_val_score to get the generalization performance. Like part a we still use negative mse to measure the performance. We also use coef_ and intercept_ to get the estimated coefficient and intercept.

```
[12] from sklearn.metrics import mean_absolute_error, mean_squared_error
     # A linear regression with multiple features
     # multiple linear regression class
     mlr = LinearRegression(fit_intercept=True,           # whether to calculate the intercept for this model (true by default, otherwise data is expected to be centered)
                            n_jobs=-1)                    # speedup computations by using multiple processors; -1 means use all processors
     mlr.fit(X, y_log)

     #Outer CV
     scores = cross_val_score(mlr,                                          # cross-validation scores
                              X,
                              y_log,
                              scoring='neg_mean_squared_error',             # optimizes for MSE
                              cv=10)                                        # fit model to the data

     print(f"Slopes:\n {mlr.coef_}")                  # estimated coefficients for the linear regression model
     print(f"Intercept:\n {mlr.intercept_}")            # estimated intercept for the linear regression model
     print(f"\n Cross Validation Scores(neg_mean_squared_error):\n{scores}\n")
     print("\n Statistics of Cross Validation Performance: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std()*2)) # estimate mean and variance from cross validation metrics
```

```
Slopes:
 [-7.47669916e-02  9.69730195e-02 -1.21867009e-01  4.55490947e-02
 -6.78771217e-03 -3.64179990e-02  3.24237686e-03 -1.83105554e-02
 -3.31628834e-01  4.49482093e-02 -1.60555568e-01 -2.44481110e-02
 -2.36471016e-02 -1.43965203e-01 -6.81910649e-02 -3.63332673e-02
  2.09968286e-01 -6.48596114e-02 -2.53821520e-02 -9.67969049e-03
 -1.47838989e-01  5.53718847e+00  3.14920305e-02]
Intercept:
 -0.5224052799313343

 Cross Validation Scores(neg_mean_squared_error):
[-0.26867163 -0.46840257 -0.28306759 -0.25736419 -0.33849702 -0.27778282
 -0.25002972 -0.25659741 -0.41991423 -0.34592955]


 Statistics of Cross Validation Performance: -0.32 (+/- 0.14)
```

It yielded a good performance so we will transform the y. In search to also improve the linear regression in terms of the Mean Squared Error, we have introduced using min-max scaling to standardize the data and the polynomial features in the model. We created a for loop to test whether when polynomial features change from 1, 2, 3, whether or not the generalization performance will change as well.

Below is the implementation of the new linear regression with polynomial features:

```
###################### Increasing Linear Regression Model Complexity    ######################
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import KFold

inner_cv = KFold(n_splits=5, random_state=42, shuffle=True)
params = {'fit_intercept': [True, False]}

#normalize data with min max scaling
sc = MinMaxScaler(feature_range=(0, 1))
sc.fit(X)                               # scaling parameters to be learned for later scaling

x_scaled = sc.transform(X)
x_sc = pd.DataFrame(x_scaled)


# Inner CV
mlr_poly = GridSearchCV(LinearRegression(),
                        params,
                        cv=inner_cv,
                        scoring='neg_mean_squared_error',             # optimizes for MSE (see note below)
                        n_jobs=-1)

for i in range(1,4):
    poly = PolynomialFeatures(degree=i)     # degree of polynomial features (degree=3)
    X_poly = poly.fit_transform(x_sc)
    mlr_poly.fit(X_poly,y_log)

    print(f"\n POLYNOMIAL FEATURES: {i} \n========================")
    print(mlr_poly.best_score_)
    print(mlr_poly.best_params_)
    print(mlr_poly.best_estimator_)

    # Outer CV
    nested_score_mlr_poly = cross_val_score(mlr_poly,
                                    X=X_poly,
                                    y=y_log,
                                    scoring='neg_mean_squared_error', # optimizes for MSE (see note below)
                                    cv=10)
    print("Nested neg_mean_squared_error value is: ", nested_score_mlr_poly.mean(), " +/- ", 2*nested_score_mlr_poly.std()) # estimate mean and 2*std from cross validation metrics
```

