ML0101EN-Clus-Hierarchical-Cars-py-v1

November 29, 2018

#

Hierarchical Clustering

Welcome to Lab of Hierarchical Clustering with Python using Scipy and Scikit-learn package.

1 Hierarchical Clustering - Agglomerative

We will be looking at a clustering technique, which is Agglomerative Hierarchical Clustering. Remember that agglomerative is the bottom up approach. In this lab, we will be looking at Agglomerative clustering, which is more popular than Divisive clustering. We will also be using Complete Linkage as the Linkage Criteria. NOTE: You can also try using Average Linkage wherever Complete Linkage would be used to see the difference!

```
In [1]: import numpy as np
        import pandas as pd
        from scipy import ndimage
        from scipy.cluster import hierarchy
        from scipy.spatial import distance_matrix
        from matplotlib import pyplot as plt
        from sklearn import manifold, datasets
        from sklearn.cluster import AgglomerativeClustering
        from sklearn.datasets.samples_generator import make_blobs
%matplotlib inline
```

1.0.1 Generating Random Data

We will be generating a set of data using the make_blobs class. Input these parameters into make_blobs:

```
<b>n_samples</b>: The total number of points equally divided among clusters. 
 Choose a number from 10-1500 
 <b>centers</b>: The number of centers to generate, or the fixed center locations. 
 Choose arrays of x,y coordinates for generating the centers. Have 1-10 centers (ex. ce
<b>cli> <b>cluster_std</b>: The standard deviation of the clusters. The larger the number, the furt
 Choose a number between 0.5-1.5
```

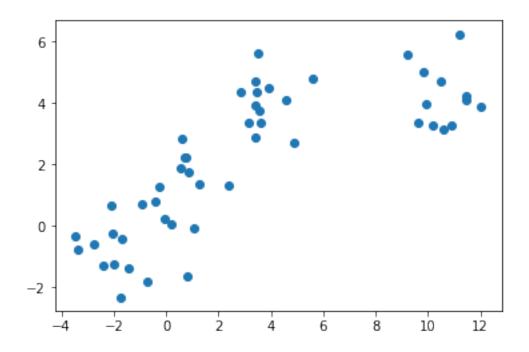
Save the result to X1 and y1.

In [2]: X1, y1 = make_blobs(n_samples=50, centers=[[4,4], [-2, -1], [1, 1], [10,4]], cluster_std

Plot the scatter plot of the randomly generated data

```
In [3]: plt.scatter(X1[:, 0], X1[:, 1], marker='o')
```

Out[3]: <matplotlib.collections.PathCollection at 0x7f761d233400>



1.0.2 Agglomerative Clustering

We will start by clustering the random data points we just created.

The Agglomerative Clustering class will require two inputs:

```
<b>n_clusters</b>: The number of clusters to form as well as the number of centroids to ger
 Value will be: 4  
<b>linkage</b>: Which linkage criterion to use. The linkage criterion determines which dist

Value will be: 'complete' 
Value will be: 'complete' 
<b>Note</b>: It is recommended you try everything with 'average' as well
```

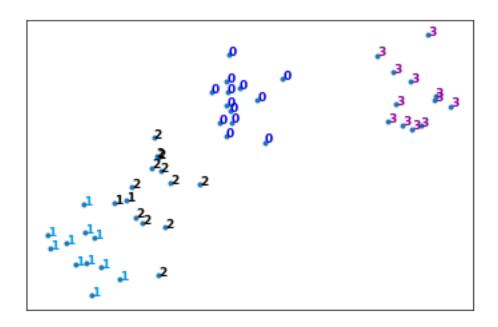
Save the result to a variable called agglom

```
In [4]: agglom = AgglomerativeClustering(n_clusters = 4, linkage = 'average')
#agglom = AgglomerativeClustering(n_clusters = 4, linkage = 'complete')
```

Fit the model with X2 and y2 from the generated data above.

