CrossValidation2

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Cross Validation2

When performing supervised machine learning analysis, it is common to withhold a portion of the data to test the final model's performance. This model testing is performed on the 'unseen' data, which the model was not trained on. This withholding of a portion of the dataset for testing is called Cross-Validation. Cross-Validation can also be used to select hyper-parameters and test the final model. In this section, we will focus on the test data only.

Cross-Validation also helps avoid over-fitting; a complex model could repeat the labels of the samples that it has just seen and, therefore, would have a perfect score but would fail to predict anything useful on the 'unseen' data. Furthermore, a complex model could just be modeling noise.

Cross validation method involves dividing the dataset into 3 parts:

training set - is a portion of the data used for training the model

validation set - is a portion of the data used to optimize the hyper-parameters of the model. This will be illustrated in the next lab

test set - is a portion of the data used to evaluate if the model generalizes enough to work on the data it was not trained on

Scikit Learn library contains many methods that can perform the splitting of the data into training, testing and validation sets. The most popular methods that we will cover now:

train test split - creates a single split into train and test sets

K-fold - creates number of k-fold splits, allowing cross validation

cross val score - evaluates model's score through cross validation

```
[1]: # Surpress warnings:
    def warn(*args, **kwargs):
        pass
    import warnings
    warnings.warn = warn
```

```
[2]: import pandas as pd
import numpy as np

import seaborn as sns
import matplotlib.pylab as plt
%matplotlib inline
```

```
from sklearn.preprocessing import StandardScaler, Normalizer
     from sklearn.model_selection import train_test_split, cross_val_score, KFold, u
      →GridSearchCV
     from sklearn.metrics import r2_score, mean_squared_error
     from sklearn.feature selection import RFE
     from sklearn.linear_model import LinearRegression
     from sklearn.pipeline import Pipeline
[3]: # load the data
     url = 'https://cf-courses-data.s3.us.cloud-object-storage.appdomain.cloud/
      →IBM-ML240EN-SkillsNetwork/labs/encoded_car_data.csv'
     data = pd.read_csv(url)
     data.head()
[3]:
        diesel
                                  convertible
                                               hardtop
                                                        hatchback
                                                                    sedan
                                                                           wagon \
                gas
                     std
                          turbo
     0
           0.0
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                1.0
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               1.0 1.0
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                                                                      1.0
                                                                             0.0
        4wd ...
                wheelbase curbweight enginesize boreratio horsepower
     0.0 ...
                     88.6
                                2548.0
                                             130.0
                                                         3.47
                                                                     111.0
     1 0.0 ...
                     88.6
                                2548.0
                                             130.0
                                                         3.47
                                                                     111.0
     2 0.0 ...
                                                                     154.0
                     94.5
                                2823.0
                                             152.0
                                                         2.68
     3 0.0 ...
                     99.8
                                                                     102.0
                                2337.0
                                             109.0
                                                         3.19
     4 1.0 ...
                     99.4
                                2824.0
                                             136.0
                                                         3.19
                                                                     115.0
        carlength
                   carwidth
                              citympg
                                      highwaympg
                                                     price
     0
                       64.1
            168.8
                                 21.0
                                             27.0 13495.0
     1
            168.8
                       64.1
                                 21.0
                                             27.0 16500.0
     2
            171.2
                       65.5
                                 19.0
                                             26.0 16500.0
     3
            176.6
                       66.2
                                 24.0
                                             30.0 13950.0
     4
            176.6
                       66.4
                                 18.0
                                             22.0 17450.0
     [5 rows x 36 columns]
[4]: data.dtypes.value_counts()
[4]: float64
     dtype: int64
[5]: data.info()
    <class 'pandas.core.frame.DataFrame'>
    RangeIndex: 205 entries, 0 to 204
```

