CA5 - Eirik H?yheim

April 28, 2021

1 CA5 - Eirik Høyheim

1.1 **Imports**

```
[1]: import pandas as pd
    import numpy as np
    import copy
    import pickle
    import matplotlib.pyplot as plt
    import seaborn as sns
    from sklearn.model_selection import train_test_split, GridSearchCV
    from sklearn.metrics import r2_score, mean_squared_error
    from sklearn.pipeline import make_pipeline
    from sklearn.ensemble import RandomForestRegressor
    from sklearn.cross_decomposition import PLSRegression
    from xgboost import XGBRegressor
```

1.2 Preprocess data, remove missing values and edit "demo_25"

```
[2]: train_raw = pd.read_pickle("train4.pkl") # read in data
   sub = pd.read_pickle("test4.pkl")
   train_raw.head()
```

```
[2]:
     demo_0
           1.37
                                     1.88
                                                       10.93
      11980
             3.10
                        91.78
                               6.50
                                           12.47
                                                 21.44
   1
    20009
            3.22
                  1.64
                       92.31
                               3.18
                                     7.15
                                           13.17
                                                 28.71
                                                       10.22
   2
     66049
           2.63
                  26.41
                        72.45
                               0.76
                                     0.72
                                           17.79
                                                 29.84
                                                       18.19
            2.39
                   0.29
   3
    11157
                        98.87
                              0.62
                                     0.61
                                           10.72
                                                 22.81
                                                       11.00
     17192
           2.69
                   0.58
                        97.40 1.07 0.76
                                           14.30
                                                 30.82
                                                       14.81
     demo_9
           ... demo_115 demo_116 demo_117 demo_118 demo_119 demo_120 \
```

```
0
    11.33 ...
                      6.5
                             1845.9
                                          9.63
                                                 missing
                                                            missing
                                                                      missing
     2.18 ...
                      4.2
1
                             4728.0
                                          0.00
                                                 missing
                                                           missing
                                                                      missing
2
    14.33
          . . .
                     51.2
                             1290.5
                                          3.33
                                                      62
                                                            5585480
                                                                        89.13
3
    17.50
                      3.0
                             3726.5
                                          0.90
                                                 missing
                                                            missing
                                                                      missing
           . . .
     9.56
                      6.8
                             2510.4
                                          2.26
          . . .
                                                 missing
                                                           missing
                                                                      missing
   demo_121 demo_122 demo_123 target
0
   missing
                  0.0
                         missing
                                    8.20
                                   71.99
1
    missing
                  0.0
                         missing
2
                         83166.8 159.32
                  5.8
                                   24.66
3
   missing
                  0.0
                         missing
   missing
                  0.0
                         missing
                                   35.62
```

[5 rows x 125 columns]

```
[3]: type(train_raw["demo_25"][0])
```

[3]: str

Both train and sub contains missing values in some of the columns and demo_25 contains string values, so need to transform these two.

```
[4]: train_with_nan = copy.copy(train_raw.replace("missing", np.nan)) # replace nan_
    →values with nan
   train_only 25_nan = copy.copy(train_with_nan[(train_with_nan.isnull().
    →sum()[train_with_nan.isnull().sum() <= 1]).index]) # remove all columns_
    → that contain more than 1 nan value
   train_only_25_nan["demo_25"] = [float(x) for x in train_only_25_nan["demo_25"]]_
    → # transforming all values from string to float
   median_demo25 = train_only_25_nan["demo_25"].median()
   train no nan = copy.copy(train only 25 nan.fillna(median demo25)) # replaces,
    → the nan value with median
   # same procedure with submission data
   sub with nan = copy.copy(sub.replace("missing", np.nan))
   sub_only_25_nan = copy.copy(sub_with_nan[(sub_with_nan.isnull().
    ⇒sum()[sub_with_nan.isnull().sum() <= 1]).index])
   sub_only_25 nan["demo_25"] = [float(x) for x in sub_only_25 nan["demo_25"]]
   sub_no_nan = copy.copy(sub_only_25 nan.fillna(median_demo25)) # replaces the__
    →nan value with median of train demo_25
   train no nan shape, sub no nan shape
```

```
[4]: ((1089, 103), (1089, 102))
```

```
[5]: train = copy.copy(train_no_nan)
```

