# model-evaluation-and-refinement

## February 3, 2019

```
<a href="http://cocl.us/DA0101EN_NotbookLink_Top">
     <img src="https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data/CognitiveClass/</pre>
</a>
  Data Analysis with Python
  Module 5: Model Evaluation and Refinement
  We have built models and made predictions of vehicle prices. Now we will determine how
accurate these predictions are.
  Table of content
<a href="#ref1">Model Evaluation </a>
<a href="#ref2">Over-fitting, Under-fitting and Model Selection </a>
<a href="#ref3">Ridge Regression </a>
<a href="#ref4">Grid Search</a>
In [1]: import pandas as pd
       import numpy as np
        # Import clean data
       path = 'https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data/CognitiveClass
       df = pd.read_csv(path)
In [3]: df.to_csv('module_5_auto.csv')
  First lets only use numeric data
In [4]: df=df._get_numeric_data()
       df.head()
Out[4]:
          Unnamed: 0 Unnamed: 0.1 symboling normalized-losses wheel-base \
       0
                                            3
                                                                         88.6
                   0
                                 0
                                                             122
                                            3
                                                             122
                                                                         88.6
       1
                   1
                                 1
       2
                   2
                                 2
                                            1
                                                             122
                                                                         94.5
       3
                   3
                                 3
                                             2
                                                              164
                                                                        99.8
       4
                                  4
                                             2
                                                                         99.4
                                                              164
            length
                       width height curb-weight engine-size ...
                                                                     stroke \
       0 0.811148 0.890278
                                48.8
                                             2548
                                                            130 ...
                                                                        2.68
       1 0.811148 0.890278
                                48.8
                                             2548
                                                           130 ...
                                                                        2.68
```

```
2 0.822681 0.909722
                                  52.4
                                               2823
                                                              152 ...
                                                                          3.47
                                  54.3
                                                              109 ...
                                                                          3.40
        3 0.848630 0.919444
                                               2337
                                                              136 ...
        4 0.848630 0.922222
                                  54.3
                                               2824
                                                                          3.40
           compression-ratio
                              horsepower
                                           peak-rpm
                                                     city-mpg highway-mpg
                                                                               price \
        0
                         9.0
                                    111.0
                                             5000.0
                                                            21
                                                                         27
                                                                            13495.0
        1
                         9.0
                                    111.0
                                             5000.0
                                                           21
                                                                         27 16500.0
        2
                         9.0
                                   154.0
                                             5000.0
                                                           19
                                                                         26 16500.0
        3
                         10.0
                                    102.0
                                             5500.0
                                                           24
                                                                         30 13950.0
        4
                         8.0
                                    115.0
                                             5500.0
                                                           18
                                                                         22 17450.0
           city-L/100km diesel
                                 gas
        0
              11.190476
        1
              11.190476
        2
              12.368421
               9.791667
        3
                              0
                                    1
        4
              13.055556
        [5 rows x 21 columns]
   Libraries for plotting
In [5]: %%capture
        ! pip install ipywidgets
In [6]: from IPython.display import display
        from IPython.html import widgets
        from IPython.display import display
        from ipywidgets import interact, interactive, fixed, interact_manual
/home/jupyterlab/conda/lib/python3.6/site-packages/IPython/html.py:14: ShimWarning: The `IPython
  "`IPython.html.widgets` has moved to `ipywidgets`.", ShimWarning)
   Functions for plotting
In [7]: def DistributionPlot(RedFunction, BlueFunction, RedName, BlueName, Title):
            width = 12
            height = 10
            plt.figure(figsize=(width, height))
            ax1 = sns.distplot(RedFunction, hist=False, color="r", label=RedName)
            ax2 = sns.distplot(BlueFunction, hist=False, color="b", label=BlueName, ax=ax1)
            plt.title(Title)
            plt.xlabel('Price (in dollars)')
            plt.ylabel('Proportion of Cars')
            plt.show()
            plt.close()
```

```
width = 12
             height = 10
             plt.figure(figsize=(width, height))
             #training data
             #testing data
             # lr: linear regression object
             #poly_transform: polynomial transformation object
             xmax=max([xtrain.values.max(), xtest.values.max()])
             xmin=min([xtrain.values.min(), xtest.values.min()])
             x=np.arange(xmin, xmax, 0.1)
             plt.plot(xtrain, y_train, 'ro', label='Training Data')
             plt.plot(xtest, y_test, 'go', label='Test Data')
             plt.plot(x, lr.predict(poly_transform.fit_transform(x.reshape(-1, 1))), label='Predict(poly_transform.fit_transform(x.reshape(-1, 1)))
             plt.ylim([-10000, 60000])
             plt.ylabel('Price')
             plt.legend()
   Part 1: Training and Testing
   An important step in testing your model is to split your data into training and testing data. We
will place the target data price in a separate dataframe y:
In [9]: y_data = df['price']
   drop price data in x data
In [10]: x_data=df.drop('price',axis=1)
   Now we randomly split our data into training and testing data using the function
train_test_split.
In [65]: from sklearn.model_selection import train_test_split
         x_train, x_test, y_train, y_test = train_test_split(x_data, y_data, test_size=0.15, ran
```

