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Hierarchical Clustering

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

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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
```

Generating Random Data

We will be generating a set of data using the **make_blobs** class.

Input these parameters into **make_blobs**:

- **n_samples**: The total number of points equally divided among clusters.
 - Choose a number from 10-1500
- **centers**: 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. centers=[[1,1], [2,5]])
- **cluster_std**: The standard deviation of the clusters. The larger the number, the further apart the clusters
 - Choose a number between 0.5-1.5

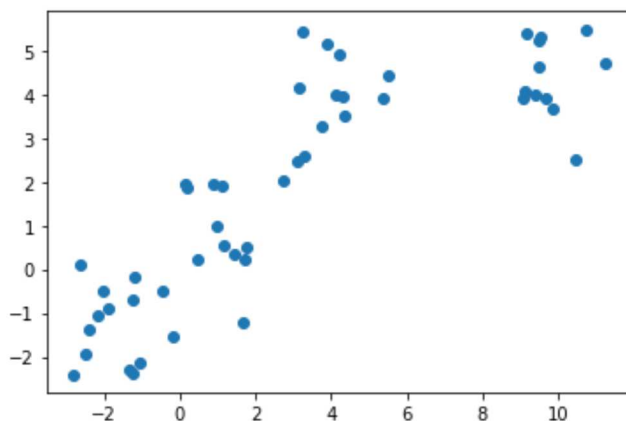
Save the result to **X1** and **y1**.

```
In [2]: X1, y1 = make_blobs(n_samples=50, centers=[[4,4], [-2, -1], [1, 1], [10,4]], cluster_std=0.9)
```

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 0x7fe205facef0>
```



Agglomerative Clustering

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

The **Agglomerative Clustering** class will require two inputs:

- **n_clusters**: The number of clusters to form as well as the number of centroids to generate.
 - Value will be: 4
- **linkage**: Which linkage criterion to use. The linkage criterion determines which distance to use between sets of observation. The algorithm will merge the pairs of cluster that minimize this criterion.
 - Value will be: 'complete'
 - **Note**: It is recommended you try everything with 'average' as well

Save the result to a variable called **agglom**

```
In [9]: #agglom = AgglomerativeClustering(n_clusters = 4, linkage = 'complete')
        #grey2018: average
        agglom = AgglomerativeClustering(n_clusters = 4, linkage = 'average')
```

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

```
In [10]: agglom.fit(X1,y1)
```

```
Out[10]: AgglomerativeClustering(affinity='euclidean', compute_full_tree='auto',
                                   connectivity=None, linkage='average', memory=None,
                                   n_clusters=4, pooling_func='deprecated')
```

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 [11]: # 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)

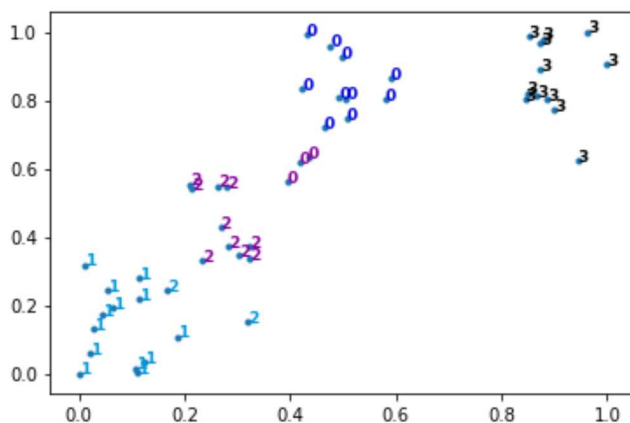
# Get the average distance for X1.
X1 = (X1 - x_min) / (x_max - x_min)

# 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()

```



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 [12]: dist_matrix = distance_matrix(X1,X1)
print(dist_matrix)

[[0.          1.03146211  1.1634196  ...  0.34090011  0.1809246  0.88282608]
 [1.03146211  0.          0.45545431  ...  0.69148334  0.88161428  0.19589229]
 [1.1634196   0.45545431  0.          ...  0.84973996  1.06746063  0.38911151]
 ...
 [0.34090011  0.69148334  0.84973996  ...  0.          0.21774462  0.54342848]
 [0.1809246   0.88161428  1.06746063  ...  0.21774462  0.          0.75048746]
 [0.88282608  0.19589229  0.38911151  ...  0.54342848  0.75048746  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 [13]: z = hierarchy.linkage(dist_matrix, 'complete')

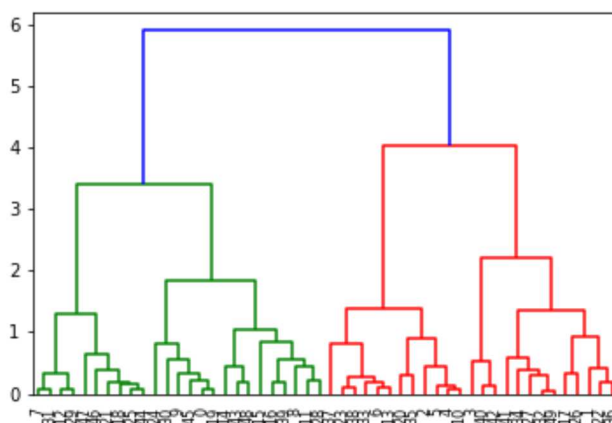
/home/jupyterlab/conda/envs/python/lib/python3.6/site-packages/ipykernel_launcher.py:1: ClusterWarning: scipy.cluster: The symmetric non-negative hollow observation matrix looks suspiciously like an uncondensed distance matrix
  """Entry point for launching an IPython kernel.
```

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 [14]: dendro = hierarchy.dendrogram(Z)
```

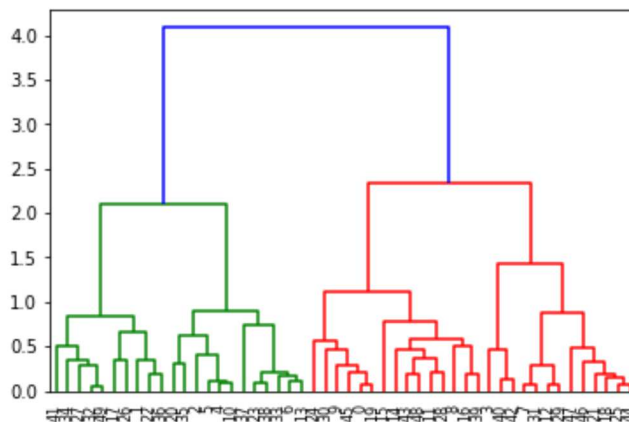


Practice

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

```
In [17]: # write your code here
Z2 = hierarchy.linkage(dist_matrix, "average")
dendro2 = hierarchy.dendrogram(Z2)
```

```
/home/jupyterlab/conda/envs/python/lib/python3.6/site-packages/ipykernel_launcher.py:2: ClusterWarning: scipy.cluster: The symmetric non-negative hollow observation matrix looks suspiciously like an uncondensed distance matrix
```



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

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.

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 \(http://cocl.us/ML0101EN-IBM-Offer-CC\)](http://cocl.us/ML0101EN-IBM-Offer-CC)

```
In [18]: !wget -O cars_clus.csv https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data/CognitiveClass/ML0101ENv3/labs/cars_clus.csv

--2020-02-04 14:23:59-- https://s3-api.us-geo.objectstorage.softlayer.net/cf-courses-data/CognitiveClass/ML0101ENv3/labs/cars_clus.csv
Resolving s3-api.us-geo.objectstorage.softlayer.net (s3-api.us-geo.objectstorage.softlayer.net)... 67.228.254.196
Connecting to s3-api.us-geo.objectstorage.softlayer.net (s3-api.us-geo.objectstorage.softlayer.net)|67.228.254.196|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 17774 (17K) [text/csv]
Saving to: 'cars_clus.csv'

cars_clus.csv      100%[=====>]  17.36K  --.-KB/s    in 0.02s

2020-02-04 14:23:59 (847 KB/s) - 'cars_clus.csv' saved [17774/17774]
```

Read data

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

```
In [19]: filename = 'cars_clus.csv'

#Read csv
pdf = pd.read_csv(filename)
print ("Shape of dataset: ", pdf.shape)

pdf.head(5)
```

Shape of dataset: (159, 16)

Out[19]:

	manufact	model	sales	resale	type	price	engine_s	horsepow	wheelbas	width	length	curb_
0	Acura	Integra	16.919	16.360	0.000	21.500	1.800	140.000	101.200	67.300	172.400	2.
1	Acura	TL	39.384	19.875	0.000	28.400	3.200	225.000	108.100	70.300	192.900	3.
2	Acura	CL	14.114	18.225	0.000	\$null\$	3.200	225.000	106.900	70.600	192.000	3.
3	Acura	RL	8.588	29.725	0.000	42.000	3.500	210.000	114.600	71.400	196.600	3.
4	Audi	A4	20.397	22.255	0.000	23.990	1.800	150.000	102.600	68.200	178.000	2.

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).

Data Cleaning

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

```
In [20]: print ("Shape of dataset before cleaning: ", pdf.size)
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: 2544

Shape of dataset after cleaning: 1872

Out[20]:

	manufact	model	sales	resale	type	price	engine_s	horsepow	wheelbas	width	length	curb_wgt
0	Acura	Integra	16.919	16.360	0.0	21.50	1.8	140.0	101.2	67.3	172.4	2.639
1	Acura	TL	39.384	19.875	0.0	28.40	3.2	225.0	108.1	70.3	192.9	3.517
2	Acura	RL	8.588	29.725	0.0	42.00	3.5	210.0	114.6	71.4	196.6	3.850
3	Audi	A4	20.397	22.255	0.0	23.99	1.8	150.0	102.6	68.2	178.0	2.998
4	Audi	A6	18.780	23.555	0.0	33.95	2.8	200.0	108.7	76.1	192.0	3.561

Feature selection

Lets select our feature set:

```
In [22]: featureset = pdf[['engine_s', 'horsepow', 'wheelbas', 'width', 'length', 'curb_wgt',
                           'fuel_cap', 'mpg']]
```

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.

```
In [23]: from sklearn.preprocessing import MinMaxScaler
x = featureset.values #returns a numpy array
min_max_scaler = MinMaxScaler()
feature_mtx = min_max_scaler.fit_transform(x)
feature_mtx [0:5]
```

```
Out[23]: array([[0.11428571, 0.21518987, 0.18655098, 0.28143713, 0.30625832,
                  0.2310559 , 0.13364055, 0.43333333],
                 [0.31428571, 0.43037975, 0.3362256 , 0.46107784, 0.5792277 ,
                  0.50372671, 0.31797235, 0.33333333],
                 [0.35714286, 0.39240506, 0.47722343, 0.52694611, 0.62849534,
                  0.60714286, 0.35483871, 0.23333333],
                 [0.11428571, 0.24050633, 0.21691974, 0.33532934, 0.38082557,
                  0.34254658, 0.28110599, 0.4          ],
                 [0.25714286, 0.36708861, 0.34924078, 0.80838323, 0.56724368,
                  0.5173913 , 0.37788018, 0.23333333]])
```

Clustering using Scipy

In this part we use Scipy package to cluster the dataset:

First, we calculate the distance matrix.


```
In [24]: import scipy
leng = feature_mtx.shape[0]
D = scipy.zeros([leng,leng])
for i in range(leng):
    for j in range(leng):
        D[i,j] = scipy.spatial.distance.euclidean(feature_mtx[i], feature_mtx[j])
```

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.

```
In [25]: import pylab
import scipy.cluster.hierarchy
Z = hierarchy.linkage(D, 'complete')
```

/home/jupyterlab/conda/envs/python/lib/python3.6/site-packages/ipykernel_launcher.py:3: ClusterWarning: scipy.cluster: The symmetric non-negative hollow observation matrix looks suspiciously like an uncondensed distance matrix
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:

```
In [26]: from scipy.cluster.hierarchy import fcluster
max_d = 3
clusters = fcluster(Z, max_d, criterion='distance')
clusters
```

```
Out[26]: array([ 1,  5,  5,  6,  5,  4,  6,  5,  5,  5,  5,  5,  4,  4,  5,  1,  6,
                5,  5,  5,  4,  2, 11,  6,  6,  5,  6,  5,  1,  6,  6, 10,  9,  8,
                9,  3,  5,  1,  7,  6,  5,  3,  5,  3,  8,  7,  9,  2,  6,  6,  5,
                4,  2,  1,  6,  5,  2,  7,  5,  5,  5,  4,  4,  3,  2,  6,  6,  5,
                7,  4,  7,  6,  6,  5,  3,  5,  5,  6,  5,  4,  4,  1,  6,  5,  5,
                5,  6,  4,  5,  4,  1,  6,  5,  6,  6,  5,  5,  5,  7,  7,  7,  2,
                2,  1,  2,  6,  5,  1,  1,  1,  7,  8,  1,  1,  6,  1,  1],
                dtype=int32)
```

Also, you can determine the number of clusters directly:

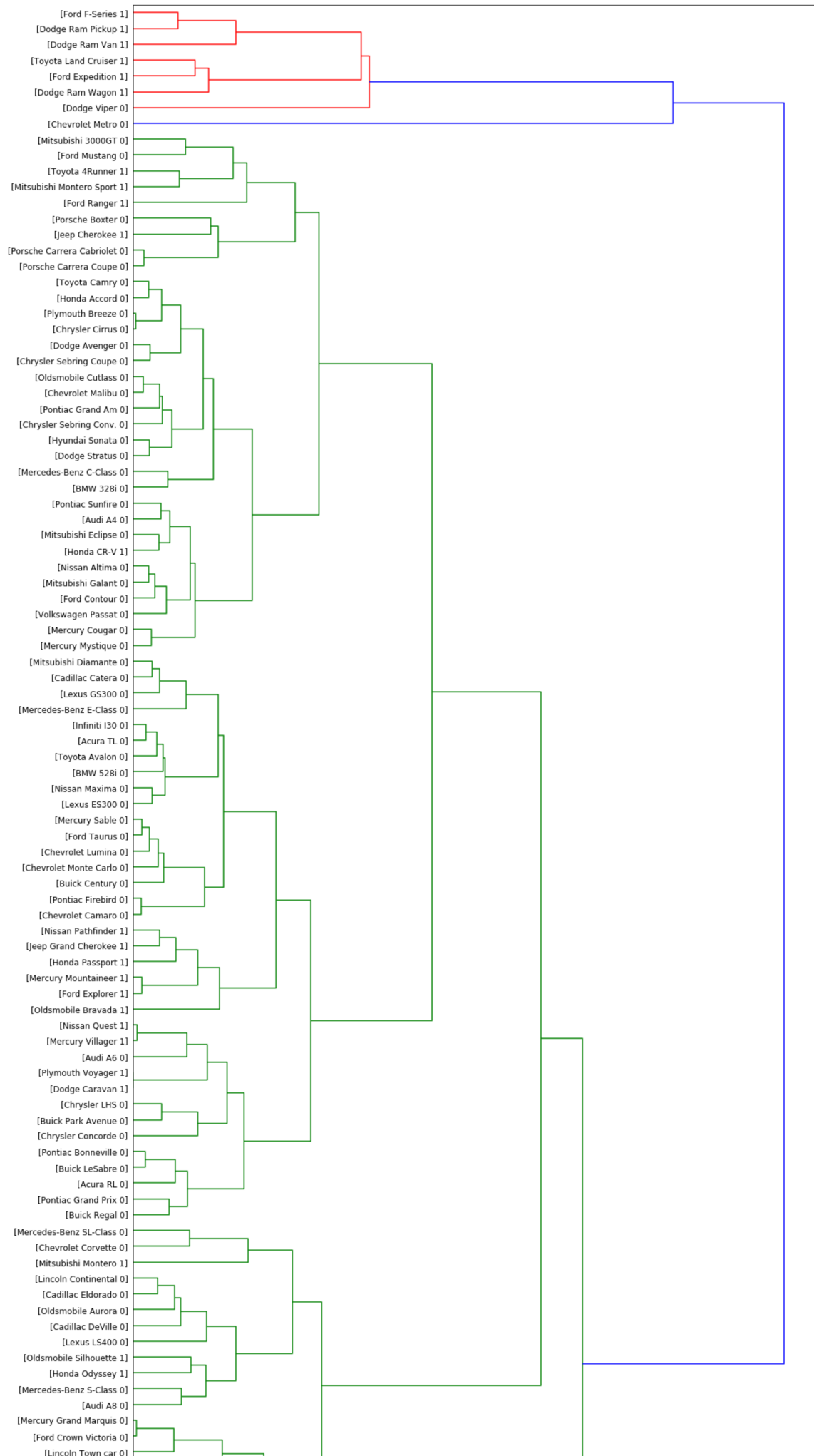
```
In [27]: from scipy.cluster.hierarchy import fcluster
         k = 5
         clusters = fcluster(Z, k, criterion='maxclust')
         clusters

Out[27]: array([1, 3, 3, 3, 3, 2, 3, 3, 3, 3, 3, 3, 2, 2, 3, 1, 3, 3, 3, 3, 2, 1,
                5, 3, 3, 3, 3, 3, 1, 3, 3, 4, 4, 4, 4, 2, 3, 1, 3, 3, 3, 2, 3, 2,
                4, 3, 4, 1, 3, 3, 3, 2, 1, 1, 3, 3, 1, 3, 3, 3, 3, 2, 2, 2, 1, 3,
                3, 3, 3, 2, 3, 3, 3, 3, 2, 3, 3, 3, 3, 2, 2, 1, 3, 3, 3, 3, 2,
                3, 2, 1, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 1, 1, 1, 1, 3, 3, 1, 1, 1,
                3, 4, 1, 1, 3, 1, 1], dtype=int32)
```

Now, plot the dendrogram:

```
In [28]: fig = pylab.figure(figsize=(18,50))
def llf(id):
    return '%s %s %s' % (pdf['manufact'][id], pdf['model'][id], int(float(pdf
['type'][id])))

dendro = hierarchy.dendrogram(Z, leaf_label_func=llf, leaf_rotation=0, leaf_font_size=12, orientation='right')
```



Clustering using scikit-learn

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

```
In [29]: dist_matrix = distance_matrix(feature_mtx, feature_mtx)
         print(dist_matrix)

[[0.          0.57777143  0.75455727 ... 0.28530295  0.24917241  0.18879995]
 [0.57777143  0.          0.22798938 ... 0.36087756  0.66346677  0.62201282]
 [0.75455727  0.22798938  0.          ... 0.51727787  0.81786095  0.77930119]
 ...
 [0.28530295  0.36087756  0.51727787 ... 0.          0.41797928  0.35720492]
 [0.24917241  0.66346677  0.81786095 ... 0.41797928  0.          0.15212198]
 [0.18879995  0.62201282  0.77930119 ... 0.35720492  0.15212198  0.          ]]
```

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 variance-minimizing 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.

```
In [30]: agglom = AgglomerativeClustering(n_clusters = 6, linkage = 'complete')
         agglom.fit(feature_mtx)
         agglom.labels_
```

```
Out[30]: array([1, 2, 2, 1, 2, 3, 1, 2, 2, 2, 2, 2, 3, 3, 2, 1, 1, 2, 2, 2, 5, 1,
                4, 1, 1, 2, 1, 2, 1, 1, 1, 5, 0, 0, 0, 3, 2, 1, 2, 1, 2, 3, 2, 3,
                0, 3, 0, 1, 1, 1, 2, 3, 1, 1, 1, 2, 1, 1, 2, 2, 2, 3, 3, 3, 1, 1,
                1, 2, 1, 2, 2, 1, 1, 2, 3, 2, 3, 1, 2, 3, 5, 1, 1, 2, 3, 2, 1, 3,
                2, 3, 1, 1, 2, 1, 1, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1,
                2, 0, 1, 1, 1, 1, 1])
```

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

```
In [31]: pdf['cluster_'] = agglom.labels_
         pdf.head()
```

```
Out[31]:
```

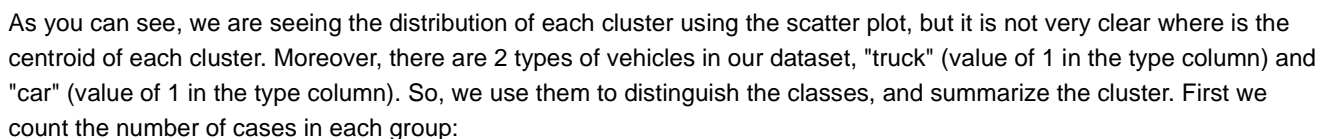
	manufact	model	sales	resale	type	price	engine_s	horsepow	wheelbas	width	length	curb_wgt
0	Acura	Integra	16.919	16.360	0.0	21.50	1.8	140.0	101.2	67.3	172.4	2.639
1	Acura	TL	39.384	19.875	0.0	28.40	3.2	225.0	108.1	70.3	192.9	3.517
2	Acura	RL	8.588	29.725	0.0	42.00	3.5	210.0	114.6	71.4	196.6	3.850
3	Audi	A4	20.397	22.255	0.0	23.99	1.8	150.0	102.6	68.2	178.0	2.998
4	Audi	A6	18.780	23.555	0.0	33.95	2.8	200.0	108.7	76.1	192.0	3.561

```
In [32]: 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=25)
    plt.scatter(subset.horsepow, subset.mpg, s= subset.price*10, c=color, label=
'cluster'+str(label),alpha=0.5)
# plt.scatter(subset.horsepow, subset.mpg)
plt.legend()
plt.title('Clusters')
plt.xlabel('horsepow')
plt.ylabel('mpg')
```

```
Out[32]: Text(0, 0.5, 'mpg')
```



```
In [33]: pdf.groupby(['cluster_', 'type'])['cluster_'].count()
```

```
Out[33]: cluster_  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: cluster_, dtype: int64
```

Now we can look at the characteristics of each cluster:

```
In [34]: agg_cars = pdf.groupby(['cluster_', 'type'])['horsepow', 'engine_s', 'mpg', 'price']
         .mean()
agg_cars
```

```
Out[34]:
```

		horsepow	engine_s	mpg	price
cluster_	type				
0	1.0	211.666667	4.483333	16.166667	29.024667
1	0.0	146.531915	2.246809	27.021277	20.306128
	1.0	145.000000	2.580000	22.200000	17.009200
2	0.0	203.111111	3.303704	24.214815	27.750593
	1.0	182.090909	3.345455	20.181818	26.265364
3	0.0	256.500000	4.410000	21.500000	42.870400
	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.


```
In [35]: plt.figure(figsize=(16,10))
for color, label in zip(colors, cluster_labels):
    subset = agg_cars.loc[(label,)]
    for i in subset.index:
        plt.text(subset.loc[i][0]+5, subset.loc[i][2], 'type='+str(int(i)) + ',
price='+str(int(subset.loc[i][3]))+'k')
    plt.scatter(subset.horsepow, subset.mpg, s=subset.price*20, c=color, label='
cluster'+str(label))
plt.legend()
plt.title('Clusters')
plt.xlabel('horsepow')
plt.ylabel('mpg')
```

'c' argument looks like a single numeric RGB or RGBA sequence, which should be avoided as value-mapping will have precedence in case its length matches with 'x' & 'y'. Please use a 2-D array with a single row if you really want to specify the same RGB or RGBA value for all points.

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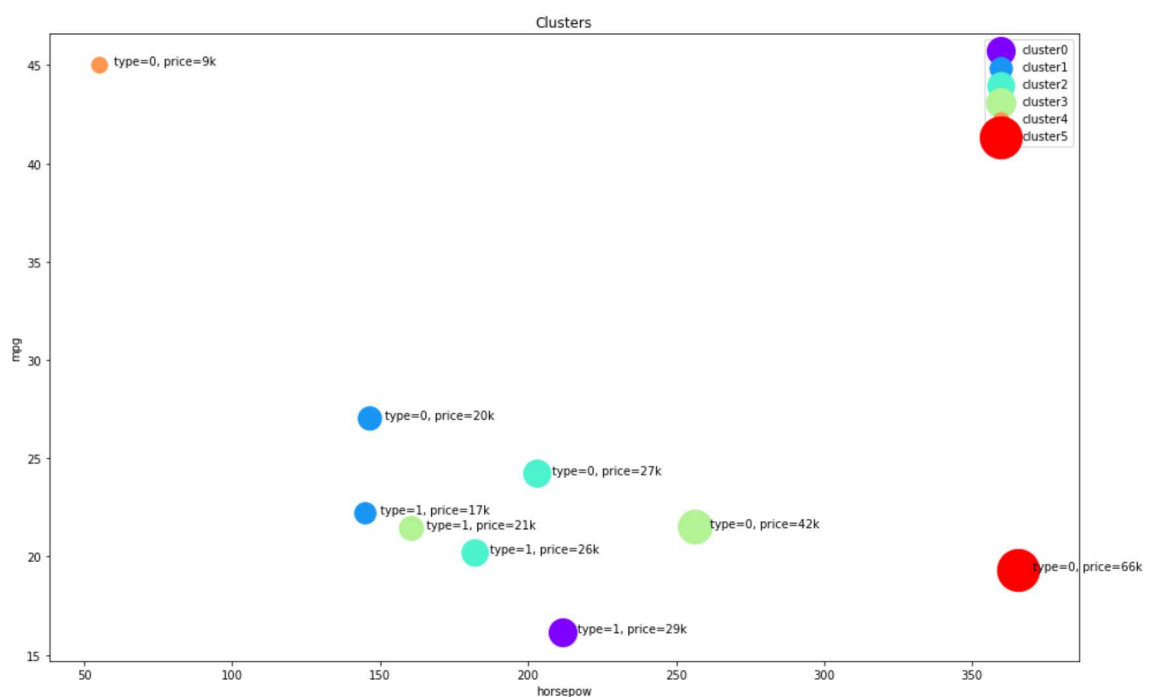
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Out[35]: Text(0, 0.5, 'mpg')



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 \(http://cocl.us/ML0101EN-SPSSModeler\)](http://cocl.us/ML0101EN-SPSSModeler).

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 \(https://cocl.us/ML0101EN_DSX\)](https://cocl.us/ML0101EN_DSX).

Thanks for completing this lesson!

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