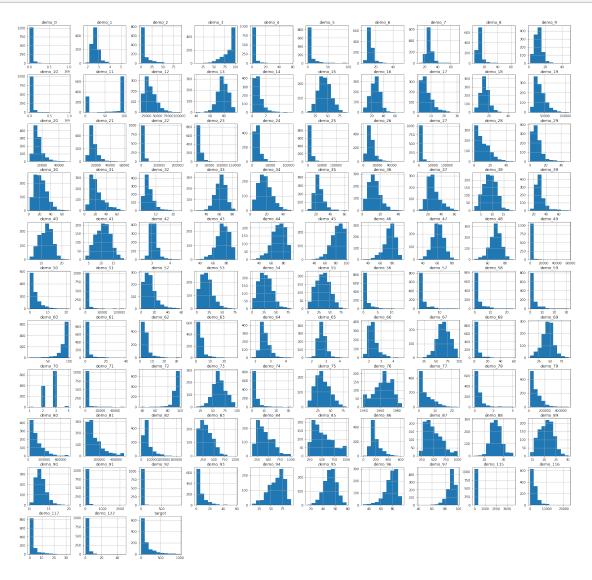
```
X = train.iloc[:, :-1]
y = train.iloc[:, -1]
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.3, random_state=1234)
```

1.3 Exploration of the data

Note: used fewer features on some of the plots to make the it faster to read through

```
[6]: train.hist(figsize=(30,30)) # see histograms of all features too see how they

→ are distributed
plt.show()
```



target is very left skewed, and a lot of the other features are skewed too. It will probably not effect prediction when using Randomforest or XGBoost, but the ones that are skewed may be

more correlated to target than those that are not skewed.

```
[7]: corr = train.corr(method="spearman") # used spearman method to see if there

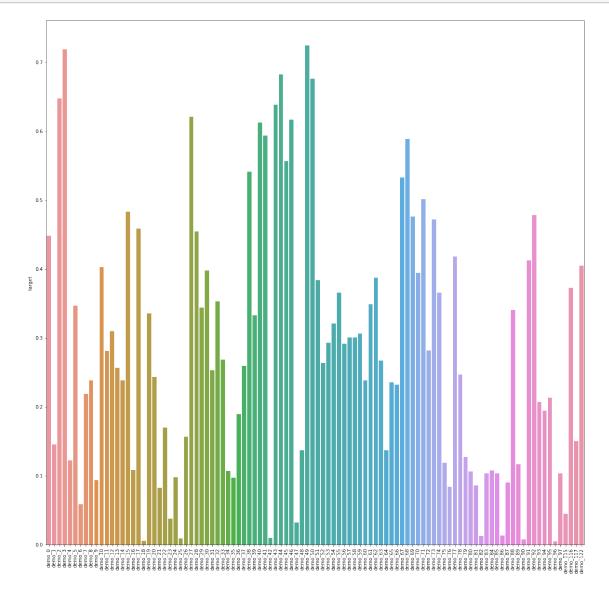
→were any non linear correlation too

fig, ax = plt.subplots(figsize=(20, 20))

sns.barplot(x=corr["target"].index[:-1], y=abs(corr["target"][:-1]))

plt.xticks(rotation=90)

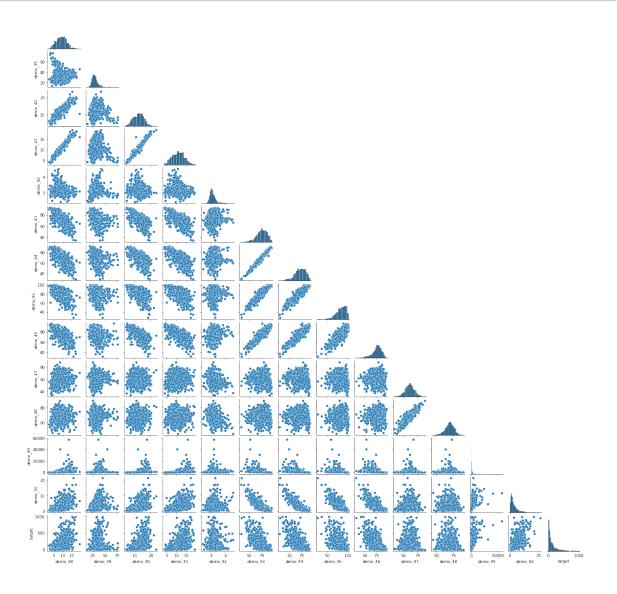
plt.show()
```