In [8]: def PollyPlot(xtrain, xtest, y\_train, y\_test, lr,poly\_transform):

print("number of test samples :", x\_test.shape[0])
print("number of training samples:",x\_train.shape[0])

number of test samples: 31 number of training samples: 170

The test\_size parameter sets the proportion of data that is split into the testing set. In the above, the testing set is set to 10% of the total dataset.

Question #1):

Use the function "train\_test\_split" to split up the data set such that 40% of the data samples will be utilized for testing, set the parameter "random\_state" equal to zero. The output of the function should be the following: "x\_train\_1", "x\_test\_1", "y\_train\_1" and "y\_test\_1".

```
In [51]: # Write your code below and press Shift+Enter to execute
         x_train_1, x_test_1, y_train_1, y_test_1 = train_test_split(x_data, y_data, test_size=0
         print("number of test samples :", x_test_1.shape[0])
         print("number of training samples:",x_train_1.shape[0])
number of test samples: 81
number of training samples: 120
   Double-click here for the solution.
   Let's import LinearRegression from the module linear_model.
In [13]: from sklearn.linear_model import LinearRegression
   We create a Linear Regression object:
In [14]: lre=LinearRegression()
   we fit the model using the feature horsepower
In [66]: lre.fit(x_train[['horsepower']], y_train)
Out[66]: LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
                   normalize=False)
   Let's Calculate the R<sup>2</sup> on the test data:
In [67]: lre.score(x_test[['horsepower']], y_test)
Out [67]: 0.707688374146705
   we can see the R<sup>2</sup> is much smaller using the test data.
In [68]: lre.score(x_train[['horsepower']], y_train)
Out [68]: 0.6449517437659684
   Question #2):
   Find the R<sup>2</sup> on the test data using 90% of the data for training data
```

Double-click here for the solution.

Sometimes you do not have sufficient testing data; as a result, you may want to perform Cross-validation. Let's go over several methods that you can use for Cross-validation.

Cross-validation Score

Lets import model\_selection from the module cross\_val\_score.

```
In [23]: from sklearn.model_selection import cross_val_score
```

We input the object, the feature in this case 'horsepower', the target data (y\_data). The parameter 'cv' determines the number of folds; in this case 4.

```
In [82]: Rcross = cross_val_score(lre, x_data[['horsepower']], y_data, cv=4)
```

The default scoring is R<sup>2</sup>; each element in the array has the average R<sup>2</sup> value in the fold:

```
In [25]: Rcross
Out[25]: array([0.7746232 , 0.51716687, 0.74785353, 0.04839605])
```

We can calculate the average and standard deviation of our estimate:

```
In [26]: print("The mean of the folds are", Rcross.mean(), "and the standard deviation is", Rcr
The mean of the folds are 0.522009915042119 and the standard deviation is 0.2911839444756029
```

We can use negative squared error as a score by setting the parameter 'scoring' metric to 'neg\_mean\_squared\_error'.

Question #3):

Calculate the average  $R^2$  using two folds, find the average  $R^2$  for the second fold utilizing the horsepower as a feature :

Double-click here for the solution.