Result

```
 POLYNOMIAL FEATURES: 1
========================
-0.3164266567500608
{'fit_intercept': False}
LinearRegression(fit_intercept=False)
Nested neg_mean_squared_error value is:  -0.31662567259381946  +/-  0.143564152997299

 POLYNOMIAL FEATURES: 2
========================
-1.2888295336883152e+20
{'fit_intercept': False}
LinearRegression(fit_intercept=False)
Nested neg_mean_squared_error value is:  -1.8436080495744444e+20  +/-  1.079765540609907e+21

 POLYNOMIAL FEATURES: 3
========================
-626659855.7850544
{'fit_intercept': False}
LinearRegression(fit_intercept=False)
Nested neg_mean_squared_error value is:  -1.1597320011260398e+22  +/-  5.824768034778826e+22
```

In the above screenshot, the linear regression model with polynomial features has outperformed the linear regression presented in Section I.5 of this report but it has not made an improvement in terms of

either MSE or MAE compared to the model built after features engineering. In addition, when the features include cubic features, the variance explodes and we get a very big MSE that cannot be displayed by the personal computer. Yet due to the MSE is not in the same scale of the part A model, we can only use train test split to generate it back to the original scale using the below code.

```
#normalize data with min max scaling
sc = MinMaxScaler(feature_range=(0, 1))
sc.fit(X_train)                                 # scaling parameters to be learned for later scaling

x_train_scaled = sc.transform(X_train)          # scaling of features in train data
x_train_sc = pd.DataFrame(x_train_scaled)       # constructing dataFrame

x_test_scaled = sc.transform(X_test)            # scaling of features in test data
x_test_sc = pd.DataFrame(x_test_scaled)         # constructing dataFrame
```

```
################################ FINAL EVALUATION ON THE TEST DATA  ########################################
#-------------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n==========================================================")
y_train_pred = np.exp(mlr_poly.predict(X_poly)) - 1/3                       # apply model to train data (in sample performance)
y_test_pred = np.exp(mlr_poly.predict(poly.fit_transform(X_test))) - 1/3    # apply model to test data with the polynomial features (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
        mean_squared_error(y_train, y_train_pred),
        mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
        mean_absolute_error(y_train, y_train_pred),
        mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
```

```
GENERAL PERFORMANCE EVALUATION
==========================================================
MSE train: 15877.895, MSE test: 15804.910
MAE train: 47.888, MAE test: 49.399
```

This feature engineering has improved the Linear Regression model in terms of Mean Absolute Error, which dropped from 67.28 to 49.4, in generalization performance evaluated on out-of-sample data (test data). However, it has not made an improvement on the Mean Squared Error on either in-sample, or out-of-sample performance.

2. **kNN Regressor built with the engineered features:**

The kNN model is very sensitive to scale. In the KNN model, if the features are not scaled the same, the scale factor will dominate the model and hence the generalization performance will suffer. Therefore, we have scaled the data for KNN and used the newly engineered features. And we built the model using nested-cross validation technique to optimize the parameters. Below are the implementation and the results.

Below is the model induction and the results:

```
################################### Optimize kNN Regressor Example      ###################################
# Pipeline of transforms with a final estimator
from sklearn.neighbors import KNeighborsRegressor
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV, KFold
from sklearn.preprocessing import MinMaxScaler
from math import sqrt
import numpy as np


# KFold splits dataset into k consecutive folds (without shuffling by default)
inner_cv = KFold(n_splits=10, shuffle=True)
outer_cv = KFold(n_splits=10, shuffle=True)

#normalize data with min max scaling
sc = MinMaxScaler(feature_range=(0, 1))
sc.fit(X)                                  # scaling parameters to be learned for later scaling

x_scaled = sc.transform(X)
x_sc = pd.DataFrame(x_scaled)


#3NN regressor
knn_regressor = neighbors.KNeighborsRegressor(n_neighbors = 8, p=2)     # euclidean_distance for p = 2

#Fit and Evaluate Model
knn_regressor.fit(x_sc, y)        # fit the model
#pred=knn_regressor.predict(x_test_sc)         # make prediction on test set
#error = sqrt(mean_squared_error(y_test,np.exp(pred)-1/3)) # calculate rmse on test set

#print('RMSE value is:', error)

# Outer CV
nested_score_knn = cross_val_score(knn_regressor,
                                   X=x_sc,
                                   y=y_log,
                                   scoring='neg_mean_squared_error', # optimizes for MSE (see note below)
                                   cv=outer_cv)

print("Nested neg_mean_squared_error value is: ", nested_score_knn.mean(), " +/- ", nested_score_knn.std())

#np.exp(nested_score_knn.mean()) -1/3, " +/- ", (np.exp(nested_score_knn.std()) - 1/3)*2)
```

```
Nested neg_mean_squared_error value is:  -0.6396415639955297  +/-  0.10148656647261313
```