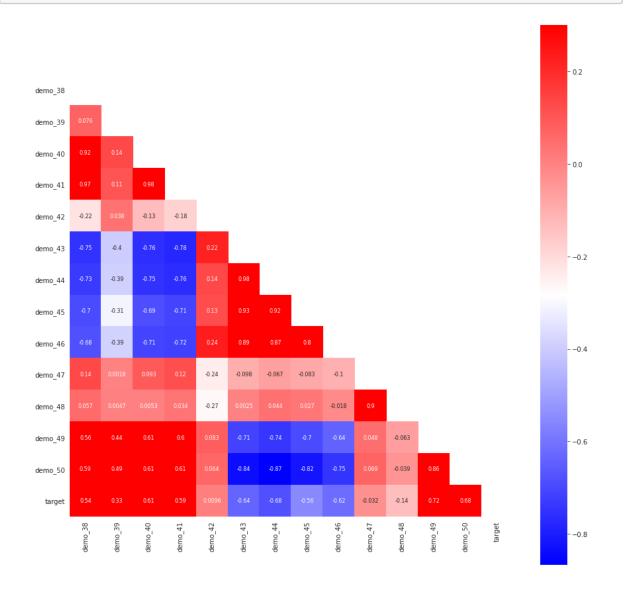
Some of the features are highly correlated to target. These features will typically help more when predicting.

```
[8]: g = sns.pairplot(train.iloc[:, [38,39,40,41,42,43,44,45,46,47,48,49,50,-1]], corner=True) # splitting up data for easier visualization g.fig.set_figheight(20)
```

```
g.fig.set_figwidth(20)
plt.show()
```



plt.show()



We want to look after features that have some type of relationship with target in the pairplot and, in the correlation matrix, we want to see which featrues that has the highest correlation too target.

In the correlation matrix, we can see that some of the features is highly correlated to each other, like demo_43 to demo_44 and demo_41 to demo_40. In the pairplot, we can see that these features also have a linear relationship with each other, which is because they are dependent on each other and/or they are the same data. Since these features have correlation, the weight when traning will be "heavier" on these observations because we are training on the same distribution more than once. This is also happening with other features that are not shown in the plots. Therefore, when traning for a better model, we should consider to remove features to get a lower within feature correlation.