Data	columns (tota	al 36	6 columns):	
#	Column	Non-	-Null Count	Dtype
0	diesel	205	non-null	float64
1	gas	205	non-null	float64
2	std	205	non-null	float64
3	turbo	205	non-null	float64
4	convertible	205	non-null	float64
5	hardtop	205	non-null	float64
6	hatchback	205	non-null	float64
7	sedan	205	non-null	float64
8	wagon	205	non-null	float64
9	4wd	205	non-null	float64
10	fwd	205	non-null	float64
11	rwd	205	non-null	float64
12	dohc	205	non-null	float64
13	dohcv	205	non-null	float64
14	1	205	non-null	float64
15	ohc	205	non-null	float64
16	ohcf	205	non-null	float64
17	ohcv	205	non-null	float64
18	rotor	205	non-null	float64
19	eight	205	non-null	float64
20	five	205	non-null	float64
21	four	205	non-null	float64
22	six	205	non-null	float64
23	three	205	non-null	float64
24	twelve	205	non-null	float64
25	two	205	non-null	float64
26	wheelbase	205	non-null	float64
27	curbweight	205	non-null	float64
28	enginesize	205	non-null	float64
29	boreratio	205	non-null	float64
30	horsepower	205	non-null	float64
31	carlength	205	non-null	float64
32	carwidth	205	non-null	float64
33	citympg	205	non-null	float64
34	highwaympg	205	non-null	float64
35	price	205	non-null	float64
dtypes: float64(36)				
memory usage: 57.8 KB				

 \rightarrow As we see from above, we now have only numeric parameters.

```
[6]: # split our data into X features and y target.
X = data.drop(columns=['price'])
y = data['price'].copy()
```

Now, let's check some evaluation statistics, such as the coefficient of determination, R^2 , using the built-in method score or r2_score, and the Root Mean Square Error, RMSE, for which we can use the mean_squared_error method, MSE.

The R^2 statistic indicates the percentage of the variance in the dependent variable that the independent variables explain collectively.

Root Mean Square Error (RMSE) is the standard deviation of the residuals (prediction errors). Residuals are a measure of how far from the regression line data points are; RMSE is a measure of how spread out these residuals are. In other words, it tells you how concentrated the data is around the line of best fit.

```
[8]: lr.score(X_train,y_train)
```

[8]: 0.9261981895971949

Using the training data only, the R^2 is ~ 0.93. So, almost 93% of variability in the training data is explained by our model.

```
[9]: lr.score(X_test,y_test)
```

[9]: 0.8500551011878996

```
[10]: # using r2_score with the same result:
print(r2_score(y_true=y_test, y_pred=predicted))
```

0.8500551011878996

Using the test data R^2 , we get ~0.85, not as good as the previous score.

Now, let's calculate the RMSE. The smaller the RMSE number the better our model is. We apply mean_squared_error to our y_test and our predicted data. Then, we take a square root of our MSE, using np.sqrt() function.

```
[11]: mse = mean_squared_error(y_true=y_test, y_pred=predicted)
    rmse = np.sqrt(mse)
    rmse
```

[11]: 3223.172216951375

Prediction Example

Let's select some random data, using iloc and see some predicted versus actual values for the car prices.

```
[12]: some_data = X.iloc[:3]
     some_labels = y.iloc[:3]
     print("Predictions:", lr.predict(some_data))
     print("Labels:", list(some_labels))
     Predictions: [13136.5 13136.5 15331.5]
     Labels: [13495.0, 16500.0, 16500.0]
[13]: predicted = lr.predict(X_test)
     predicted
[13]: array([27673. , 21306.5 , 10731.75, 12098.5 , 26182.5 ,
             8206.75, 7521.25, 10133.25, 9568.25, 17289.25,
                                                              7369.25.
            16499.5 , 10778.75 , 39805.5 , 5530.25 ,
                                                    2453. , 15548.5 ,
            10740.75, 11435.25, 10798. , 15860.5 , 10356. ,
                                                              3644.75.
             6992.5 , 28662.75 , 18291. , 15265.75 , 4490.5 , 16435.25 ,
            26810.75, 5815.5, 4933.75, 16826.5,
                                                    8276.5, 30296.75,
            12268.5 , 12934.25 , 6289.75 , 15975.5 ,
                                                    8184. , 15277.75,
            14764.25, 5273.5, 6240.5, 9097.
                                                    5815.5 , 7237.25,
            16745. , 15406.75, 5050.5 , 21925. ,
                                                   7226.75, 11396.
             4428.25, 16473.5 , 18310. , 12934.25, 29684.25,
                                                              5446.25,
             9815.5 , 17210.5 ])
```

We can also use the pipeline to run operations on our data. For example we can standardize our data then perform linear regression by applying the method fit.

```
[14]: pipe = Pipeline([('ss',StandardScaler() ),('lr', LinearRegression())])
    pipe.fit(X_train,y_train)
    pipe
```