Run the following code to show the clustering! Remember to read the code and comments to gain more understanding on how the plotting works.

```
In [6]: # Create a figure of size 6 inches by 4 inches.
        plt.figure(figsize=(6,4))
        # These two lines of code are used to scale the data points down,
        # Or else the data points will be scattered very far apart.
        # Create a minimum and maximum range of X1.
        x_{min}, x_{max} = np.min(X1, axis=0), np.max(X1, axis=0)
        # Get the average distance for X1.
        X1 = (X1 - x_min) / (x_max - x_min)
        # This loop displays all of the datapoints.
        for i in range(X1.shape[0]):
            # Replace the data points with their respective cluster value
            # (ex. 0) and is color coded with a colormap (plt.cm.spectral)
            plt.text(X1[i, 0], X1[i, 1], str(y1[i]),
                     color=plt.cm.nipy_spectral(agglom.labels_[i] / 10.),
                     fontdict={'weight': 'bold', 'size': 9})
        # Remove the x ticks, y ticks, x and y axis
        plt.xticks([])
        plt.yticks([])
        #plt.axis('off')
        # Display the plot of the original data before clustering
        plt.scatter(X1[:, 0], X1[:, 1], marker='.')
        # Display the plot
        plt.show()
```



1.0.3 Dendrogram Associated for the Agglomerative Hierarchical Clustering

Remember that a distance matrix contains the distance from each point to every other point of a dataset . Use the function distance_matrix, which requires two inputs. Use the Feature Matrix, X2 as both inputs and save the distance matrix to a variable called dist_matrix Remember that the distance values are symmetric, with a diagonal of 0's. This is one way of making sure your matrix is correct. (print out dist_matrix to make sure it's correct)

```
In [7]: dist_matrix = distance_matrix(X1,X1)
       print(dist_matrix)
[[0.
           Γ0.7127667 0.
                     0.73318222 ... 0.88954675 1.09165685 0.85612432]
 [0.12820861 0.73318222 0.
                               ... 0.1693065 0.37318947 0.14118721]
 [0.26923777 0.88954675 0.1693065 ... 0.
                                            0.20513762 0.034014 ]
 [0.45732344 1.09165685 0.37318947 ... 0.20513762 0.
                                                     0.23712687]
 [0.25001
           0.85612432 0.14118721 ... 0.034014
                                           0.23712687 0.
                                                              ]]
```

Using the linkage class from hierarchy, pass in the parameters:

```
 The distance matrix 
'complete' for complete linkage 

Save the result to a variable called Z

In [8]: Z = hierarchy.linkage(dist_matrix, 'complete')
```

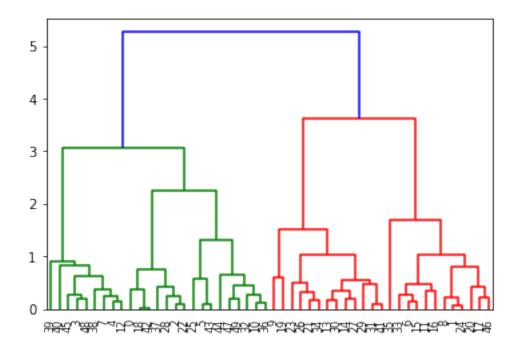
/home/jupyterlab/conda/lib/python3.6/site-packages/ipykernel_launcher.py:1: ClusterWarning: scip """Entry point for launching an IPython kernel.

A Hierarchical clustering is typically visualized as a dendrogram as shown in the following cell. Each merge is represented by a horizontal line. The y-coordinate of the horizontal line is the similarity of the two clusters that were merged, where cities are viewed as singleton clusters. By moving up from the bottom layer to the top node, a dendrogram allows us to reconstruct the history of merges that resulted in the depicted clustering.

Next, we will save the dendrogram to a variable called dendro. In doing this, the dendrogram will also be displayed. Using the dendrogram class from hierarchy, pass in the parameter:

Z

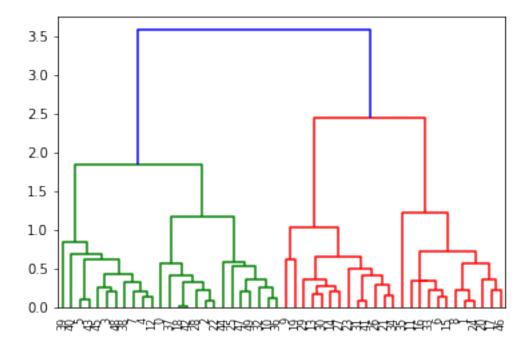
In [9]: dendro = hierarchy.dendrogram(Z)



1.1 Practice

We used **complete** linkage for our case, change it to **average** linkage to see how the dendogram changes.

/home/jupyterlab/conda/lib/python3.6/site-packages/ipykernel_launcher.py:2: ClusterWarning: scip



Double-click **here** for the solution.

