

Introduction to Business Data Analytics

Homework #4



(put your name above (incl. any nicknames))

| Total grade: | out of | _165 | _ points |
|--------------|--------|------|----------|
| | | | |
| | | | |
| | | | |

Please answer all the questions and submit your assignment as a single PDF by uploading it on Canvas.

1) (20 points) Assume that you built a model for predicting consumer credit ratings and evaluated it on the test dataset of 5 records. Based the following 5 actual and predicted credit ratings (see table below), calculate the following performance metrics for your model: MAE, MAPE, RMSE, and Average error.

| Actual Credit Rating | Predicted Credit Rating |
|-----------------------------|--------------------------------|
| 670 | 710 |
| 680 | 660 |
| 550 | 600 |
| 740 | 800 |
| 700 | 600 |

[4 points MAE – 1 point for formula and 3 points for correct application of formula

- 4 points MAPE- 1 point for formula and 3 points for correct application of formula
- 4 points RMSE-1 point for formula and 3 points for correct application of formula
- 4 points Average Error– 1 point for formula and 3 points for correct application of formula]

$$e_i = \hat{y} - y = p_i - a_i$$

$$(\mathbf{MAE}) = \frac{\sum_{i=1}^{n} |e_i|}{n}$$

MAE = (|710-670| + |660-680| + |600-550| + |800-740| + |600-700|) / 5 = (40+20+50+60+100) / 5 = 54

(MAPE) =
$$\frac{\sum_{i=1}^{n} |e_i/a_i|}{n}$$

MAPE = (40/670 + 20/680 + 50/550 + 60/740 + 100/700) / 5 = 8.08%

$$(\mathsf{RMSE}) = \sqrt{\frac{\sum_{i=1}^n e_i^2}{n}}$$

 $RMSE = SQRT((40^{2} + (-20)^{2} + 50^{2} + 60^{2} + (-100)^{2})/5) = SQRT((1600 + 400 + 2500 + 3600 + 10000)/5) = SQRT(3620) = 60.17$

Average error =
$$\frac{\sum_{i=1}^{n} e_i}{n}$$

Average Error = (40 + (-20) + 50 + 60 + (-100)) / 5 = 6

2) (145 points) Use numeric prediction techniques to build a predictive model for the HW4.xlsx dataset. This dataset is provided on Canvas and contains data about whether or not different consumers made a purchase in response to a test mailing of a certain catalog and, in case of a purchase, how much money each consumer spent. The data file has a brief description of all the attributes in a separate worksheet. We would like to build predictive models to predict how much will the customers spend; Spending is the target variable (numeric value: amount spent).

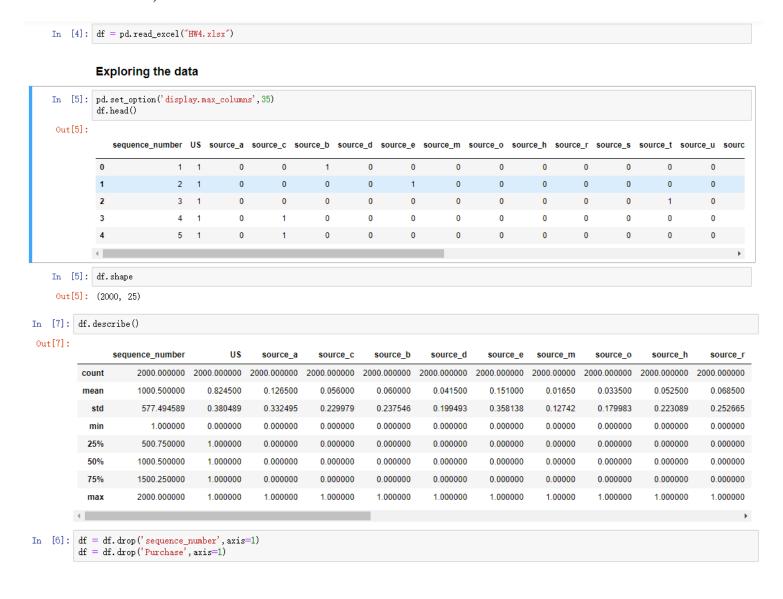
Use Python for this exercise.

Whenever applicable use random state 42 (10 points).

(a) (50 points) After exploring the data, build numeric prediction models that predict Spending. Use linear regression, k-NN, and regression tree techniques. Briefly discuss the models you have built. Use cross-validation with 10 folds to estimate the generalization performance. Present the results for each of the three techniques and discuss which one yields the best performance.

[part a is worth 50 points in total:

15 points for exploring the data (i.e., descriptive statistics including min max mean and stdv, visualizations, target variable distribution)

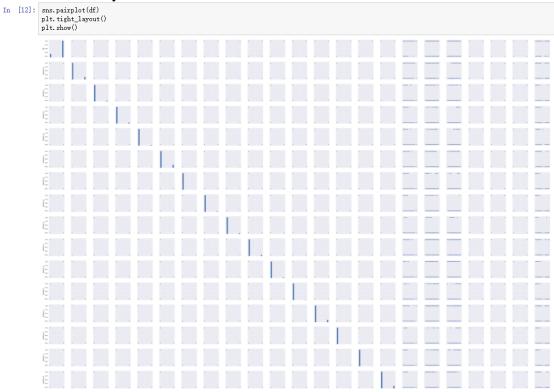


Drop the 'sequence_number' column because it's an ID column. Drop the 'Purchase' column because it's data leakage.

```
In [9]: df.shape
Out[9]: (2000, 23)
In [7]: df.isnull().sum(axis=0)
Out[7]: US
                                0
         source_a
                                0
         source_c
         source_b
                                0
         source_d
                                0
                                0
         source_e
                                0
         source_m
                                0
         source_o
                                0
         source_h
         source_r
                                0
         source_s
                                0
         source_t
                                0
         source_u
         source_p
                                0
         source_x
                                0
         source_w
         Freq
                                0
         last_update_days_ago
                                0
         1st_update_days_ago
                                0
         Web order
                                0
         \texttt{Gender=male}
                                0
         Address_is_res
                                0
                                0
         Spending
         dtype: int64
```

Check data.frame.shape after dropping two columns.

Check if there's any null data.



Visualization of pairplot of the data.frame.

```
[13]: cols = ['Freq', 'last_update_days_ago', 'lst_update_days_ago', 'Spending']
         {\tt sns.pairplot(df[cols])}
        plt.tight_layout()
plt.show()
                15
                10
            Freq
                0
         last_update_days_ago
          1500
         Spending
             1000
              500
                 0
                                                                                                                           1000
```

last_update_days_ago

1st_update_days_ago

Spending

Visualization of pairplot of 4 non-binary numeric variables.

Freq

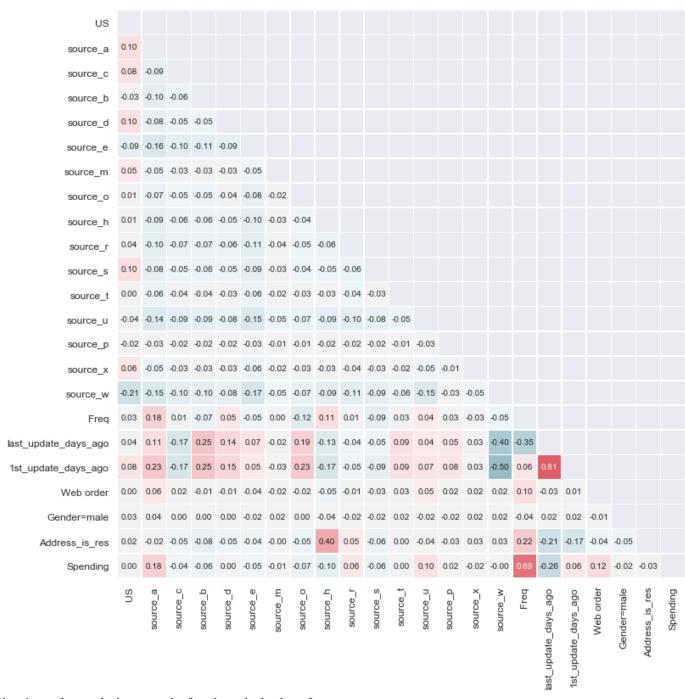
[17]: sns. distplot(df['Spending']) Out[17]: <matplotlib.axes._subplots.AxesSubplot at 0x2ef3e3837b8> 0.0175 0.0150 0.0125 0.0100 0.0075 0.0050 0.0025 0.0000 1000 0 250 500 750 1250 1500

Spending

Visualization of target variable distribution.

```
In [14]: #Correlation heatmap
          corr = df.corr()
          # Generate a mask for the upper triangle
          mask = np.zeros_like(corr, dtype=np.bool)
          mask[np.triu_indices_from(mask)] = True
          # Set up the matplotlib figure
          f, ax = plt.subplots(figsize=(15, 15))
          # Generate a custom diverging colormap
          cmap = sns.diverging_palette(220, 10, as_cmap=True)
          # Draw the heatmap with the mask and correct aspect ratio
          sns.heatmap(corr, mask=mask, cmap=cmap, vmax=1, vmin=-1, center=0,
                     square=True, linewidths=.5, cbar_kws={"shrink": .5}, annot=True, fmt='.2f')
                                                            - 1.00
                            1.00-0.35 0.06
                                                            - 0.75
                            -0.35 1.00 0.81 -0.26
  last_update_days_ago
                                                             0.50
                                                             0.25
                            0.06 0.81 1.00 0.06
  1st_update_days_ago
                                                             0.00
                                   -0.26 0.06
                Spending
                                                              -0.25
                                                  Spending
```

Visualization of correlation matrix for 4 non-binary numeric variables.



Visualization of correlation matrix for the whole data.frame.

10 points for correctly building linear regression model - provide screenshots and explain what you are doing and the corresponding results

Model Building

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import GridSearchCV, KFold

X= df.iloc[:,:-1].values
y= df.iloc[:,-1].values
ccv = KFold(n_splits=10, shuffle=True, random_state=42)
```

Set up X and y, specify random_state=42 for 10-fold cross validation.

Since my target variable "Spending" in this problem is numeric rather than categorical, I use Root Mean Squared Error (RMSE) to evaluate the performance of different models in terms of prediction error.

In addition, I use 10-fold cross validation to measure generalization performance.

X and y here are from original dataset after dropping 2 variables ('sequence_number', 'Purchase').

```
In [9]: ### Linear Regression
          np.random.seed(42)
          slr2 = LinearRegression()
          slr2.fit(X, y)
          scores = cross_val_score(slr2, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
          print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
          Cross-Validation RMSE: 127.75 (+/- 142.89)
 In [10]: ### Lasso Regression
            from sklearn.linear_model import Lasso # Lasso Regression class
            np.random.seed(42)
            lasso = Lasso(alpha=0.1, random_state=42)
            lasso.fit(X, y) # Fit model to data
            scores = cross_val_score(lasso, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
            print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
            Cross-Validation RMSE: 127.64 (+/- 143.00)
In [11]: ### Ridge Regression
          from sklearn.linear_model import Ridge
          np. random. seed (42)
          ridge = Ridge()
          ridge.fit(X, y) # Fit model to data
          scores = cross_val_score(ridge, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
          print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
          Cross-Validation RMSE: 127.74 (+/- 142.91)
```

For linear regression, I build 3 models, linear regression without penalty, lasso regression, and ridge regression. Their performance evaluated by 10-fold cross-validation are:

| | RMSE |
|---------------------|--------|
| Simple Linear | 127.75 |
| <u>Lasso Linear</u> | 127.64 |
| Ridge Linear | 127.74 |

Lasso Regression with alpha = 0.1 specified is slightly better than the other two models.

10 points for correctly building k-NN model - provide screenshots and explain what you are doing and the corresponding results

```
In [13]: ### kNW
from sklearn.neighbors import KNeighborsClassifier
from sklearn.preprocessing import StandardScaler
import warnings
warnings.filterwarnings("ignore")

np.random.seed(42)

sc = StandardScaler()
sc.fit(X)
X_scaled = sc.transform(X)

knn_regressor = neighbors.KNeighborsRegressor(n_neighbors=3)
knn_regressor.fit(X_scaled, y)

scores = cross_val_score(knn_regressor, X_scaled, y, cv=ccv, scoring = 'neg_mean_squared_error')

print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))

Cross-Validation RMSE: 150.54 (+/- 171.61)
```

For kNN model, I use StandardScaler() to standardize X into X_scaled. I then use X_scaled and y to train the model. In addition, I specify n_neighbors = 3 to make this kNN a 3NN model. The 10-fold cross-validation performance is RMSE = 150.54.

10 points for correctly building regression tree model - provide screenshots and explain what you are doing and the corresponding results

```
In [12]: ### Decision Tree from sklearn. tree import DecisionTreeRegressor #Documentation available here http://scikit-learn.org/stannp.random.seed(42)

tree = DecisionTreeRegressor(max_depth=3)
tree.fit(X, y)

scores = cross_val_score(tree, X, y, cv=ccv, scoring = 'neg_mean_squared_error')

print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))