[14]: Pipeline(steps=[('ss', StandardScaler()), ('lr', LinearRegression())])

```
[15]: # Let's calculate the R squared
pipe.score(X_train,y_train)
```

[15]: 0.9262722224294516

 \rightarrow Using the training data only, the R squared is \sim 0.93. Now, let's check the R squared on the test set.

```
[16]: pipe.score(X_test,y_test)
```

[16]: 0.8419174509630335

→ The R squared is much lower. This value provides more accurate evaluation of our model since we test our model on the 'unseen' data set. In case if the R squared is negative, it is because

the model is too complex and the data is overfitting. For more information, please, visit this documentation on overfitting.

This will make more sense when we explore polynomial regression.

Exercise 1

Create a pipeline object called pipe1, replace standardization with normalization. Calculate the R^2 using the built-in method score and for RMSE, using mean_squared_error method.

```
[17]: pipe1 = Pipeline([('norm', Normalizer()),('lr', LinearRegression())])
      pipe1.fit(X_train,y_train)
      # Calculate R2 and RMSE on the test set
      y pred = pipe1.predict(X test)
      r2 = pipe1.score(X_test, y_test)
      rmse = mean_squared_error(y_test, y_pred, squared=False)
      print("R2:", r2)
      print("RMSE:", rmse)
     R2: -1.346604622143935e+18
     RMSE: 9659123380530.787
     Note, you can also use normalize by setting the LinearRegression(normalize=True):
     pipe1 = Pipeline([
         ('norm', Normalizer()),
         ('lr', LinearRegression(normalize=True))
     1)
     # rest of the code is the same
```

One feature

We can use the test data to select a feature with the best performance. We have a list of features:

```
[19]: features=list(X)
print(features, sep=' | ')
```

```
['diesel', 'gas', 'std', 'turbo', 'convertible', 'hardtop', 'hatchback', 'sedan', 'wagon', '4wd', 'fwd', 'rwd', 'dohc', 'dohcv', 'l', 'ohc', 'ohcf', 'ohcv', 'rotor', 'eight', 'five', 'four', 'six', 'three', 'twelve', 'two', 'wheelbase', 'curbweight', 'enginesize', 'boreratio', 'horsepower', 'carlength', 'carwidth', 'citympg', 'highwaympg']
```

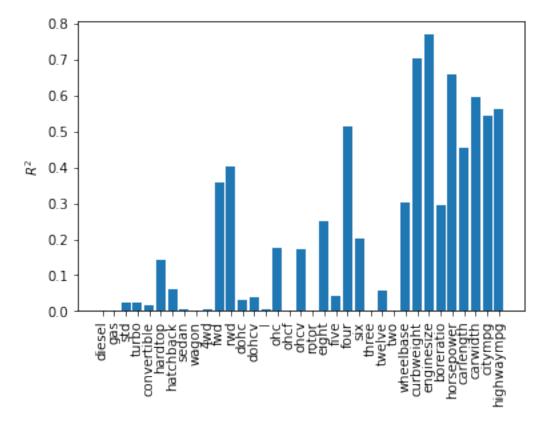
We can train a linear regression model using each feature and use the test data to obtain the best feature.

```
[20]: R_2=[]
pipe = Pipeline([('ss',StandardScaler() ),('lr', LinearRegression())])
for feature in features:
```

```
pipe.fit(X_train[[feature]], y_train)
R_2.append(pipe.score(X_train[[feature]], y_train))
```

We can plot the \mathbb{R}^2 for each feature:

```
[21]: plt.bar(features,R_2)
   plt.xticks(rotation=90)
   plt.ylabel("$R^2$")
   plt.show()
```



Now, we select the feature that works best, using argmax() function.

```
[22]: best=features[np.argmax(R_2)] best
```

[22]: 'enginesize'

So, 'enginesize' is the feature that produces the highest \mathbb{R}^2 . We then train the feature that works best using all the data.

```
[23]: pipe.fit(X[[best]],y)
```

