

1. Hyper-parameter Tuning

October 28, 2021

Hyperparameter Tuning for Multiple Regression

We will find optimal number of features using recursive feature elimination (RFE) and k-fold cross validation.

```
[56]: # Import necessary package
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import warnings # suppress warnings
warnings.filterwarnings('ignore')
```

0.0.1 Step 1: Load the dataset

```
[57]: df = pd.read_csv('E:\\MY LECTURES\\DATA SCIENCE\\3.Programs\\dataset\\Housing.
    ↪ csv')
df.head()
```

```
[57]:
```

	price	area	bedrooms	bathrooms	stories	mainroad	guestroom	basement	\
0	13300000	7420	4	2	3	yes	no	no	
1	12250000	8960	4	4	4	yes	no	no	
2	12250000	9960	3	2	2	yes	no	yes	
3	12215000	7500	4	2	2	yes	no	yes	
4	11410000	7420	4	1	2	yes	yes	yes	

	hotwaterheating	airconditioning	parking	prefarea	furnishingstatus
0	no	yes	2	yes	furnished
1	no	yes	3	no	furnished
2	no	no	2	yes	semi-furnished
3	no	yes	3	yes	furnished
4	no	yes	2	no	furnished

0.0.2 Step 2: Apply EDA

Univariate and bivariate analysis

0.0.3 Step 3. Pre-process and extract the features

```
[58]: # data preparation - list of all the "yes-no" binary categorical variables
# we will map yes to 1 and no to 0
binary_vars_list = ['mainroad', 'guestroom', 'basement', 'hotwaterheating',
                    ↪ 'airconditioning', 'prefarea']

# defining the map function
def binary_map(x):
    return x.map({'yes': 1, "no": 0})

# applying the function to the housing variables list
df[binary_vars_list] = df[binary_vars_list].apply(binary_map)
df.head()
```

```
[58]:
```

	price	area	bedrooms	bathrooms	stories	mainroad	guestroom	\
0	13300000	7420	4	2	3	1	0	
1	12250000	8960	4	4	4	1	0	
2	12250000	9960	3	2	2	1	0	
3	12215000	7500	4	2	2	1	0	
4	11410000	7420	4	1	2	1	1	

	basement	hotwaterheating	airconditioning	parking	prefarea	\
0	0	0	1	2	1	
1	0	0	1	3	0	
2	1	0	0	2	1	
3	1	0	1	3	1	
4	1	0	1	2	0	

	furnishingstatus
0	furnished
1	furnished
2	semi-furnished
3	furnished
4	furnished

```
[59]: # 'dummy' variables
# get dummy variables for 'furnishingstatus'
# also, drop the first column of the resulting df (since n-1 dummy vars suffice)
status = pd.get_dummies(df['furnishingstatus'], drop_first = True)
status.head()
```

```
[59]:
```

	semi-furnished	unfurnished
0	0	0
1	0	0
2	1	0
3	0	0

4 0 0

```
[60]: # concat the dummy variable df with the main df
df = pd.concat([df, status], axis = 1)
df.head()
```

```
[60]:
```

	price	area	bedrooms	bathrooms	stories	mainroad	guestroom	\
0	13300000	7420	4	2	3	1	0	
1	12250000	8960	4	4	4	1	0	
2	12250000	9960	3	2	2	1	0	
3	12215000	7500	4	2	2	1	0	
4	11410000	7420	4	1	2	1	1	

	basement	hotwaterheating	airconditioning	parking	prefarea	\
0	0	0	1	2	1	
1	0	0	1	3	0	
2	1	0	0	2	1	
3	1	0	1	3	1	
4	1	0	1	2	0	

	furnishingstatus	semi-furnished	unfurnished
0	furnished	0	0
1	furnished	0	0
2	semi-furnished	1	0
3	furnished	0	0
4	furnished	0	0

```
[61]: # remove 'furnishingstatus' since we already have the dummy vars
df.drop(['furnishingstatus'], axis = 1, inplace = True)
df.head()
```

```
[61]:
```

	price	area	bedrooms	bathrooms	stories	mainroad	guestroom	\
0	13300000	7420	4	2	3	1	0	
1	12250000	8960	4	4	4	1	0	
2	12250000	9960	3	2	2	1	0	
3	12215000	7500	4	2	2	1	0	
4	11410000	7420	4	1	2	1	1	

	basement	hotwaterheating	airconditioning	parking	prefarea	\
0	0	0	1	2	1	
1	0	0	1	3	0	
2	1	0	0	2	1	
3	1	0	1	3	1	
4	1	0	1	2	0	