You can also use the function 'cross\_val\_predict' to predict the output. The function splits up the data into the specified number of folds, using one fold to get a prediction while the rest of the folds are used as test data. First import the function:

```
In [30]: from sklearn.model_selection import cross_val_predict
```

We input the object, the feature in this case 'horsepower', the target data y\_data. The parameter 'cv' determines the number of folds; in this case 4. We can produce an output:

Part 2: Overfitting, Underfitting and Model Selection

It turns out that the test data sometimes referred to as the out of sample data is a much better measure of how well your model performs in the real world. One reason for this is overfitting; let's go over some examples. It turns out these differences are more apparent in Multiple Linear Regression and Polynomial Regression so we will explore overfitting in that context.

Let's create Multiple linear regression objects and train the model using 'horsepower', 'curbweight', 'engine-size' and 'highway-mpg' as features.

Prediction using training data:

16667.18254832])

Prediction using test data:

Let's perform some model evaluation using our training and testing data separately. First we import the seaborn and matplotlibb library for plotting.

Let's examine the distribution of the predicted values of the training data.

/home/jupyterlab/conda/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWarning: Usi return np.add.reduce(sorted[indexer] \* weights, axis=axis) / sumval

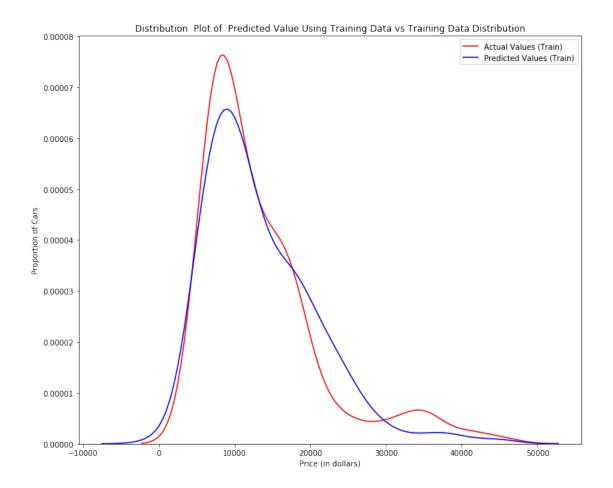
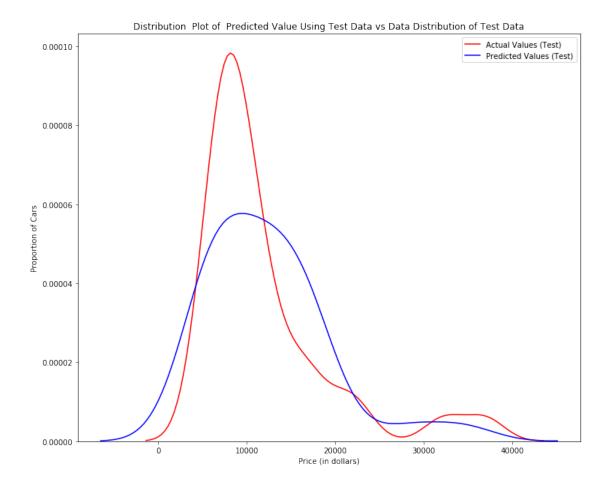


Figure 1: Plot of predicted values using the training data compared to the training data. So far the model seems to be doing well in learning from the training dataset. But what happens when the model encounters new data from the testing dataset? When the model generates new values from the test data, we see the distribution of the predicted values is much different from the actual target values.

In [89]: Title='Distribution Plot of Predicted Value Using Test Data vs Data Distribution of T DistributionPlot(y\_test,yhat\_test,"Actual Values (Test)","Predicted Values (Test)",Titl



Figur 2: Plot of predicted value using the test data compared to the test data.

Comparing Figure 1 and Figure 2; it is evident the distribution of the test data in Figure 1 is much better at fitting the data. This difference in Figure 2 is apparent where the ranges are from 5000 to 15 000. This is where the distribution shape is exceptionally different. Let's see if polynomial regression also exhibits a drop in the prediction accuracy when analysing the test dataset.

#### In [90]: from sklearn.preprocessing import PolynomialFeatures

### Overfitting

Overfitting occurs when the model fits the noise, not the underlying process. Therefore when testing your model using the test-set, your model does not perform as well as it is modelling noise, not the underlying process that generated the relationship. Let's create a degree 5 polynomial model.

Let's use 55 percent of the data for testing and the rest for training:

In [92]: x\_train, x\_test, y\_train, y\_test = train\_test\_split(x\_data, y\_data, test\_size=0.45, ran

We will perform a degree 5 polynomial transformation on the feature 'horse power'.

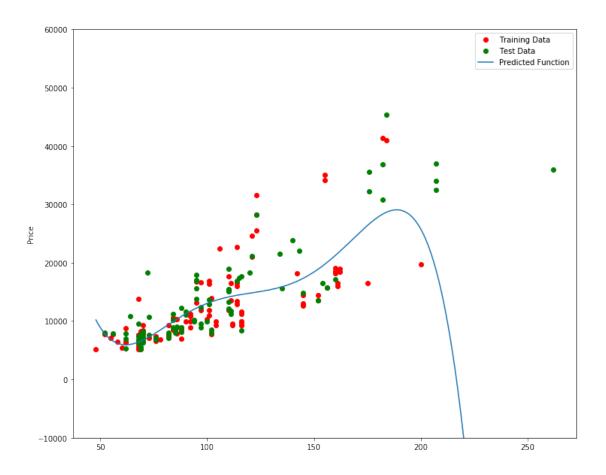
Now let's create a linear regression model "poly" and train it.

We can see the output of our model using the method "predict." then assign the values to "yhat".

Let's take the first five predicted values and compare it to the actual targets.

We will use the function "PollyPlot" that we defined at the beginning of the lab to display the training data, testing data, and the predicted function.

```
In [97]: PollyPlot(x_train[['horsepower']], x_test[['horsepower']], y_train, y_test, poly,pr)
```



Figur 4 A polynomial regression model, red dots represent training data, green dots represent test data, and the blue line represents the model prediction.

We see that the estimated function appears to track the data but around 200 horsepower, the function begins to diverge from the data points.

R<sup>2</sup> of the training data:

```
In [98]: poly.score(x_train_pr, y_train)
```

Out[98]: 0.5567716902028981

R<sup>2</sup> of the test data:

```
In [99]: poly.score(x_test_pr, y_test)
```

Out[99]: -29.87162132967278

We see the R<sup>2</sup> for the training data is 0.5567 while the R<sup>2</sup> on the test data was -29.87. The lower the R<sup>2</sup>, the worse the model, a Negative R<sup>2</sup> is a sign of overfitting.

Let's see how the R^2 changes on the test data for different order polynomials and plot the results:

```
In [100]: Rsqu_test = []

order = [1, 2, 3, 4]
for n in order:
    pr = PolynomialFeatures(degree=n)

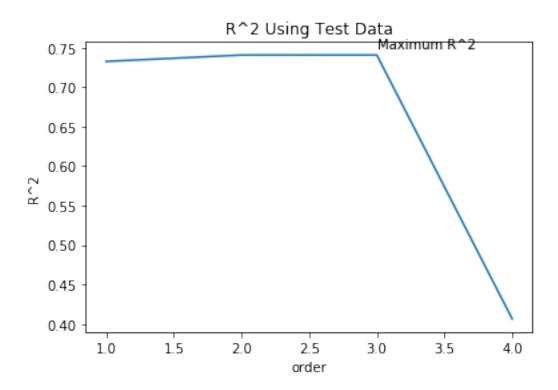
x_train_pr = pr.fit_transform(x_train[['horsepower']])

x_test_pr = pr.fit_transform(x_test[['horsepower']])

lr.fit(x_train_pr, y_train)

Rsqu_test.append(lr.score(x_test_pr, y_test))

plt.plot(order, Rsqu_test)
    plt.xlabel('order')
    plt.ylabel('R^2')
    plt.title('R^2 Using Test Data')
    plt.text(3, 0.75, 'Maximum R^2 ')
Out[100]: Text(3, 0.75, 'Maximum R^2 ')
```

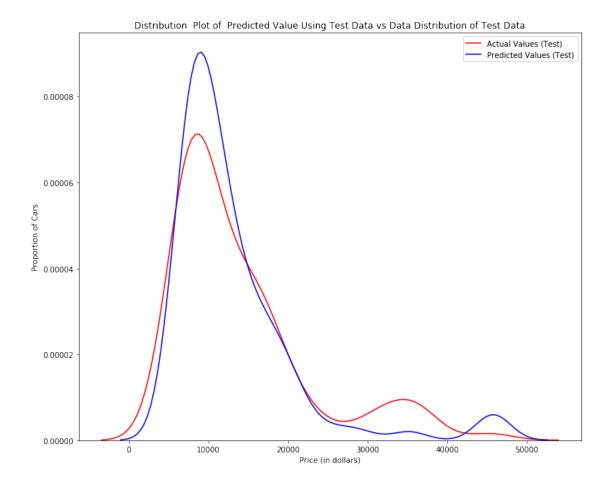


We see the R^2 gradually increases until an order three polynomial is used. Then the R^2 dramatically decreases at four.

The following function will be used in the next section; please run the cell.

The following interface allows you to experiment with different polynomial orders and different amounts of data.

/home/jupyterlab/conda/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWarning: Usi return np.add.reduce(sorted[indexer] \* weights, axis=axis) / sumval



Question #4a):

We can perform polynomial transformations with more than one feature. Create a "PolynomialFeatures" object "pr1" of degree two?

Double-click here for the solution.

Question #4b):

Transform the training and testing samples for the features 'horsepower', 'curb-weight', 'engine-size' and 'highway-mpg'. Hint: use the method "fit\_transform"?

Double-click here for the solution.

Question #4c):

How many dimensions does the new feature have? Hint: use the attribute "shape"

Double-click here for the solution.

Question #4d):

Create a linear regression model "poly1" and train the object using the method "fit" using the polynomial features?

Double-click here for the solution.

Ouestion #4e):

Use the method "predict" to predict an output on the polynomial features, then use the function "DistributionPlot" to display the distribution of the predicted output vs the test data?

Double-click here for the solution.

Question #4f):

Use the distribution plot to determine the two regions were the predicted prices are less accurate than the actual prices.

Double-click here for the solution.

In [126]: print('predicted:', yhat[0:4])

test set : [ 6295. 10698. 13860. 13499.]

print('test set :', y\_test[0:4].values)

predicted: [ 6567.83081933 9597.97151399 20836.22326843 19347.69543463]

Part 3: Ridge regression

In this section, we will review Ridge Regression we will see how the parameter Alfa changes the model. Just a note here our test data will be used as validation data.

Let's perform a degree two polynomial transformation on our data.

```
In [130]: pr=PolynomialFeatures(degree=2)
          x_train_pr=pr.fit_transform(x_train[['horsepower', 'curb-weight', 'engine-size', 'high
          x_test_pr=pr.fit_transform(x_test[['horsepower', 'curb-weight', 'engine-size', 'highwa
   Let's import Ridge from the module linear models.
In [120]: from sklearn.linear_model import Ridge
   Let's create a Ridge regression object, setting the regularization parameter to 0.1
In [121]: RigeModel=Ridge(alpha=0.1)
   Like regular regression, you can fit the model using the method fit.
In [123]: RigeModel.fit(x_train_pr, y_train)
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/linear_model/ridge.py:125: LinAlgWarr
Ill-conditioned matrix detected. Result is not guaranteed to be accurate.
Reciprocal condition number1.029716e-16
  overwrite a=True).T
Out[123]: Ridge(alpha=0.1, copy_X=True, fit_intercept=True, max_iter=None,
             normalize=False, random_state=None, solver='auto', tol=0.001)
   Similarly, you can obtain a prediction:
In [125]: yhat = RigeModel.predict(x_test_pr)
   Let's compare the first five predicted samples to our test set
```

We select the value of Alfa that minimizes the test error, for example, we can use a for loop.