1.4 Pipeline containing a compression step

Will use PLSReggression to compress data into a lower dim space then use a regression algorithm to predict data.

```
[10]: ## Class taken from lecture notes about PLSRegression
     class PLSRegressionWrapper(PLSRegression):
         def transform(self, X):
             return super().transform(X)
         def fit_transform(self, X, Y):
             return self.fit(X,Y).transform(X) # Only use X for transform when both \Box
      \rightarrow X and Y are supplied
[11]: my_pipe = make_pipeline(PLSRegressionWrapper(n_components=5, scale=True),__
      →RandomForestRegressor(n_estimators=1000, random_state=0))
     my_pipe.get_params()
[11]: {'memory': None,
      'steps': [('plsregressionwrapper', PLSRegressionWrapper(n_components=5)),
       ('randomforestregressor',
        RandomForestRegressor(n_estimators=1000, random_state=0))],
      'verbose': False,
      'plsregressionwrapper': PLSRegressionWrapper(n_components=5),
      'randomforestregressor': RandomForestRegressor(n_estimators=1000,
     random_state=0),
      'plsregressionwrapper_copy': True,
      'plsregressionwrapper_max_iter': 500,
      'plsregressionwrapper_n_components': 5,
      'plsregressionwrapper_scale': True,
      'plsregressionwrapper__tol': 1e-06,
      'randomforestregressor_bootstrap': True,
      'randomforestregressor ccp alpha': 0.0,
      'randomforestregressor__criterion': 'mse',
      'randomforestregressor_max_depth': None,
      'randomforestregressor__max_features': 'auto',
      'randomforestregressor__max_leaf_nodes': None,
      'randomforestregressor_max_samples': None,
      'randomforestregressor_min_impurity_decrease': 0.0,
      'randomforestregressor_min_impurity_split': None,
      'randomforestregressor_min_samples_leaf': 1,
      'randomforestregressor_min_samples_split': 2,
      'randomforestregressor__min_weight_fraction_leaf': 0.0,
      'randomforestregressor_n_estimators': 1000,
      'randomforestregressor_n_jobs': None,
      'randomforestregressor_oob_score': False,
```

```
'randomforestregressor_random_state': 0,
      'randomforestregressor_verbose': 0,
      'randomforestregressor_warm_start': False}
[12]: param_grid
                  = [
         {'randomforestregressor_max_depth': [8,9,10,11,12],
          'randomforestregressor__criterion': ["mae", "mse"],
          'plsregressionwrapper_n_components': [5,6,7]
     ]
     gs = GridSearchCV(estimator=my pipe,
                       param_grid=param_grid,
                       scoring='r2',
                       cv=10,
                       n_{jobs}=-1
[13]: %%time
     gs = gs.fit(X_train, y_train)
    Wall time: 16min 44s
[14]: print(gs.best_score_)
     print(gs.best_params_)
    0.6976553929636007
    {'plsregressionwrapper__n_components': 6, 'randomforestregressor__criterion':
    'mae', 'randomforestregressor_max_depth': 9}
[15]: for r, _ in enumerate(gs.cv_results_['mean_test_score']):
         print("%0.4f +/- %0.4f %r"
               % (gs.cv_results_['mean_test_score'][r],
                  gs.cv_results_['std_test_score'][r],
                  gs.cv_results_['params'][r]))
    0.6946 +/- 0.0876 {'plsregressionwrapper_n_components': 5,
    'randomforestregressor__criterion': 'mae', 'randomforestregressor__max_depth':
    0.6932 +/- 0.0871 {'plsregressionwrapper_n_components': 5,
    'randomforestregressor_criterion': 'mae', 'randomforestregressor_max_depth':
    0.6928 +/- 0.0867 {'plsregressionwrapper_n_components': 5,
    'randomforestregressor criterion': 'mae', 'randomforestregressor max depth':
    10}
```

```
0.6916 +/- 0.0860 {'plsregressionwrapper_n_components': 5,
'randomforestregressor_criterion': 'mae', 'randomforestregressor_max_depth':
11}
0.6903 +/- 0.0860 {'plsregressionwrapper_n_components': 5,
'randomforestregressor criterion': 'mae', 'randomforestregressor max depth':
0.6907 +/- 0.0880 {'plsregressionwrapper n components': 5,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
0.6895 +/- 0.0876 {'plsregressionwrapper_n_components': 5,
'randomforestregressor criterion': 'mse', 'randomforestregressor max depth':
0.6887 +/- 0.0872 {'plsregressionwrapper_n_components': 5,
'randomforestregressor__criterion': 'mse', 'randomforestregressor__max_depth':
0.6882 +/- 0.0866 {'plsregressionwrapper_n_components': 5,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
0.6884 +/- 0.0867 {'plsregressionwrapper_n_components': 5,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
0.6973 +/- 0.0765 {'plsregressionwrapper n components': 6,
'randomforestregressor__criterion': 'mae', 'randomforestregressor__max_depth':
0.6977 +/- 0.0757 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mae', 'randomforestregressor_max depth':
9}
0.6966 +/- 0.0745 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mae', 'randomforestregressor_max depth':
10}
0.6966 +/- 0.0752 {'plsregressionwrapper_n_components': 6,
'randomforestregressor__criterion': 'mae', 'randomforestregressor__max_depth':
11}
0.6960 +/- 0.0748 {'plsregressionwrapper_n_components': 6,
'randomforestregressor criterion': 'mae', 'randomforestregressor max depth':
12}
0.6921 +/- 0.0778 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
8}
0.6922 +/- 0.0778 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
9}
0.6923 +/- 0.0772 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
10}
0.6925 +/- 0.0762 {'plsregressionwrapper_n_components': 6,
'randomforestregressor__criterion': 'mse', 'randomforestregressor__max_depth':
11}
```

```
0.6914 +/- 0.0768 {'plsregressionwrapper_n_components': 6,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
0.6920 +/- 0.0706 {'plsregressionwrapper_n_components': 7,
'randomforestregressor criterion': 'mae', 'randomforestregressor max depth':
0.6908 +/- 0.0691 {'plsregressionwrapper n components': 7,
'randomforestregressor__criterion': 'mae', 'randomforestregressor__max_depth':
0.6906 +/- 0.0681 {'plsregressionwrapper_n_components': 7,
'randomforestregressor criterion': 'mae', 'randomforestregressor max depth':
0.6902 +/- 0.0673 {'plsregressionwrapper_n_components': 7,
'randomforestregressor__criterion': 'mae', 'randomforestregressor__max_depth':
0.6903 +/- 0.0672 {'plsregressionwrapper_n_components': 7,
'randomforestregressor_criterion': 'mae', 'randomforestregressor_max_depth':
0.6866 +/- 0.0706 {'plsregressionwrapper_n_components': 7,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max_depth':
0.6856 +/- 0.0709 {'plsregressionwrapper n components': 7,
'randomforestregressor__criterion': 'mse', 'randomforestregressor__max_depth':
0.6858 +/- 0.0697 {'plsregressionwrapper_n_components': 7,
'randomforestregressor_criterion': 'mse', 'randomforestregressor_max depth':
10}
0.6859 +/- 0.0703 {'plsregressionwrapper_n_components': 7,
'randomforestregressor criterion': 'mse', 'randomforestregressor max depth':
11}
0.6860 +/- 0.0692 {'plsregressionwrapper_n_components': 7,
'randomforestregressor__criterion': 'mse', 'randomforestregressor__max_depth':
12}
```

1.4.1 Lets see how it handles unseen data

```
mean_squared_error(y_test, y_test_pred)))
print('R^2 train: %.3f, test: %.3f' % (
    r2_score(y_train, y_train_pred),
    r2_score(y_test, y_test_pred)))
```

```
MSE train: 1983.824, test: 11739.705 R^2 train: 0.932, test: 0.652
```

Overfits on training data, and does not perform that as well on test data as the model did while training.

1.5 Pipeline using only regression method directly on the pre-processed data.

```
gs.cv_results_['params'][r]))
```

```
0.7143 +/- 0.0778 {'randomforestregressor__criterion': 'mae',
'randomforestregressor__max_depth': 8}
0.7153 +/- 0.0766 {'randomforestregressor__criterion': 'mae',
'randomforestregressor__max_depth': 9}
```

1.5.1 Lets see how it handles unseen data

```
MSE train: 1462.909, test: 12021.246 R^2 train: 0.950, test: 0.644
```

Overfitted even more than the model with compression and got a worse r^2 score on the test data. The two models does produce somewhat equal results, but RandomForest without compression got a higher avareage training score. Therefore, I will use that model to send in a submission.

1.6 Submission of my best score between the two models

```
[22]: submission = copy.copy(sub_no_nan)
```

Kaggle score: 0.67968.

1.7 Summary regression with and without compression step

In this example, when training for best scores, the regression that did not contain a compression step first managed to get a better result. Reasoning for this is not very obvious, but I could imagine that the PLS compression step was effected by having all features, even the features with high correlation to each other. If I tried to remove some of the between feature correlation, it may have given a different result.

When it comes to working with wide data in contrast to tall data, it is much harder to see which features that correlated to eachother, which features that are correlated to the target and, because of high dimension, we need to take into consideration the curse of dimensionality. Since this data has many featrues, it's harder to obtain a model that is statistically reliable. Therefore, it would probably be a good idea to compress data into a lower dimension using either PCA, LDA, KPCA or PLS. In this notebook, the algorithm that did not have a compression step managed to get the best results when training, but this could of course be because of between feature correlation or some other factor like RandomForestRegression does not need any preprocessing before training.

Another thing to take into consideration when using wide data is that it is way more time consuming to run through, therefore it would be a good idea to either remove features that are not necescerry, or, as mentioned, use a compressor to lower the dimension of the data.

NOTE: got a lower score when compressing before using regression model when using ElasticNet too.