After cross validation, we get an MSE is 0.63 +/- 0.1014. Yet due to the MSE is not in the same scale of the part a model, we can only use train test split to generate it back to the original scale using the below code.

```
#3NN regressor
knn_regressor = neighbors.KNeighborsRegressor(n_neighbors = 8, p=2)     # euclidean_distance for p = 2

#Fit and Evaluate Model
knn_regressor.fit(x_train_sc, y_train_log)        # fit the model
pred=knn_regressor.predict(x_test_sc)         # make prediction on test set
error = sqrt(mean_squared_error(y_test,np.exp(pred)-1/3)) # calculate rmse on test set

print('RMSE value is:', error)
```

```
################################ FINAL EVALUATION ON THE TEST DATA  ########################################
#-------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n=====================================================")
y_train_pred = np.exp(knn_regressor.predict(x_train_sc)) - 1/3                    # apply model to train data (in sample performance)
y_test_pred = np.exp(knn_regressor.predict(x_test_sc)) - 1/3        # apply model to test data (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
       mean_squared_error(y_train, y_train_pred),
       mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                                  # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
       mean_absolute_error(y_train, y_train_pred),
       mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                       # y_test_pred: Estimated target values
```

```
GENERAL PERFORMANCE EVALUATION
=====================================================
MSE train: 21556.789, MSE test: 22710.619
MAE train: 55.809, MAE test: 62.027
```

These results were an improvement to the kNN regression generalization performance in terms of both MSE and MAE. Below is the generalization performance comparison for the two models

Before	Now
MSE train: 0.000, test: 29513.228 MAE train: 0.000, test: 99.403	MSE train: 21556.789, MSE test: 22710.619 MAE train: 55.809, MAE test: 62.027

This comparison shows that the kNN was overfitting before and now, the feature engineering has solved the issue.

3. Regression Tree built with the engineered features:

For this regression tree, we have used the newly engineered features as described above, and the scaled dataset as the input for our cross validation.

```
[27] ################################### Regressor Tree - Nested CV     ###################################

     # Find optimal paramater for DecisionTreeRegressor with GridSearchCV
     from sklearn.model_selection import KFold
     from sklearn.tree import DecisionTreeRegressor

     # KFold splits dataset into k consecutive folds (without shuffling by default)
     inner_cv = KFold(n_splits=10, shuffle=True, random_state=42)
     outer_cv = KFold(n_splits=10, shuffle=True, random_state=42)

     # Find the max_depth and max_features that minimizes MSE
     # Inner CV
     dt = DecisionTreeRegressor(random_state=42)
     dt.fit(x_sc, y_log)                                # fit model

     # Outer CV
     nested_score_dt = cross_val_score(dt,
                                       X=x_sc,
                                       y=y_log,
                                       scoring='neg_mean_squared_error', # optimizes for MSE (see note below)
                                       cv=outer_cv)
     print("Nested MSE value for log-transofrmed data is: ", nested_score_dt.mean(), " +/- ", nested_score_dt.std()*2)
```

```
Nested MSE value for log-transofrmed data is:  -0.5510108963682656  +/-  0.10999716507347168
```

The mse value for log transformed data is 0.55 +/- 0.1099. And because it is not of the same scale, we again use the generalization performance of the test dataset to compare with the original dataset.

```
################################ FINAL EVALUATION ON THE TEST DATA  ##########################################
#-------------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n==================================================")
y_train_pred = np.exp(dt.predict(x_train_sc)) - 1/3                          # apply model to train data (in sample performance)
y_test_pred = np.exp(dt.predict(x_test_sc)) - 1/3         # apply model to test data (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
        mean_squared_error(y_train, y_train_pred),
        mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                           # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
        mean_absolute_error(y_train, y_train_pred),
        mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                           # y_test_pred: Estimated target values
```

```
Nested MSE value for log-transofrmed data is:  -0.587154554315627  +/-  0.3899066597628915
GENERAL PERFORMANCE EVALUATION
==================================================
MSE train: 1.125, MSE test: 24919.922
MAE train: 0.040, MAE test: 66.612
```

This result shows the improvement of the decision tree after the feature engineering. Below is the comparison of train test the before and after feature engineering.

Before

```
MSE train: 0.000, test: 30104.140
MAE train: 0.000, test: 70.609
```

Now

```
MSE train: 1.125, MSE test: 24919.922
MAE train: 0.040, MAE test: 66.612
```

4. **Generalization performance with features engineering.**

Because after normalization using min-max scaling and log transformation, the performance of each individual models are of different scale, so we use the MSE for each of the model to compare the performance.

Linear Regression has improved in its general performance in terms of MAE but it has slightly suffered in terms of MSE which we wanted to optimize. Feature engineering has not helped linear regression. While this can be due to some other reasons, the tentative reason is that our dataset contained a lot of binary explanatory variables. Even after feature engineering, these variables were still categorical(binary) and hence still not a good variable to choose for linear regression that predicts numerical/continuous value.

In k-Nearest Neighbors Regression, the generalization significantly improved in both MSE and MAE. This is what we expected for a kNN regressor because KNN is very sensitive to the scaling factor that we tackled with feature engineering. In part (I), on the test dataset, MSE test: 29513.228, MAE test: 99.403 and after feature engineering we had MSE test: 22710.619, MAE test: 62.027. This is a significant improvement that feature engineering has brought to the performance of kNN regression. Both kNN modes were trained with 8 nearest neighbors and minkowski distance and the rest of the parameters were left to take default values.

Decision Tree Regressor has also achieved a huge improvement after the feature engineering. The generalization performance was as follows, MSE test: 30104.140, MAE test: 70.609 and after the feature engineering the generalization performance was as follows: MSE test: 24919.922, MAE test: 66.612. This was also a significant improvement. Both of the above regression trees were trained on default parameters with only random forest enforced to be 42.

III. OPTIMIZING THE MODELS' PERFORMANCE WITH PARAMETER TUNING

1. Linear Regression built with parameter tuning:

```
from sklearn.metrics import mean_absolute_error, mean_squared_error
# A linear regression with multiple features
# multiple linear regression class

inner_cv = KFold(n_splits=10, shuffle=True, random_state=42)
parameters={'fit_intercept':[True, False]}
           #'normalize':[True, False]}  #This parameter is ignored when fit_intercept is set to False.
                                        # If True, the regressors X will be normalized before regression by subtracting the mean and dividing by the l2-norm.

mlr = GridSearchCV(LinearRegression(n_jobs=-1),  # GridSearchCV
                   parameters,
                   scoring='neg_mean_squared_error',             # optimizes for MSE
                   n_jobs=4,
                   cv=inner_cv)

mlr.fit(X_train, y_train_log)

#Outer CV
scores = cross_val_score(mlr,                                          # cross-validation scores
                         X_train,
                         y_train_log,
                         cv=10)                                      # fit model to the data

mlr = mlr.best_estimator_
print(f"Slopes:\n {mlr.coef_}")                  # estimated coefficients for the linear regression model
print(f"Intercept:\n {mlr.intercept_}")            # estimated intercept for the linear regression model
print(f"\n Cross Validation Scores(R-squares):\n{scores}\n")
print("\n Statistics of Cross Validation Performance: %0.2f (+/- %0.2f)" % (scores.mean(), scores.std()*2)) # estimate mean and variance from cross validation metrics

################################## FINAL EVALUATION ON THE TEST DATA  ###########################################
#-------------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n=====================================================")
y_train_pred = np.exp(mlr.predict(X_train)) - 1/3                  # apply model to train data (in sample performance)
y_test_pred = np.exp(mlr.predict(X_test)) - 1/3                    # apply model to test data (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
        mean_squared_error(y_train, y_train_pred),
        mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
        mean_absolute_error(y_train, y_train_pred),
        mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
```

```
Slopes:
 [-7.09092798e-02  9.61846804e-02 -1.49290821e-01  2.74652949e-02
 -2.17630856e-02 -5.68251469e-02 -1.35239749e-02 -2.59919958e-02
 -3.34595814e-01  4.87361281e-02 -2.23708107e-01  2.88278224e-02
 -7.29000950e-02 -1.86521219e-01 -5.87545987e-02 -1.78370053e-02
  2.04283940e-01 -6.34732750e-02 -1.09952308e-02 -5.08563129e-03
 -1.52331042e-01  5.50838185e+00  3.62623253e-02]
Intercept:
 -0.5284955790794803

 Cross Validation Scores(R-squares):
[-0.35882675 -0.29797386 -0.3931856  -0.27323076 -0.35558566 -0.33099814
 -0.15321666 -0.35889326 -0.34347557 -0.33582459]


 Statistics of Cross Validation Performance: -0.32 (+/- 0.13)
GENERAL PERFORMANCE EVALUATION
==================================================
MSE train: 15877.895, MSE test: 15804.910
MAE train: 47.888, MAE test: 49.399
```

This parameter tuning has not improved the Linear Regression model performance in terms of Mean Absolute Error or Mean Squared error in either in-sample or out-of-sample performance.

2. **kNN Regressor built with parameter tuning:**

```
################################### Optimize kNN Regressor Example      ###################################
# Pipeline of transforms with a final estimator
from sklearn.neighbors import KNeighborsRegressor
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV, KFold


# KFold splits dataset into k consecutive folds (without shuffling by default)
inner_cv = KFold(n_splits=5, shuffle=True)
outer_cv = KFold(n_splits=5, shuffle=True)


params = {'knn__n_neighbors':[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15],
          'knn__p':[1,2]}                                   # when p = 1, this is equivalent to using manhattan_distance (l1),
                                                            # and euclidean_distance for p = 2
pipe = Pipeline([
        ('knn', KNeighborsRegressor())
      ])

# Inner CV
knn2_optk = GridSearchCV(pipe,
                         params,
                         cv=inner_cv,
                         scoring='neg_mean_squared_error',              # optimizes for MSE (see note below)
                         n_jobs=-1)
knn2_optk.fit(X_train,y_train_log)

print(knn2_optk.best_score_)
print(knn2_optk.best_params_)
print(knn2_optk.best_estimator_)

print('Non-nested R-squared value is:', knn2_optk.best_score_)

# Outer CV
nested_score_knn2_optk = cross_val_score(knn2_optk,
                                         X=X_train,
                                         y=y_train_log,
                                         scoring='neg_mean_squared_error', # optimizes for MSE
                                         cv=outer_cv)
print("Nested R-squared value is: ", nested_score_knn2_optk.mean(), " +/- ", nested_score_knn2_optk.std()*2)

################################ FINAL EVALUATION ON THE TEST DATA  ########################################
#-------------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n====================================================")
y_train_pred = np.exp(knn2_optk.predict(X_train)) - 1/3                  # apply model to train data (in sample performance)
y_test_pred = np.exp(knn2_optk.predict(X_test)) - 1/3                    # apply model to test data (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
        mean_squared_error(y_train, y_train_pred),
        mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
        mean_absolute_error(y_train, y_train_pred),
        mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                                   # y_test_pred: Estimated target values
```

```
-1.2334203025984045
{'knn__n_neighbors': 6, 'knn__p': 1}
Pipeline(steps=[('knn', KNeighborsRegressor(n_neighbors=6, p=1))])
Non-nested R-squared value is: -1.2334203025984045
Nested R-squared value is:  -1.2834325552159722  +/-  0.19344473120113967
GENERAL PERFORMANCE EVALUATION
====================================================
MSE train: 13562.701, MSE test: 17717.465
MAE train: 47.452, MAE test: 56.164
```

These results were an improvement to the kNN regression generalization performance in terms of both MSE and MAE. Below is the generalization performance comparison for the two models

Before	Now
MSE train: 21556.789, MSE test: 22710.619 MAE train: 55.809, MAE test: 62.027	MSE train: 13562.701, MSE test: 17717.465 MAE train: 47.452, MAE test: 56.164