2 Clustering on Vehicle dataset

Imagine that an automobile manufacturer has developed prototypes for a new vehicle. Before introducing the new model into its range, the manufacturer wants to determine which existing vehicles on the market are most like the prototypes--that is, how vehicles can be grouped, which group is the most similar with the model, and therefore which models they will be competing against.

Our objective here, is to use clustering methods, to find the most distinctive clusters of vehicles. It will summarize the existing vehicles and help manufacturers to make decision about the supply of new models.

2.0.1 Download data

To download the data, we will use !wget to download it from IBM Object Storage.

Did you know? When it comes to Machine Learning, you will likely be working with large datasets. As a business, where can you host your data? IBM is offering a unique opportunity for businesses, with 10 Tb of IBM Cloud Object Storage: Sign up now for free

In [11]: !wget -O cars_clus.csv https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data-courses-dat

2.1 Read data

lets read dataset to see what features the manufacturer has collected about the existing models.

```
In [12]: #filename = 'cars_clus.csv'
        #Read csv
        #pdf = pd.read_csv(filename)
        pdf = pd.read_csv('cars_clus.csv')
        print ("Shape of dataset: ", pdf.shape)
        print('Column Names:', list(pdf))
        pdf.head(5)
Shape of dataset: (159, 16)
Column Names: ['manufact', 'model', 'sales', 'resale', 'type', 'price', 'engine_s', 'horsepow',
Out[12]:
          manufact
                      model
                              sales resale
                                             type
                                                    price engine_s horsepow wheelbas
             Acura Integra 16.919 16.360 0.000 21.500
                                                             1.800 140.000 101.200
        0
        1
             Acura
                         TL 39.384 19.875 0.000 28.400
                                                             3.200 225.000 108.100
        2
                         CL 14.114 18.225 0.000 $null$
                                                             3.200 225.000 106.900
             Acura
                              8.588 29.725 0.000 42.000
        3
                         RL
                                                             3.500 210.000 114.600
             Acura
        4
              Audi
                         A4 20.397 22.255 0.000 23.990
                                                             1.800 150.000 102.600
            width
                   length curb_wgt fuel_cap
                                                mpg lnsales
                                                            partition
        0 67.300 172.400
                              2.639
                                     13.200 28.000
                                                      2.828
                                                                   0.0
        1 70.300 192.900
                              3.517
                                     17.200 25.000
                                                      3.673
                                                                   0.0
        2 70.600 192.000
                              3.470
                                     17.200 26.000
                                                      2.647
                                                                   0.0
        3 71.400 196.600
                              3.850
                                     18.000 22.000
                                                                   0.0
                                                      2.150
        4 68.200 178.000
                              2.998
                                     16.400 27.000
                                                      3.015
                                                                   0.0
```

The feature sets include price in thousands (price), engine size (engine_s), horsepower (horsepow), wheelbase (wheelbas), width (width), length (length), curb weight (curb_wgt), fuel capacity (fuel_cap) and fuel efficiency (mpg).

2.1.1 Data Cleaning

lets simply clear the dataset by dropping the rows that have null value:

```
In [13]: print ("Shape of dataset before cleaning: ", pdf.size)
        print('\n')
        pdf[[ 'sales', 'resale', 'type', 'price', 'engine_s',
                'horsepow', 'wheelbas', 'width', 'length', 'curb_wgt', 'fuel_cap',
                'mpg', 'lnsales']] = pdf[['sales', 'resale', 'type', 'price', 'engine_s',
                'horsepow', 'wheelbas', 'width', 'length', 'curb_wgt', 'fuel_cap',
                'mpg', 'lnsales']].apply(pd.to_numeric, errors='coerce')
        pdf = pdf.dropna()
        pdf = pdf.reset_index(drop=True)
        print ("Shape of dataset after cleaning: ", pdf.size)
        pdf.head(5)
Shape of dataset before cleaning:
Shape of dataset after cleaning: 1872
Out[13]:
          manufact
                      model
                              sales resale type price engine_s
                                                                   horsepow \
             Acura Integra 16.919 16.360
                                                                       140.0
                                              0.0 21.50
                                                               1.8
        0
        1
                         TL 39.384 19.875
                                              0.0 28.40
                                                               3.2
                                                                       225.0
             Acura
        2
                                              0.0 42.00
             Acura
                         R.I.
                              8.588 29.725
                                                               3.5
                                                                       210.0
        3
              Audi
                         A4 20.397 22.255
                                              0.0 23.99
                                                               1.8
                                                                       150.0
        4
              Audi
                         A6 18.780 23.555
                                              0.0 33.95
                                                               2.8
                                                                       200.0
           wheelbas width length curb_wgt fuel_cap
                                                         mpg lnsales partition
        0
              101.2
                      67.3
                             172.4
                                       2.639
                                                  13.2 28.0
                                                                2.828
                                                                             0.0
              108.1
                      70.3 192.9
                                                                             0.0
        1
                                       3.517
                                                  17.2 25.0
                                                                3.673
        2
              114.6
                     71.4 196.6
                                       3.850
                                                  18.0 22.0
                                                                2.150
                                                                             0.0
        3
                      68.2
                                                  16.4 27.0
              102.6
                             178.0
                                       2.998
                                                                3.015
                                                                             0.0
              108.7
                      76.1 192.0
                                       3.561
                                                  18.5 22.0
                                                                2.933
                                                                             0.0
```