Cross-Validation RMSE: 137.51 (+/- 165.45)
```

For regression tree model, I specify max_depth =3. The 10-fold cross-validation performance is RMSE = 137.51.

5 points for discussing which of the three models yields the best performance]

| | KIVISE |
|---------------------|--------|
| Simple Linear | 127.75 |
| <u>Lasso Linear</u> | 127.64 |
| Ridge Linear | 127.74 |
| <u>k-NN</u> | 150.54 |
| Regression Tree | 137.51 |

Compiling the RMSE results from previous models, I find that using 10-fold cross-validation, all of the three linear regression models perform better than k-NN and regression tree. However, within the three linear models, Lasso Regression wins slightly with an RMSE of 127.64. Thus, the best performing model in term of RMSE is Lasso Regression with 10-fold cross-validation and original dataset.

(b) (50 points) Engage in feature engineering (i.e., create new features based on existing features) to optimize the performance of linear regression, k-NN, and regression tree techniques. Present the results for each of the three techniques (choose the best performing model for each technique in case you try multiple models) and discuss which of the three yields the best performance. Use cross-validation with 10 folds to estimate the generalization performance. Discuss whether and why the generalization performance was improved or not.

[part a is worth 50 points in total:

10 points for correctly building the new linear regression model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [35]: from scipy.stats import skew
           df1 = df.copv()
           for i in [16, 17, 18, 22]:
              ori = skew(df1.iloc[:,i].values)
               log = skew(np.log(df1.iloc[:,i].values))
               sqrt = skew(np.sqrt(df1.iloc[:,i].values))
               cbrt = skew(np.cbrt(df1.iloc[:,i].values))
               square = skew(np.square(df1.iloc[:,i].values))
                exp = skew(np.exp(df1.iloc[:,i].values))
               cube = skew(np.power(df1.iloc[:,i].values,3))
               a = [ori, log, sqrt, cbrt, square, exp, cube]
               a = [our, logs, sqt, count, square, exp, count]
b = ['origin', 'log', 'sqrt', 'cbrt', 'square', 'exp', 'cube']
print(df1.columns[i])
               print('origin', ori)
               print(b[np.nanargmin(np.abs(a))], a[np.nanargmin(np.abs(a))])
               print()
           origin 2.978831957861886
           sqrt -0.0007524462984254756
           last update days ago
           origin -0.1877302916019205
           origin -0.1877302916019205
           1st update days ago
           origin -0.48919431348535225
           square 0.15425388263790038
           Spending
           origin 3.925494392575958
           cbrt 0.5102390986256735
```

Before I build any new model, I run a FOR loop to find the current skewness of 4 non-binary numeric variables in the dataset ('Freq', 'last_update_days_ago', '1st_update_days_ago', 'Spending') and the skewness after using log, sqrt, and cbrt. After the transformation of these 4 variables, the RMSEs of different models only get bigger. So I start to look for a new approach.

```
df1['period'] = df['1st_update_days_ago'] - df['last_update_days_ago']
df1['Ratio'] = df1['Freq'] / (df1['period']+0.00001)
df1.head()
   US source_a source_c source_b source_e source_m source_o source_h source_r source_t source_t source_u source_p source_x sou
                                          0
                                                   0
                                                             0
                                                                       0
                                                                                0
                                                                                         0
                                                                                                  0
                                                                                                           0
                                                                                                                                        0
              n
                       0
                                 0
                                          0
                                                   1
                                                             0
                                                                       0
                                                                                0
                                                                                         0
                                                                                                  0
                                                                                                           0
                                                                                                                     0
                                                                                                                              0
                                                                                                                                        0
                                                   0
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                                                                                                           0
                                                                                                                     0
                                                                                                                              0
                                                                                                                                        0
              0
              0
                                                   0
                                                                                                  0
                                                                                                                                        0
```