	semi-furnished	unfurnished
0	0	0

1	0	0
2	1	0
3	0	0
4	0	0

```
[62]: # extracting relevant features
numeric_vars = ['area', 'bedrooms', 'bathrooms', 'stories', 'parking', 'price']
temp = df[numeric_vars]
temp.head()
```

```
[62]:
```

	area	bedrooms	bathrooms	stories	parking	price
0	7420	4	2	3	2	13300000
1	8960	4	4	4	3	12250000
2	9960	3	2	2	2	12250000
3	7500	4	2	2	3	12215000
4	7420	4	1	2	2	11410000

```
[63]: # pre-process: Scale the values of those features between 0 and 1
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
temp1 = scaler.fit_transform(temp)
temp1 = pd.DataFrame(temp1, columns=['area', 'bedrooms', 'bathrooms', 'stories',
    ↪ 'parking', 'price'])
temp1.head()
```

```
[63]:
```

	area	bedrooms	bathrooms	stories	parking	price
0	0.396564	0.6	0.333333	0.666667	0.666667	1.000000
1	0.502405	0.6	1.000000	1.000000	1.000000	0.909091
2	0.571134	0.4	0.333333	0.333333	0.666667	0.909091
3	0.402062	0.6	0.333333	0.333333	1.000000	0.906061
4	0.396564	0.6	0.000000	0.333333	0.666667	0.836364

```
[64]: df1 = df[["mainroad", "guestroom", "basement", "hotwaterheating",
    ↪ "airconditioning", "prefarea", "semi-furnished"]]
df1.head()
```

```
[64]:
```

	mainroad	guestroom	basement	hotwaterheating	airconditioning	prefarea	\
0	1	0	0	0	1	1	
1	1	0	0	0	1	0	
2	1	0	1	0	0	1	
3	1	0	1	0	1	1	
4	1	1	1	0	1	0	

	semi-furnished
0	0
1	0
2	1

```
3          0
4          0
```

```
[65]: pre_processed_data = pd.concat([df1,temp1],axis=1)
pre_processed_data.head()
```

```
[65]:
```

	mainroad	guestroom	basement	hotwaterheating	airconditioning	prefarea	\
0	1	0	0	0	1	1	
1	1	0	0	0	1	0	
2	1	0	1	0	0	1	
3	1	0	1	0	1	1	
4	1	1	1	0	1	0	

	semi-furnished	area	bedrooms	bathrooms	stories	parking	price
0	0	0.396564	0.6	0.333333	0.666667	0.666667	1.000000
1	0	0.502405	0.6	1.000000	1.000000	1.000000	0.909091
2	1	0.571134	0.4	0.333333	0.333333	0.666667	0.909091
3	0	0.402062	0.6	0.333333	0.333333	1.000000	0.906061
4	0	0.396564	0.6	0.000000	0.333333	0.666667	0.836364

```
[66]: pre_processed_data.shape
```

```
[66]: (545, 13)
```

0.0.4 Step 4. Split the data for training and testing

```
[67]: # split into train and test
from sklearn.model_selection import train_test_split
train, test = train_test_split(pre_processed_data, train_size = 0.8, test_size=
↳ 0.2, random_state = 100)
```

```
[68]: # divide into x_train, y_train, x_test, y_test
y_train = train.pop('price')
x_train = train

y_test = test.pop('price')
x_test = test
```

Using RFE (recursive feature elimination) to find optimal number of features Now, we have 13 input features. To build the model using RFE, we need to tell RFE how many features we want in the final model. It then runs a feature elimination algorithm.

Note that the number of features to be used in the model is a **hyperparameter**.

```
[69]: # num of max features
len(x_train.columns)
```

[69]: 12

demanding 10 features

```
[70]: # first model with an arbitrary choice of n_features (say 10) using Recursive_
      ↪ Feature Elimination (RFE)
from sklearn.feature_selection import RFE
from sklearn.linear_model import LinearRegression

lm = LinearRegression()

rfe = RFE(lm, n_features_to_select = 10)

rfe = rfe.fit(x_train, y_train)
```

```
[71]: # tuples of (feature name, whether selected, ranking)
      # note that the 'rank' is > 1 for non-selected features
list(zip(x_train.columns, rfe.support_, rfe.ranking_))
```

```
[71]: [('mainroad', True, 1),
      ('guestroom', True, 1),
      ('basement', False, 2),
      ('hotwaterheating', True, 1),
      ('airconditioning', True, 1),
      ('prefarea', True, 1),
      ('semi-furnished', False, 3),
      ('area', True, 1),
      ('bedrooms', True, 1),
      ('bathrooms', True, 1),
      ('stories', True, 1),
      ('parking', True, 1)]
```

```
[72]: import sklearn.metrics

      # predict prices of X_test
      y_pred = rfe.predict(x_test)

      # evaluate the model on test set
      r2 = sklearn.metrics.r2_score(y_test, y_pred)
      print("R2 score for 10 features is ", np.round(r2,2)*100,"%")
```

R2 score for 10 features is 66.0 %

demanding 6 features

```
[73]: # try with another value of RFE

rfe = RFE(lm, n_features_to_select = 6)
rfe = rfe.fit(x_train, y_train)

# predict prices of X_test
y_pred = rfe.predict(x_test)

# evaluate the model on test set
r2 = sklearn.metrics.r2_score(y_test, y_pred)
print("R2 score for 6 features is ", np.round(r2,2)*100,"%")
```

R2 score for 6 features is 61.0 %

Using k-fold cross-validation

```
[74]: # number of features in X_train
len(x_train.columns)
```

[74]: 12

```
[75]: from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV

# step-1: create a cross-validation scheme
folds = KFold(n_splits = 5, shuffle = True, random_state = 100)

# step-2: specify range of hyperparameters to tune
hyper_params = [{'n_features_to_select': list(range(1, 14))}]

# step-3: perform grid search
# 3.1 specify model
lm = LinearRegression()
rfe = RFE(lm)

# 3.2 call GridSearchCV()
model_cv = GridSearchCV(estimator = rfe, param_grid = hyper_params, scoring=
↳ 'r2', cv = folds, verbose = 1, return_train_score=True)

# fit the model
model_cv.fit(x_train, y_train)
```

Fitting 5 folds for each of 13 candidates, totalling 65 fits

```
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.
[Parallel(n_jobs=1)]: Done 65 out of 65 | elapsed: 0.6s finished
```

```
[75]: GridSearchCV(cv=KFold(n_splits=5, random_state=100, shuffle=True),
                  estimator=RFE(estimator=LinearRegression()),
                  param_grid=[{'n_features_to_select': [1, 2, 3, 4, 5, 6, 7, 8, 9,
                                                         10, 11, 12, 13]}],
                  return_train_score=True, scoring='r2', verbose=1)
```

```
[76]: # cv results
cv_results = pd.DataFrame(model_cv.cv_results_)
cv_results
```

```
[76]:
```

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	\
0	0.010394	0.001020	0.002399	4.893565e-04	
1	0.010787	0.003189	0.002399	4.897265e-04	
2	0.009394	0.001021	0.001999	6.315051e-04	
3	0.008196	0.000748	0.001799	3.998047e-04	
4	0.008156	0.003756	0.001208	9.861814e-04	
5	0.009488	0.006468	0.001207	9.855652e-04	
6	0.006742	0.005462	0.001599	7.997275e-04	
7	0.005597	0.000489	0.001999	7.478899e-07	
8	0.004523	0.000445	0.002399	4.898045e-04	
9	0.004397	0.000489	0.001599	4.896873e-04	
10	0.003399	0.000799	0.001599	4.894147e-04	
11	0.002598	0.000490	0.001599	4.894537e-04	
12	0.000999	0.001264	0.003924	5.917418e-03	

	param_n_features_to_select	params	\
0	1	{'n_features_to_select': 1}	
1	2	{'n_features_to_select': 2}	
2	3	{'n_features_to_select': 3}	
3	4	{'n_features_to_select': 4}	
4	5	{'n_features_to_select': 5}	
5	6	{'n_features_to_select': 6}	
6	7	{'n_features_to_select': 7}	
7	8	{'n_features_to_select': 8}	
8	9	{'n_features_to_select': 9}	
9	10	{'n_features_to_select': 10}	
10	11	{'n_features_to_select': 11}	
11	12	{'n_features_to_select': 12}	
12	13	{'n_features_to_select': 13}	

	split0_test_score	split1_test_score	split2_test_score	\
0	0.276949	0.387262	0.100131	
1	0.429683	0.556214	0.406671	
2	0.495335	0.585472	0.491629	
3	0.533694	0.612475	0.481561	
4	0.531246	0.625839	0.531517	
5	0.548520	0.634265	0.550628	

6	0.572115	0.669321	0.588741
7	0.582022	0.674105	0.616321
8	0.567159	0.678084	0.643983
9	0.595612	0.686668	0.660261
10	0.589047	0.695003	0.671007
11	0.592462	0.693810	0.672526
12	0.592462	0.693810	0.672526

	split3_test_score	...	mean_test_score	std_test_score	rank_test_score	\
0	0.296618	...	0.251887	0.096787	13	
1	0.508769	...	0.462183	0.059862	12	
2	0.550714	...	0.523759	0.037856	11	
3	0.548044	...	0.536108	0.044583	10	
4	0.518539	...	0.542786	0.042524	9	
5	0.529404	...	0.552411	0.044890	8	
6	0.555967	...	0.596075	0.039000	7	
7	0.572281	...	0.608162	0.036143	6	
8	0.601480	...	0.617711	0.038855	5	
9	0.609489	...	0.632374	0.034953	4	
10	0.615245	...	0.636593	0.039712	3	
11	0.620823	...	0.637518	0.038926	1	
12	0.620823	...	0.637518	0.038926	1	

	split0_train_score	split1_train_score	split2_train_score	\
0	0.280964	0.233348	0.315899	
1	0.491680	0.447678	0.492970	
2	0.549716	0.519267	0.546667	
3	0.597053	0.571504	0.551180	
4	0.600922	0.584481	0.596180	
5	0.623425	0.599596	0.606989	
6	0.632366	0.626130	0.634878	
7	0.641664	0.640590	0.644835	
8	0.661629	0.641990	0.654508	
9	0.680275	0.653070	0.663458	
10	0.687217	0.655536	0.666639	
11	0.687616	0.657890	0.667863	
12	0.687616	0.657890	0.667863	

	split3_train_score	split4_train_score	mean_train_score	std_train_score
0	0.270183	0.300176	0.280114	0.028176
1	0.471062	0.496231	0.479924	0.018399
2	0.533585	0.548466	0.539540	0.011666
3	0.540888	0.573760	0.566877	0.019500
4	0.604684	0.611186	0.599491	0.008967
5	0.635190	0.620695	0.617179	0.012560
6	0.647244	0.648303	0.637784	0.008646
7	0.658142	0.662905	0.649627	0.009131

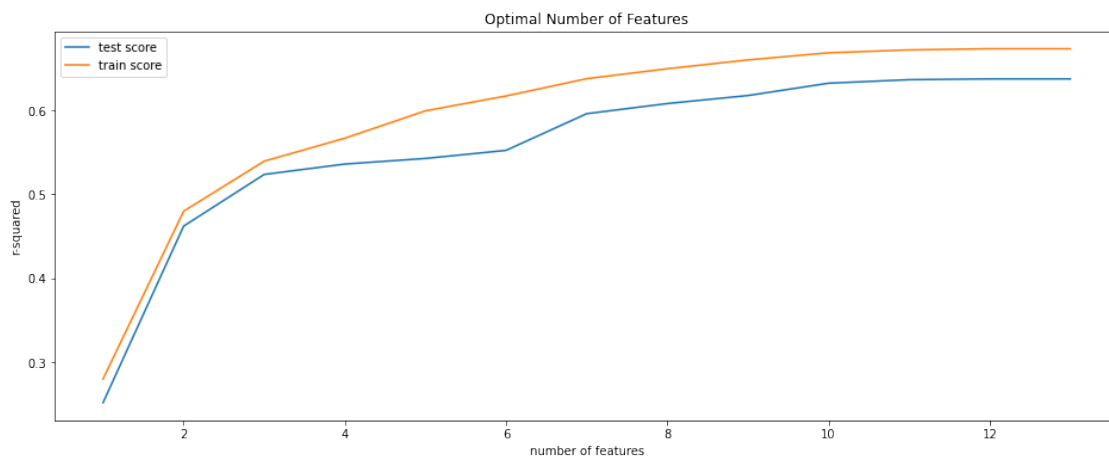
8	0.666207	0.676354	0.660138	0.011516
9	0.667128	0.679152	0.668617	0.010173
10	0.671415	0.679437	0.672049	0.010835
11	0.672042	0.681946	0.673471	0.010470
12	0.672042	0.681946	0.673471	0.010470

[13 rows x 21 columns]

```
[77]: # plotting cv results
plt.figure(figsize=(16,6))

plt.plot(cv_results["param_n_features_to_select"],
         ↪cv_results["mean_test_score"])
plt.plot(cv_results["param_n_features_to_select"],
         ↪cv_results["mean_train_score"])
plt.xlabel('number of features')
plt.ylabel('r-squared')
plt.title("Optimal Number of Features")
plt.legend(['test score', 'train score'], loc='upper left')
```

[77]: <matplotlib.legend.Legend at 0x1a2c3c6ba90>



From the graph above, we can observe that R_{square} value keeps increasing as we incrementally add features.

After adding 12 features, there is no much increase in the score. Therefore, we can select first 10 features for building the model.

```
[78]: # final model
n_features_optimal = 10

lm = LinearRegression()
```

```
rfe = RFE(lm, n_features_to_select = n_features_optimal)
rfe = rfe.fit(x_train, y_train)

# predict prices of x_test
y_pred = rfe.predict(x_test)
r2 = sklearn.metrics.r2_score(y_test, y_pred)
print(r2)
```

0.656129343365103

Notice that the test score is very close to the ‘mean test score’ on the k-folds (about 60%). In general, the mean score estimated by CV will usually be a good estimate of the test score.