1.8 My best performing model, XGBoost.

The function bellow was found from https://github.com/aprilypchen/depy2016/blob/master/DePy_Talk.ipg It finds all combinations of 2 columns, then, in the PolynomialFeatures step, it multiples all these combinations together. E.g. demo_1 * demo_2 = demo_1demo_2

```
[24]: from itertools import combinations
from sklearn.preprocessing import PolynomialFeatures

def addinteractions(df):
    # Get feature names
    combos = list(combinations(list(df.columns), 2))
    colnames = list(df.columns) + [''.join(x) for x in combos]

# Find interactions
poly = PolynomialFeatures(interaction_only=True, include_bias=False)
    df = poly.fit_transform(df)
    df = pd.DataFrame(df)
    df.columns = colnames

# Remove interaction terms with all 0 values
```

```
noint_indicies = [i for i, x in enumerate(list((df == 0).all())) if x]
df = df.drop(df.columns[noint_indicies], axis=1)
return df
```

1.8.1 Uses addinteractions, then, since there is too many features now, find features that highly correlates to target and use them when training

```
[25]: train = copy.copy(train_no_nan)
     submisson = copy.copy(sub_no_nan)
     X = train.iloc[:, :-1]
     y = train.iloc[:, -1]
     new_X = addinteractions(X)
     new_submisson = addinteractions(submisson)
     new_X["target"] = y
     new_X.shape, new_submisson.shape # As we can see, alot of new columns, way too⊔
[25]: ((1089, 5254), (1089, 5253))
[26]: %%time
     corr = new_X.corr(method="spearman") # find the correlation between all_
      \rightarrow features
    Wall time: 5min 1s
[27]: wanted columns = []
     for column, corr in zip(corr["target"].index, abs(corr["target"])):
         if corr > 0.5: # Only take features that have higher than 0.5 in
      →correlation to target
             wanted_columns.append(column)
[28]: | train = copy.copy(new_X[wanted_columns]) # Now train contains only features_
      →that have higher than 0.5 correlation to target
     X = train.iloc[:, :-1].values
     y = train.iloc[:, -1].values
```

X_train, X_test, y_train, y_test = train_test_split(

X, y, test_size=0.3, random_state=1)

train.shape

[28]: (1089, 759)

There are still a lot of features. It would probably be smarter to use a compressor or chose features in another way. But it was too time consuming...

1.8.2 Training for a good model

```
[29]: | xgb_reg = XGBRegressor(n_jobs=-1, random_state=1)
     # trained for more parameters, but removed those when going through the
      \rightarrownotebook to take less time
     param_grid = [
         {'learning_rate': [0.001],
          'max_depth': [3],
          'n_estimators': [8000]}
     ]
     gs = GridSearchCV(estimator=xgb_reg,
                      param_grid=param_grid,
                       scoring="r2",
                        cv=5,
                      n_{jobs=-1}
[30]: | %%time
     gs = gs.fit(X_train, y_train)
    Wall time: 17min 31s
[31]: print(gs.best_score_)
     print(gs.best_params_)
    0.6839682561559277
    {'learning_rate': 0.001, 'max_depth': 3, 'n_estimators': 8000}
[32]: for r, _ in enumerate(gs.cv_results_['mean_test_score']):
         print("%0.3f +/- %0.4f %r"
               % (gs.cv_results_['mean_test_score'][r],
                  gs.cv_results_['std_test_score'][r],
                  gs.cv_results_['params'][r]))
```

0.684 +/- 0.0306 {'learning_rate': 0.001, 'max_depth': 3, 'n_estimators': 8000}

This gets me a fearly high r^2 score with low standard deviation. This may be an indication of a more stabile model than the previous ones.

1.8.3 Lets see how it handles unseen data

MSE train: 1319.281, test: 9928.263 R² train: 0.953, test: 0.727

Overfit the training data, but performed quite decent on the test set. Possibly overfitting/luck to get this result on the test set.

1.8.4 Send in a submission to kaggle

```
[35]: model = XGBRegressor(max_depth=3,learning_rate=0.001,n_estimators=8000) model.fit(X, y)
```

```
[35]: XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1, colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1, importance_type='gain', interaction_constraints='', learning_rate=0.001, max_delta_step=0, max_depth=3, min_child_weight=1, missing=nan, monotone_constraints='()', n_estimators=8000, n_jobs=8, num_parallel_tree=1, random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method='exact', validate_parameters=1, verbosity=None)
```

Kaggle score: 0.73807, maybe an overfit but seems like it is inside the CI of scores.