I first create a new variable 'period' to measure the difference between '1st_update_days_ago' and 'lsat_update_days_ago'. Then, I create another variable 'Ratio' to get 'Freq' per day. Here, due to a large number of zeros in 'period', I add 0.00001 to 'period' to avoid inf values in 'Ratio'.

```
In [90]: from sklearn.preprocessing import PolynomialFeatures
            o= df.iloc[:,:-1].values
            X= df1.iloc[:,np.r_[0:22,-1,-2]]
            y= df1.iloc[:,-3]
            quadratic = PolynomialFeatures(degree=2)
            cubic = PolynomialFeatures(degree=3)
            X_quad = quadratic.fit_transform(X)
            print (X. shape)
            print (X_quad. shape)
            (2000, 24)
            (2000, 325)
In [78]: ### Linear Regression
           np.random.seed(42)
           slr2 = LinearRegression()
            slr2.fit(X, y)
            s=cross_val_score(slr2, o, y, cv=ccv, scoring = 'neg_mean_squared_error')
            scores = cross_val_score(slr2, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
            scores2 = cross_val_score(slr2, X_quad, y, cv=ccv, scoring = 'neg_mean_squared_error')
           print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-s.mean()), np.sqrt(s.std()) * 2))
print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores2.mean()), np.sqrt(scores2.std()) * 2))
           Cross-Validation RMSE: 127.75 (+/- 142.89)
           Cross-Validation RMSE: 127.04 (+/- 141.92)
           Cross-Validation RMSE: 133.66 (+/- 140.69)
In [79]: ### Lasso Regression
            from sklearn.linear_model import Lasso # Lasso Regression class
            np.random.seed(42)
            lasso = Lasso()
            lasso.fit(X, y) # Fit model to data
            s=cross_val_score(lasso, o, y, cv=ccv, scoring = 'neg_mean_squared_error')
           scores = cross_val_score(lasso, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
scores2 = cross_val_score(lasso, X_quad, y, cv=ccv, scoring = 'neg_mean_squared_error')
           Cross-Validation RMSE: 127.77 (+/- 143.69)
            Cross-Validation RMSE: 127.04 (+/- 142.98)
            Cross-Validation RMSE: 127.83 (+/- 144.17)
```

```
In [80]: ### Ridge Regression
from sklearn.linear_model import Ridge

np.random.seed(42)
ridge = Ridge()
ridge.fit(X, y) # Fit model to data

s=cross_val_score(ridge, o, y, cv=ccv, scoring = 'neg_mean_squared_error')
scores = cross_val_score(ridge, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
scores2 = cross_val_score(ridge, X_quad, y, cv=ccv, scoring = 'neg_mean_squared_error')

print("Cross_validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-s.mean()), np.sqrt(s.std()) * 2))
print("Cross_validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))

Cross_validation RMSE: 127.74 (+/- 142.91)
Cross_validation RMSE: 127.02 (+/- 141.94)
Cross_validation RMSE: 127.03 (+/- 142.23)
```

For each model, it reports RMSE for original dataset, RMSE with 2 new variables ('period', 'Ratio'), and RMSE after quadratic transformation. Their performance evaluated by 10-fold cross-validation are:

| | Original RMSE | RMSE with 2 new variables | RMSE with quadratic transformation |
|---------------|------------------|---------------------------|------------------------------------|
| Simple Linear | 127.75 | 127.04 | 133.66 |
| Lasso Linear | 127.64 | 127.04 | 127.83 |
| Ridge Linear | 127.74 | 127.02 | 129.39 |

The best performance happens when using Ridge Regression and dataset with 2 new variables. The best performing RMSE is 127.02, better than the original RMSE.

10 points for correctly building the new k-NN model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [61]: ### kNW
          from sklearn.neighbors import KNeighborsClassifier
          from sklearn import neighbors
          from sklearn.preprocessing import StandardScaler
          import warnings
          warnings.filterwarnings("ignore")
          np.random.seed(42)
          sc = StandardScaler()
          sc.fit(o)
          knn_regressor = neighbors. KNeighborsRegressor (n_neighbors=3)
          knn_regressor.fit(X_scaled,y)
          scores = cross_val_score(knn_regressor, X_scaled, y, cv=ccv, scoring = 'neg_mean_squared_error')
          print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
          Cross-Validation RMSE: 150.54 (+/- 171.61)
 In [87]: ### kNW
           import warnings
           warnings.filterwarnings("ignore")
           np.random.seed(42)
           sc = StandardScaler()
           X_scaled = sc. transform(X)
           knn regressor = neighbors. KNeighborsRegressor(n neighbors=3)
           knn_regressor.fit(X_scaled,y)
           scores = cross_val_score(knn_regressor, X_scaled, y, cv=ccv, scoring = 'neg_mean_squared_error')
           print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
           Cross-Validation RMSE: 149.77 (+/- 172.37)
```

```
In [88]: ### kNW
import warnings
warnings.filterwarnings("ignore")

np.random.seed(42)

sc = StandardScaler()
sc.fit(X_quad)
    X_scaled = sc.transform(X_quad)

knm_regressor = neighbors.KNeighborsRegressor(n_neighbors=3)
knm_regressor.fit(X_scaled, y)

scores = cross_val_score(knm_regressor, X_scaled, y, cv=ccv, scoring = 'neg_mean_squared_error')
print("Cross_Validation RMSE: $0.2f (+/- $0.2f)" $ (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))