3. **Regression Tree built with parameter tuning:**

```
################################## Regressor Tree - Nested CV      ##################################

# Find optimal paramater for DecisionTreeRegressor with GridSearchCV
from sklearn.model_selection import GridSearchCV, KFold
from sklearn.tree import DecisionTreeRegressor

# KFold splits dataset into k consecutive folds (without shuffling by default)
inner_cv = KFold(n_splits=10, shuffle=True, random_state=42)
outer_cv = KFold(n_splits=10, shuffle=True, random_state=42)

# Find the max_depth that minimizes MSE
# Inner CV
parameters = {'max_depth': range(3,20),                    # range of parameters for the depth of the tree
              'max_features':range(1, new_df.shape[1])}           # Try enforcing number of max features contributing to the decision tree
gs_dt = GridSearchCV(DecisionTreeRegressor(random_state=42),  # GridSearchCV
                     parameters,
                     scoring='neg_mean_squared_error', # optimizes for MSE+
                     n_jobs=4,
                     cv=inner_cv)
gs_dt.fit(X_train, y_train_log)                               # fit model

gs_dt = gs_dt.fit(X_train,y_train_log)
print(" Parameter Tuning")
print("Non-nested Performance: ", gs_dt.best_score_)
print("Optimal Parameter: ", gs_dt.best_params_)    # parameter setting that gave the best results on the inner cross-validation
print("Optimal Estimator: ", gs_dt.best_estimator_) # estimator that was chosen by the search, i.e. estimator which gave best score

# Outer CV
nested_score_gs_dt = cross_val_score(gs_dt,        # estimate generalization performance (outer cross-validation)
                                     X=X_train,
                                     y=y_train_log,
                                     scoring='neg_mean_squared_error', # optimizes for MSE+
                                     cv=outer_cv)
print("Nested CV Performance: ",nested_score_gs_dt.mean(), " +/- ", nested_score_gs_dt.std())

################################ FINAL EVALUATION ON THE TEST DATA  ########################################
#-------------------------------------------------------------------------------------------------------------
print("GENERAL PERFORMANCE EVALUATION\n=====================================================")
y_train_pred = np.exp(gs_dt.predict(X_train)) - 1/3                  # apply model to train data (in sample performance)
y_test_pred = np.exp(gs_dt.predict(X_test)) - 1/3                    # apply model to test data (out of sample performance)

print('MSE train: %.3f, MSE test: %.3f' % ( # mean_absolute_error
       mean_squared_error(y_train, y_train_pred),
       mean_squared_error(y_test, y_test_pred)))  # y_test: Ground truth (correct) target values
                                                  # y_test_pred: Estimated target values
print('MAE train: %.3f, MAE test: %.3f' % ( # mean_squared_error
       mean_absolute_error(y_train, y_train_pred),
       mean_absolute_error(y_test, y_test_pred))) # y_test: Ground truth (correct) target values
                                                  # y_test_pred: Estimated target values
```

```
 Parameter Tuning
Non-nested Performance:  -0.3238884409117332
Optimal Parameter:  {'max_depth': 5, 'max_features': 14}
Optimal Estimator:  DecisionTreeRegressor(max_depth=5, max_features=14, random_state=42)
Nested CV Performance:  -0.3438943686361674  +/-  0.08957798534080867
GENERAL PERFORMANCE EVALUATION
=====================================================
MSE train: 12705.363, MSE test: 16129.248
MAE train: 45.467, MAE test: 49.821
```

For this regression tree, we have used the new tuned parameters as described above, and the scaled dataset.
This result does not show any improvement of the regression tree after the parameter tuning.

Before	Now
MSE train: 10612.008, MSE test: 16011.985 MAE train: 40.156, MAE test: 49.715	MSE train: 12705.363, MSE test: 16129.248 MAE train: 45.467, MAE test: 49.821

4. Results

The overall MSE and MAE are lowest for the linear regression model and thus, yields the best performance out of the 3 models.

Linear Regression:
MSE train: 15877.895, MSE test: 15804.910
MAE train: 47.888, MAE test: 49.399

kNN Regressor:
MSE train: 13562.701, MSE test: 17717.465
MAE train: 47.452, MAE test: 56.164

Regression Tree:
MSE train: 12705.363, MSE test: 16129.248
MAE train: 45.467, MAE test: 49.821