Out[128]: <matplotlib.legend.Legend at 0x7f0d30286518>

plt.xlabel('alpha')
plt.ylabel('R^2')

plt.legend()

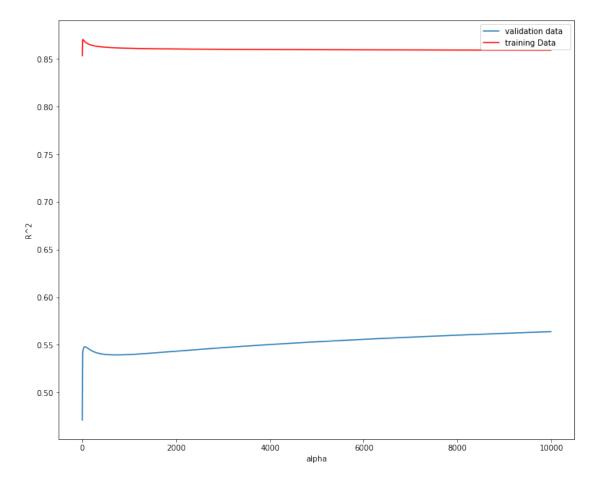


Figure 6:The blue line represents the R<sup>2</sup> of the test data, and the red line represents the R<sup>2</sup> of the training data. The x-axis represents the different values of Alfa

The red line in figure 6 represents the R<sup>2</sup> of the test data, as Alpha increases the R<sup>2</sup> decreases; therefore as Alfa increases the model performs worse on the test data. The blue line represents the R<sup>2</sup> on the validation data, as the value for Alfa increases the R<sup>2</sup> decreases.

Question #5):

Perform Ridge regression and calculate the R<sup>2</sup> using the polynomial features, use the training data to train the model and test data to test the model. The parameter alpha should be set to 10.

```
In [133]: # Write your code below and press Shift+Enter to execute
    RigeModel1=Ridge(alpha=10)
    RigeModel1.fit(x_train_pr, y_train)
    #yhat = RigeModel1.predict(x_test_pr)
    #print('predicted:', yhat[0:4])
    #print('test set :', y_test[0:4].values)
    RigeModel1.score(x_test_pr, y_test)
Out[133]: 0.5418576440207072
```

Double-click here for the solution.

Part 4: Grid Search

Fit the model

The term Alfa is a hyperparameter, sklearn has the class GridSearchCV to make the process of finding the best hyperparameter simpler.

Let's import GridSearchCV from the module model\_selection.

```
In [141]: Grid1.fit(x_data[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']], y_data)
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/model_selection/_search.py:841: Depre
  DeprecationWarning)
Out[141]: GridSearchCV(cv=4, error_score='raise-deprecating',
                 estimator=Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=None,
             normalize=False, random_state=None, solver='auto', tol=0.001),
                 fit_params=None, iid='warn', n_jobs=None,
                 param_grid=[{'alpha': [0.001, 0.1, 1, 10, 100, 1000, 10000, 100000]}],
                 pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
                 scoring=None, verbose=0)
   The object finds the best parameter values on the validation data. We can obtain the estimator
with the best parameters and assign it to the variable BestRR as follows:
In [142]: BestRR=Grid1.best_estimator_
          BestRR
Out[142]: Ridge(alpha=10000, copy_X=True, fit_intercept=True, max_iter=None,
             normalize=False, random_state=None, solver='auto', tol=0.001)
   We now test our model on the test data
In [143]: BestRR.score(x_test[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']], y_te
Out[143]: 0.8411649831036149
   Question #6):
   Perform a grid search for the alpha parameter and the normalization parameter, then find the
best values of the parameters
In [150]: # Write your code below and press Shift+Enter to execute
          parameters2= [{'alpha': [0.001,0.1,1, 10, 100, 10000, 100000, 100000], 'normalize
          Grid2 = GridSearchCV(RR, parameters2,cv=4)
          Grid2.fit(x_data[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg']], y_data)
          BestRR2=Grid2.best_estimator_
          BestRR2, BestRR2.score(x_test[['horsepower', 'curb-weight', 'engine-size', 'highway-mpg
/home/jupyterlab/conda/lib/python3.6/site-packages/sklearn/model_selection/_search.py:841: Depre
  DeprecationWarning)
Out[150]: (Ridge(alpha=0.1, copy_X=True, fit_intercept=True, max_iter=None,
              normalize=True, random_state=None, solver='auto', tol=0.001),
           0.840859719294301)
   Double-click here for the solution.
```

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