Cross_Validation RMSE: 151.07 (+/- 172.05)
```

Within all three k-NN models (original, original+2 new variables, original+2 new variables+quadratic transformed), the best performing model is the one with 2 new variables but not transformed quadratically. The best 10-fold cross-validation RMSE is 149.77, better than the original RMSE.

| | | RMSE with 2 | RMSE with |
|-------------|----------|-------------|----------------|
| | Original | new | quadratic |
| | RMSE | variables | transformation |
| <u>k-NN</u> | 150.54 | 149.77 | 151.07 |

10 points for correctly building the new regression tree model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [86]: ### Decision Tree
from sklearn. tree import DecisionTreeRegressor #Documentation available here http://scikit-learn.org/stable

np.random.seed(42)
tree = DecisionTreeRegressor(max_depth=3)
tree.fit(X, y)

s=cross_val_score(tree, o, y, cv=ccv, scoring = 'neg_mean_squared_error')
scores = cross_val_score(tree, X, y, cv=ccv, scoring = 'neg_mean_squared_error')
scores2 = cross_val_score(tree, X_quad, y, cv=ccv, scoring = 'neg_mean_squared_error')

print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-s.mean()), np.sqrt(s.std()) * 2))
print("Cross-Validation RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-scores.mean()), np.sqrt(scores.std()) * 2))
print("Cross-Validation RMSE: $0.2f (+/- %0.2f)" % (np.sqrt(-scores2.mean()), np.sqrt(scores2.std()) * 2))

Cross-Validation RMSE: 137.51 (+/- 165.45)
Cross-Validation RMSE: 134.68 (+/- 148.82)
Cross-Validation RMSE: 134.24 (+/- 167.05)
```

Within all three regression tree models (original, original+2 new variables, original+2 new variables+quadratic transformed), the best performing model is the one with 2 new variables and transformed quadratically. The best 10-fold cross-validation RMSE is 134.24, better than the original RMSE.

| | Original | RMSE with 2 new | RMSE with quadratic |
|-------------------|----------|-----------------------|---------------------|
| Daguagian | RMSE | variables | transformation |
| <u>Regression</u> | | | |
| <u>Tree</u> | 137.51 | 134.68 | 134.24 |

20 points for discussing if the generalization performance was improved or not for each of the techniques (linear regression, kNN, and regression tree) and justifying why it was improved or alternatively why it was not improved]

| | Original RMSE | RMSE with 2 new variables | RMSE with quadratic transformation |
|-----------------|------------------|---------------------------|------------------------------------|
| Simple Linear | 127.75 | 127.04 | 133.66 |
| Lasso Linear | 127.64 | 127.04 | 127.83 |
| Ridge Linear | 127.74 | 127.02 | 129.39 |
| <u>k-NN</u> | 150.54 | 149.77 | 151.07 |
| Regression Tree | 137.51 | 134.68 | 134.24 |

RMSE with 2 new variables ('period', 'Ratio'):

Under 10-fold cross-validation, all models have improvement in RMSE, although most of the improvements are limited (less than 1). For regression tree, the improvement is bigger (almost 3). This is because the 2 new variables capture more information from the original 3 variables ('Freq', '1st_update_days_ago', 'last_update_days_ago'). This increase in information helps models to predict more accurately.

RMSE with 2 new variables and quadratic transformation:

Under 10-fold cross-validation, most models have worse performance than original RMSE. This is probably because quadratic transformation generates redundant variables that affects the accuracy and robustness of the original model. However, for regression tree, RMSE with 2 new variables and quadratic transformation performs better than both original RMSE and RMSE with 2 new variables but without quadratic transformation. This is probably because that after quadratic transformation, the new model has more variables and information to perform more partition of the data to predict more accurately.

Overall, the best performing model is Ridge Regression with 2 new variables, yielding an RMSE of 127.02.

(c) (35 points) Engage in parameter tuning to optimize the performance of linear regression, k-NN, and regression tree techniques. Use cross-validations with 10 folds to estimate the generalization performance. Present the results for each of the three techniques and discuss which one yields the best performance.