2.1.2 Feature selection

Lets select our feature set:

```
In [14]: featureset = pdf[['engine_s', 'horsepow', 'wheelbas', 'width', 'length', 'curb_wgt', '
```

2.1.3 Normalization

Now we can normalize the feature set. **MinMaxScaler** transforms features by scaling each feature to a given range. It is by default (0, 1). That is, this estimator scales and translates each feature individually such that it is between zero and one.

2.2 Clustering using Scipy

In this part we use Scipy package to cluster the dataset: First, we calculate the distance matrix.

In agglomerative clustering, at each iteration, the algorithm must update the distance matrix to reflect the distance of the newly formed cluster with the remaining clusters in the forest. The following methods are supported in Scipy for calculating the distance between the newly formed cluster and each: - single - complete - average - weighted - centroid

We use **complete** for our case, but feel free to change it to see how the results change.

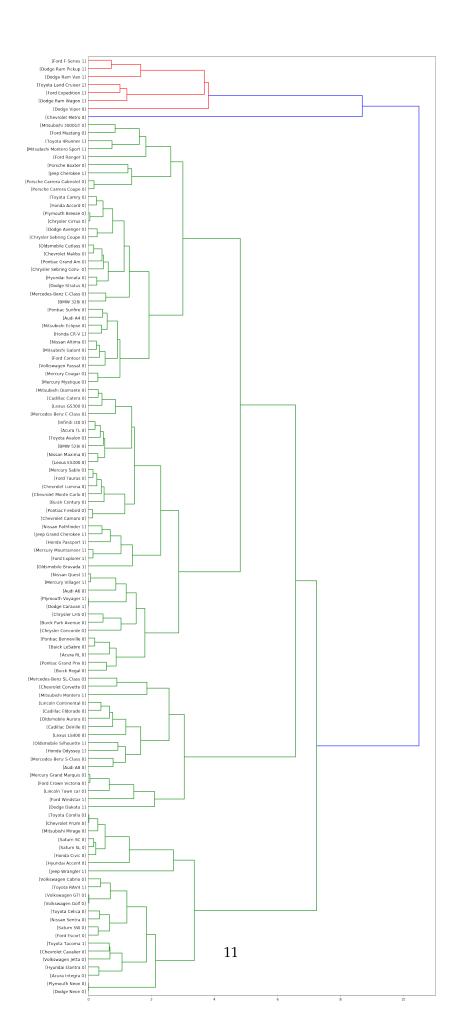
/home/jupyterlab/conda/lib/python3.6/site-packages/ipykernel_launcher.py:3: ClusterWarning: scip This is separate from the ipykernel package so we can avoid doing imports until

Essentially, Hierarchical clustering does not require a pre-specified number of clusters. However, in some applications we want a partition of disjoint clusters just as in flat clustering. So you can use a cutting line:

```
6,
Out[18]: array([ 1, 5, 5,
                               5, 4, 6, 5, 5, 5, 5, 4, 4, 5,
                                                                              6,
                                               5,
                                                       5,
                5,
                    5,
                        5,
                            4,
                                2, 11,
                                       6,
                                           6,
                                                   6,
                                                           1,
                                                               6,
                                                                  6, 10,
                                                                              8,
                9, 3,
                               7,
                                           3,
                                               5,
                                                   3,
                                                           7,
                                                               9,
                                                                  2,
                                                                              5,
                        5,
                           1,
                                   6,
                                       5,
                                                       8,
                                                                      6,
                4, 2,
                        1,
                            6,
                               5,
                                   2,
                                       7,
                                           5,
                                               5,
                                                   5,
                                                       4,
                                                           4,
                                                               3,
                                                                  2,
                                                                      6,
                                                                              5,
                               6,
                                       3,
                                           5,
                                               5,
                                                   6,
                7, 4,
                       7,
                            6,
                                   5,
                                                       5,
                                                           4,
                                                               4,
                                                                  1,
                       4,
                            5,
                                           5,
                                               6,
                                                   6,
                                                          5,
                5, 6,
                               4,
                                   1,
                                       6,
                                                       5,
                                                              5,
                            6,
                2, 1,
                        2,
                               5,
                                  1, 1,
                                          1,
                                               7,
                                                   8, 1,
                                                          1,
                                                               6,
                                                                 1,
              dtype=int32)
```