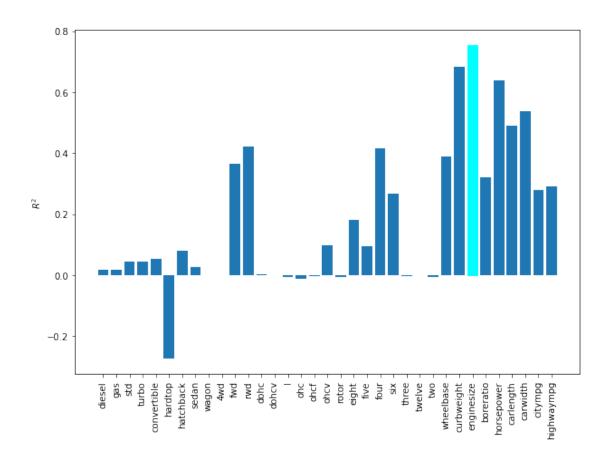
[23]: Pipeline(steps=[('ss', StandardScaler()), ('lr', LinearRegression())])

Exercise 2

Find the best feature using the test data, without standardization.

```
[37]: R_2=[]
      for feature in features:
          lr.fit(X_train[[feature]], y_train)
          R_2.append(lr.score(X_test[[feature]],y_test))
      best = features[np.argmax(R_2)]
      print("\nBest feature using test data w/o standardization:\t", best, "\n")
      best_index = np.argmax(R_2)
      fig, ax = plt.subplots(figsize=(10, 7))
      bars = ax.bar(features, R_2)
      plt.xticks(rotation=90)
      plt.ylabel("$R^2$")
      # Conditional formatting for best bar
      for i in range(len(bars)):
          if R_2[i] == R_2[best_index]:
              bars[i].set_color('cyan')
      plt.show()
```

Best feature using test data w/o standardization: enginesize



K Fold Cross Validation

Cross-validation is a resampling procedure used to evaluate machine learning models on a limited data sample.

The procedure has a single parameter called k that refers to the number of groups that a given data sample is to be split into. As such, the procedure is often called k-fold cross-validation. When a specific value for k is chosen, it may be used in place of k in the reference to the model, such as k=5 becoming 5-fold cross-validation, as shown in the Diagram below. In this case, we would use K-1 (or 4 folds) for testing a 1 fold for training. K-fold is also used for hyper-parameters selection that we will discuss later.

Cross Validation Score

Now, let's use *Scikit-Learn's K-fold cross-validation* method to see whether we can assess the performance of our model. The *K-fold cross-validation* method splits the training set into the number of folds (n_splits), as now in the Diagram above, if we have K folds, K-1 is used for training and one fold is used for testing. The input parameters are as follows:

estimatorestimator: The object to use to fit the data. X: array-like of shape (n_samples, n_features). The data to fit. Can be for example a list, or an array. y: array-like of shape (n_samples,) or (n_samples, n_outputs), default=None. The target variable to try to predict in the case of supervised learning. scoring: A str or a scorer callable object/ function with signature

scorer (estimator, X, y) which should return only a single value. See model evaluation

```
[38]: N=len(X)
N
```

[38]: 205

```
[39]: # create a Linear Regression object
lr = LinearRegression()
# calculate cross validation scores based on our testing sets
scores = cross_val_score(lr, X, y, scoring ="r2", cv=3)
scores
```

[39]: array([0.81508001, 0.7238302 , -0.0913317])

We can calculate mean and standard deviation using the following function of the scores:

```
[40]: def display_scores(scores, print_=False):
    print("Scores:", scores)
    print("Mean:", scores.mean())
    print("Standard deviation:", scores.std())

display_scores(scores)
```

Scores: [0.81508001 0.7238302 -0.0913317]

Mean: 0.4825261694103302

Standard deviation: 0.40748519272512795

The larger the fold, the better the model performance is, as we are using more samples for training; the variance also decreases. Cross Validation Scores are RMSE values for training the data on each of our folds, in our case cv = 3, so we get 3 scores, 1 for each fold.