[part a is worth 35 points in total:

10 points for correctly optimizing at least two parameters for linear regression model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [94]: inner_cv = KFold(n_splits=10, shuffle=True, random_state=42)
outer_cv = KFold(n_splits=10, shuffle=True, random_state=42)
```

Specify random_state = 42 for both inner_cv and outer_cv.

For all models, I use original dataset + 2 new variables as X. For the k-NN model, I then standardize X into X_std.

```
In [95]: gs_lasso = GridSearchCV(estimator=Lasso(
                                        random state=42),
                               param_grid=[{'alpha': [ 0.00001, 0.0001, 0.001, 0.01, 0.1 ,1 ,10 ,100, 1000, 10000, 100000, 1000000],
                                              'fit_intercept':['True','False']}],
                               scoring='neg_mean_squared_error',
                               cv=inner cv,
                               n_jobs=5)
           gs_lasso = gs_lasso.fit(X,y)
           print("\n Parameter Tuning #LASSO")
           print("Non-nested CV performance: ", gs_lasso.best_score_)
           print("Optimal Parameter: ", gs_lasso.best_params_)
print("Optimal Estimator: ", gs_lasso.best_estimator_) # Estimator that was chosen by the search, i.e. estimator which gave highes
           nested_score_gs_lasso = cross_val_score(gs_lasso, X=X, y=y, cv=outer_cv)
print("Nested CV performance: ", nested_score_gs_lasso.mean(), " +/- ", nested_score_gs_lasso.std())
           print("Nested CV RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-nested_score_gs_lasso.mean()), np.sqrt(nested_score_gs_lasso.std()) * 2))
            Parameter Tuning #LASSO
           Non-nested CV performance: -16106.355145865382
           Optimal Parameter: {'alpha': 0.1, 'fit_intercept': 'True'}
           Optimal Estimator: Lasso(alpha=0.1, copy_X=True, fit_intercept='True', max_iter=1000,
              normalize=False, positive=False, precompute=False, random_state=42,
              selection='cyclic', tol=0.0001, warm_start=False)
           Nested CV performance: -16106.355145865382 +/- 5046.510486052244
           Nested CV RMSE: 126.91 (+/- 142.08)
```

For the Lasso Model, optimal parameters are alpha = 0.1, fit_intercept = 'True'. The 10-fold cross-validation performance is RMSE = 126.91.

```
In [96]: gs_ridge = GridSearchCV(estimator=Ridge(
                                     random_state=42),
                            param_grid=[{'alpha': [ 0.00001, 0.0001, 0.001, 0.01, 0.1 ,1 ,10 ,100, 1000, 10000, 100000, 1000000],
                                          'fit_intercept':['True','False']}],
                            scoring='neg_mean_squared_error',
                            cv=inner_cv,
                            n jobs=5)
          gs_ridge = gs_ridge.fit(X,y)
          print("\n Parameter Tuning #LASSO")
          print("Non-nested CV performance: ", gs_ridge.best_score_)
          print("Optimal Parameter: ", gs_ridge.best_params_)
          print("O<mark>ptimal Estimator: ", gs_ridge.best_estimator_)</mark> # Estimator that was chosen by the search, i.e. estimator which gave highest score
          nested_score_gs_ridge = cross_val_score(gs_ridge, X=X, y=y, cv=outer_cv)
          print("Nested CV performance: ", nested_score_gs_ridge.mean(), " +/- ", nested_score_gs_ridge.std())
          print("Nested CV RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-nested_score_gs_ridge.mean()), np.sqrt(nested_score_gs_ridge.std()) * 2))
           Parameter Tuning #LASSO
          Non-nested CV performance: -16118.450916616299
          Optimal Parameter: {'alpha': 10, 'fit_intercept': 'True'}
          Optimal Estimator: Ridge(alpha=10, copy_X=True, fit_intercept='True', max_iter=None,
             normalize=False, random_state=42, solver='auto', tol=0.001)
          Nested CV performance: -16118.4509166163 +/- 5051.591188936467
          Nested CV RMSE: 126.96 (+/- 142.15)
```

For the Ridge Model, optimal parameters are alpha = 10, fit_intercept = 'True'. The 10-fold cross-validation performance is RMSE = 126.96.

10 points for correctly optimizing at least two parameters for linear k-NN model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [102]: sc = StandardScaler()
                sc.fit(X)
                X_std = sc. transform(X)
                gs_knn = GridSearchCV(estimator=neighbors.KNeighborsRegressor(
                                         metric='minkowski'),
param_grid=[{'n_neighbors': range(1,25),
                                                             'weights':['uniform','distance'],'p':[1,2]}],
                                         scoring='neg_mean_squared_error',
                                         cv=inner_cv,
                                         n_jobs=5)
                gs_knn = gs_knn.fit(X_std,y)
                print("Non-nested CV performance: ", gs_knn.best_score_)

print("Optimal Parameter: ", gs_knn.best_params_)

print("Optimal Estimator: ", gs_knn.best_estimator_) # Estimator that was chosen by the search, i.e. estimator which gave his
                nested_score_gs_kmn = cross_val_score(gs_kmn, N=N_std, y=y, cv=outer_cv)
print("Nested_CV performance: ",nested_score_gs_kmn.mean(), " +/- ", nested_score_gs_kmn.std())
print("Nested_CV RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-nested_score_gs_kmn.mean()), np.sqrt(nested_score_gs_kmn.std()) * 2))
                 Parameter Tuning #KNN
                Non-nested CV performance: -20040.605387697447
                Optimal Parameter: {'n_neighbors': 14, 'p': 2, 'weights': 'uniform'}
Optimal Estimator: KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
                             metric_params=None, n_jobs=None, n_neighbors=14, p=2,
                              weights='uniform')
                Nested CV performance: -20186.140538579803 +/- 6739.3885866555775
                Nested CV RMSE: 142.08 (+/- 164.19)
```

For the k-NN Model, optimal parameters are n_neighbors = 14, p = 2, weights = 'uniform'. The 10-fold cross-validation is RMSE = 142.08.

10 points for correctly optimizing at least two parameters for linear regression tree model and improving the performance as much as possible - provide screenshots and explain what you are doing and the corresponding results

```
In [101]: gs_dt = GridSearchCV(estimator=DecisionTreeRegressor(random_state=42, criterion='mse'),
                                      param_grid=[{'max_depth': [1,3,5,7,9,11,13]
                                                        'min_samples_leaf':[1,2,3,4,5]}],
                                      scoring='neg_mean_squared_error',
                                      cv=inner cv,
                                       n_jobs=5)
               gs_dt = gs_dt.fit(X,y)
              print("\n Parameter Tuning #DT")
print("Non-nested CV performance: ", gs_dt.best_score_)
               print("Optimal Parameter: ", gs_dt.best_params_)
print("Optimal Estimator: ", gs_dt.best_estimator_)
               nested_score_gs_dt = cross_val_score(gs_dt, X=X, y=y, cv=outer_cv)
               print("Nested CV performance: ",nested_score_gs_dt.mean(), " +/- ", nested_score_gs_dt.std())
print("Nested CV RMSE: %0.2f (+/- %0.2f)" % (np.sqrt(-nested_score_gs_dt.mean()), np.sqrt(nested_score_gs_dt.std()) * 2))
                Parameter Tuning #DT
               Non-nested CV performance: -17854.57881832836
              Optimal Parameter: {'max_depth': 5, 'min_samples_leaf': 5}
Optimal Estimator: DecisionTreeRegressor(criterion='mse', max_depth=5, max_features=None,
                             {\tt max\_leaf\_nodes=None,\ min\_impurity\_decrease=0.0,}
                             min_impurity_split=None, min_samples_leaf=5,
                             min_samples_split=2, min_weight_fraction_leaf=0.0,
               presort=False, random_state=42, splitter='best')
Nested CV performance: -17479.326622895744 +/- 5669.079814673664
               Nested CV RMSE: 132.21 (+/- 150.59)
```

For the regression tree model, optimal parameters are max_depth = 5, min_samples_leaf = 5. The 10-fold cross-validation is RMSE = 132.21.

5 points for discussing which of the three models yields the best performance]

| | Original RMSE | RMSE with 2 new variables | RMSE with quadratic transformation | RMSE after parameter tuning |
|-----------------|------------------|------------------------------|------------------------------------|-----------------------------------|
| Simple Linear | 127.75 | 127.04 | 133.66 | - |
| Lasso Linear | 127.64 | 127.04 | 127.83 | 126.91 |
| Ridge Linear | 127.74 | 127.02 | 129.39 | 126.96 |
| <u>k-NN</u> | 150.54 | 149.77 | 151.07 | 142.08 |
| Regression Tree | 137.51 | 134.68 | 134.24 | 132.21 |

Overall, linear regression models perform much better than k-NN model and regression tree model. One possible reason is the dataset is relatively small with only 2000 instances. Within linear regression models, the difference is minimal among linear regression without penalty, lasso regression, and ridge regression. Ridge regression wins by only 0.05.