Also, you can determine the number of clusters directly:

Now, plot the dendrogram:



2.3 Clustering using scikit-learn

Lets redo it again, but this time using scikit-learn package:

Now, we can use the 'AgglomerativeClustering' function from scikit-learn library to cluster the dataset. The AgglomerativeClustering performs a hierarchical clustering using a bottom up approach. The linkage criteria determines the metric used for the merge strategy:

- Ward minimizes the sum of squared differences within all clusters. It is a varianceminimizing approach and in this sense is similar to the k-means objective function but tackled with an agglomerative hierarchical approach.
- Maximum or complete linkage minimizes the maximum distance between observations of pairs of clusters.
- Average linkage minimizes the average of the distances between all observations of pairs of clusters.

And, we can add a new field to our dataframe to show the cluster of each row:

```
2
              Acura
                               8.588 29.725
                                               0.0 42.00
                                                                 3.5
                                                                         210.0
                          RL
                                               0.0 23.99
                                                                         150.0
         3
               Audi
                          A4 20.397 22.255
                                                                 1.8
         4
               Audi
                          A6 18.780 23.555
                                               0.0 33.95
                                                                 2.8
                                                                         200.0
            wheelbas width
                             length
                                    curb_wgt
                                               fuel_cap
                                                           mpg
                                                               lnsales
                                                                         partition \
         0
               101.2
                       67.3
                              172.4
                                        2.639
                                                    13.2
                                                         28.0
                                                                  2.828
                                                                               0.0
               108.1
                       70.3
                                        3.517
                                                    17.2 25.0
                                                                               0.0
         1
                              192.9
                                                                  3.673
         2
               114.6
                       71.4
                              196.6
                                        3.850
                                                    18.0 22.0
                                                                  2.150
                                                                               0.0
                                                                  3.015
                                                                               0.0
         3
               102.6
                       68.2
                              178.0
                                        2.998
                                                    16.4 27.0
         4
               108.7
                       76.1
                              192.0
                                        3.561
                                                    18.5 22.0
                                                                  2.933
                                                                               0.0
            cluster_
         0
                   1
                   2
         1
         2
                   2
         3
                   1
         4
                   2
In [24]: import matplotlib.cm as cm
         n_clusters = max(agglom.labels_)+1
         colors = cm.rainbow(np.linspace(0, 1, n_clusters))
         cluster_labels = list(range(0, n_clusters))
         # Create a figure of size 6 inches by 4 inches.
         plt.figure(figsize=(16,14))
         for color, label in zip(colors, cluster_labels):
             subset = pdf[pdf.cluster_ == label]
             for i in subset.index:
                     plt.text(subset.horsepow[i], subset.mpg[i],str(subset['model'][i]), rotation
             plt.scatter(subset.horsepow, subset.mpg, s= subset.price*10, c=color, label='cluster'
             plt.scatter(subset.horsepow, subset.mpg)
         plt.legend()
         plt.title('Clusters')
         plt.xlabel('horsepow')
         plt.ylabel('mpg')
Out[24]: Text(0,0.5,'mpg')
```

0.0 28.40

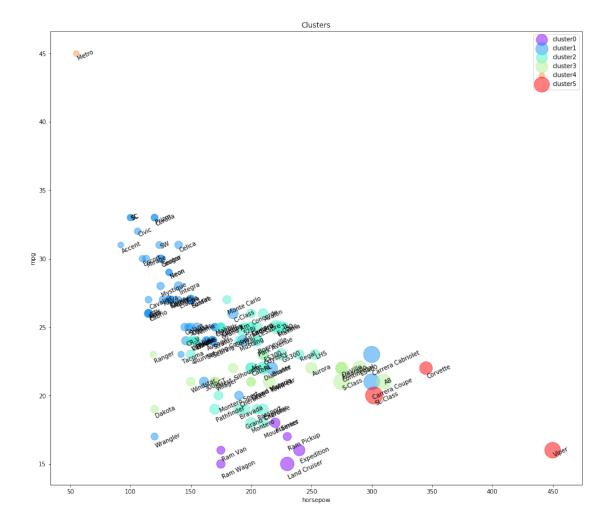
3.2

225.0

1

Acura

TL 39.384 19.875



As you can see, we are seeing the distribution of each cluster using the scatter plot, but it is not very clear where is the centroid of each cluster. Moreover, there are 2 types of vehicles in our dataset, "truck" (value of 1 in the type column) and "car" (value of 1 in the type column). So, we use them to distinguish the classes, and summarize the cluster. First we count the number of cases in each group:

```
In [25]: pdf.groupby(['cluster_','type'])['cluster_'].count()
```

Out[25]:	cluste	r_	type		
	0		1.0	6	
	1		0.0	47	
			1.0	5	
	2		0.0	27	
			1.0	11	
	3		0.0	10	
			1.0	7	
	4		0.0	1	
	5		0.0	3	
	Name:	clus	ter_,	dtype:	int64

Now we can look at the characteristics of each cluster:

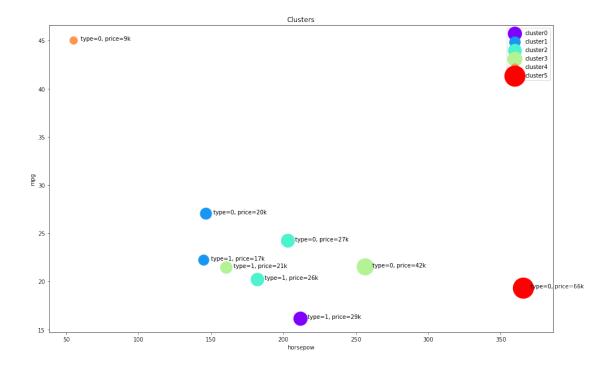
```
In [26]: agg_cars = pdf.groupby(['cluster_','type'])['horsepow','engine_s','mpg','price'].mean()
        agg_cars
Out [26]:
                         horsepow engine_s
                                                          price
                                                  mpg
        cluster_ type
                       211.666667 4.483333 16.166667 29.024667
                 1.0
        1
                 0.0
                       146.531915 2.246809 27.021277 20.306128
                 1.0
                     145.000000 2.580000 22.200000 17.009200
                      203.111111 3.303704 24.214815 27.750593
        2
                 0.0
                 1.0
                     182.090909 3.345455 20.181818 26.265364
                 0.0 256.500000 4.410000 21.500000 42.870400
        3
                 1.0
                      160.571429 3.071429 21.428571 21.527714
        4
                 0.0
                        55.000000 1.000000 45.000000
                                                      9.235000
        5
                 0.0
                       365.666667 6.233333 19.333333 66.010000
```

It is obvious that we have 3 main clusters with the majority of vehicles in those.

Cars: - Cluster 1: with almost high mpg, and low in horsepower. - Cluster 2: with good mpg and horsepower, but higher price than average. - Cluster 3: with low mpg, high horsepower, highest price.

Trucks: - Cluster 1: with almost highest mpg among trucks, and lowest in horsepower and price. - Cluster 2: with almost low mpg and medium horsepower, but higher price than average. - Cluster 3: with good mpg and horsepower, low price.

Please notice that we did not use **type**, and **price** of cars in the clustering process, but Hierarchical clustering could forge the clusters and discriminate them with quite high accuracy.



2.4 Want to learn more?

IBM SPSS Modeler is a comprehensive analytics platform that has many machine learning algorithms. It has been designed to bring predictive intelligence to decisions made by individuals, by groups, by systems – by your enterprise as a whole. A free trial is available through this course, available here: SPSS Modeler.

Also, you can use Watson Studio to run these notebooks faster with bigger datasets. Watson Studio is IBM's leading cloud solution for data scientists, built by data scientists. With Jupyter notebooks, RStudio, Apache Spark and popular libraries pre-packaged in the cloud, Watson Studio enables data scientists to collaborate on their projects without having to install anything. Join the fast-growing community of Watson Studio users today with a free account at Watson Studio

2.4.1 Thanks for completing this lesson!

Notebook created by: Saeed Aghabozorgi

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