Exercise 3

Compute the cross validation scores for 5 folds, using the linear regression object 1r and neg_mean_squared_error method for scoring.

```
[44]: lr = LinearRegression()
scores5 = cross_val_score(lr, X, y, scoring='neg_mean_squared_error', cv=5)
scores5 = np.sqrt(-scores5)
display_scores(scores5)
```

Scores: [3155.3045326 11345.67407101 3025.79039538 5629.2248323

5549.16298134]

Mean: 5741.031362524296

Standard deviation: 3017.2786021293505

K Fold

In many cases, we would like to train models that are not available in Scikit-learn or are too large to fit in the memory. We can create a KFold object that Provides train/test indices to split data into train/test sets in an iterative manner.

n_splitsint: A number of folds. Must be at least 2. Changed in version 0.22: n_splits default value changed from 3 to 5. shuffle: Indicates whether to shuffle the data before splitting into batches. Note, the samples within each split will not be shuffled. random_state: the random state.

```
[45]: # We create the `KFold` object `kf`, setting the number of splits to 2.

n_splits=2

kf = KFold(n_splits = n_splits)
```

We train the model using the split(X,y) method. It provides the train/test indices for X and y. Half the data is used for training in the first iteration, and the rest is used for testing and displaying the indexes for each set. For the second iteration, the data used for training is used for testing, and the testing data is used for training. We store the R^2 for each iteration in the array R_2. The np.zeros() function returns a new array of given shape and type, filled with zeros. Then, we calculate the R^2 for each of the X train and X test splits.

```
[46]: y = data['price'].copy()
    X = data.drop(columns=['price'])
    R_2 = np.zeros((n_splits,1))
    pipe = Pipeline([('ss',StandardScaler() ),('lr', LinearRegression())])
    n = 0

for k,(train_index, test_index) in enumerate(kf.split(X,y)):
    print("TRAIN:", train_index)
    print("TEST:", test_index)
    X_train, X_test = X.iloc[train_index], X.iloc[test_index]

    y_train, y_test = y[train_index], y[test_index]
    pipe.fit(X_train, y_train)
    n += 1
    R_2[k]=pipe.score(X_test, y_test)
```

```
TRAIN: [103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138
 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156
 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174
 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192
 193 194 195 196 197 198 199 200 201 202 203 204]
                                                                    14
TEST: [
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                                        99 100 101 102]
  90
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              93
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                            96
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TRAIN: [
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```

```
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                                       99 100 101 102]
     91
                          96
                                   98
TEST: [103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138
 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156
 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174
 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192
 193 194 195 196 197 198 199 200 201 202 203 204]
```

We can calculate the average R^2 :

```
[47]: R_2.mean()
```

[47]: 0.39256530180315163

If we set the number of splits to three, we see 2/3's of the data is used for training.

```
[48]: n_{splits} = 3
      kf = KFold(n_splits = n_splits)
      y = data['price'].copy()
      X = data.drop(columns=['price'])
      R_2 = np.zeros((n_splits, 1))
      pipe = Pipeline([('ss',StandardScaler() ),('lr', LinearRegression())])
      n = 0
      for k,(train_index, test_index) in enumerate(kf.split(X,y)):
          print("TRAIN:", train index)
          print("TEST:", test_index)
          X_train, X_test = X.iloc[train_index], X.iloc[test_index]
          y_train, y_test = y[train_index], y[test_index]
          pipe.fit(X_train, y_train)
          n += 1
          R_2[k] = pipe.score(X_test, y_test)
      R_2.mean()
```

```
70 71 72
                        73
                            74 75
                                    76
                                            78
                                               79
                                                        81 82
TRAIN: [ 69
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                                                99 100 101 102 103 104
 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122
 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140
 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158
 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176
 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194
 195 196 197 198 199 200 201 202 203 204]
```

```
TEST: [ 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68]
TRAIN: [
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[48]: 0.47719341451693237

Exercise 4

It many applications, it is useful to randomly select samples for K fold cross validation. In this Exercise, randomly select samples by setting shuffle to True in the KFold constructor. Use all the parameters, as above.

```
[49]: n_splits = 3
kf = KFold(n_splits=n_splits, shuffle=True, random_state=42)
y = data['price'].copy()
X = data.drop(columns=['price'])
R_2 = np.zeros((n_splits, 1))
pipe = Pipeline([('ss', StandardScaler()), ('lr', LinearRegression())])
n = 0
for k, (train_index, test_index) in enumerate(kf.split(X, y)):
    print("TRAIN:", train_index)
    print("TEST:", test_index)
X_train, X_test = X.iloc[train_index], X.iloc[test_index]
y_train, y_test = y[train_index], y[test_index]
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n += 1
         R_2[k] = pipe.score(X_test, y_test)
     R_2.mean()
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[49]: 0.6904823744622521
```

pipe.fit(X_train, y_train)

[]: