# Unsupervised Learning

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## Agenda: Fundamentals of Unsupervised Learning

Clustering - Understanding Distance

Hierarchical clustering

K-Means and K-medoids

# Why clustering and its applications

#### Why clustering?

- 1) To group similar objects/data points
- 2) To find homogeneous sets of customers
- 3) To segment the data in similar groups

#### Applications:

- 1) Marketing: Customer Segmentation & Profiling
- 2) Libraries: Book classification
- 3) Retail: Store Categorization

#### What is Clustering?

Clustering is a technique for finding similar groups in data, called clusters

Clustering is an Unsupervised Learning Technique

Clustering can also be thought of as a case reduction technique wherein it groups together similar records in cluster

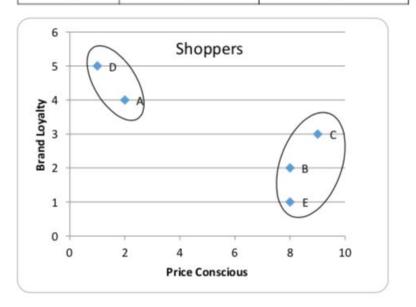
#### What is a Cluster?

A cluster can be defined as a collection of objects which are "similar" between them and are "dissimilar" to the objects belonging to other clusters

How do we define "Similar" in clustering?

**Based on Distance** 

Shoppers	Price Conscious	<b>Brand Loyalty</b>
Α	2	4
В	8	2
С	9	3
D	1	5
E	8	1



#### How do we define "(dis) Similar"?

Similar in clustering is based on Distance

Various distance measures

**Euclidean Distance** 

Chebyshev Distance

Manhattan Distance ...and more

Α

Block

Manhattan Distance = 8 + 4 = 12

Block

Chebyshev Distance = Max (8, 4) = 8

Block

Eucledian Distance =  $sqrt(8^2 + 4^2) = 8.94$ 

Block

Block

Block

Block | E

Block

Block

Block

Block

В

#### Chebyshev Distance

In mathematics, Chebyshev distance is a metric defined on a vector space where the distance between two vectors is the greatest of their differences along any coordinate dimension

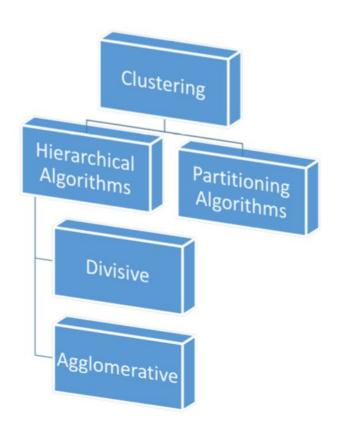
Assume two vectors: A (x1, y1, ... z1) & B (x2, y2, ... z2)

Chebyshev Distance = Max ( | x2 - x1 | , | y2 - y1 | , ..... | z2 - z1 | )

Application: Survey / Research Data where the responses are Ordinal Reference

Link: https://en.wikipedia.org/wiki/Chebyshev\_distance

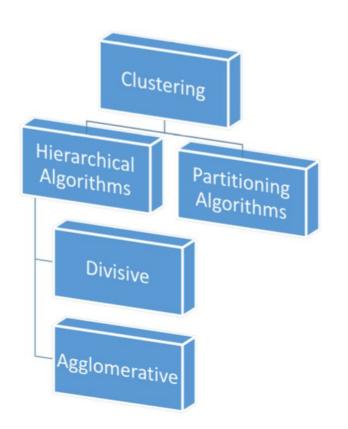
#### Types of Clustering Procedures



- •Hierarchical clustering is characterized by a tree like structure and uses distance as a measure of (dis)similarity
- Partitioning Algorithms starts with a set of partitions as clusters and iteratively refines the partitions to form stable clusters

Agglomerative: This is a "bottom-up" approach: each observation starts in its own cluster, and pairs of clusters are

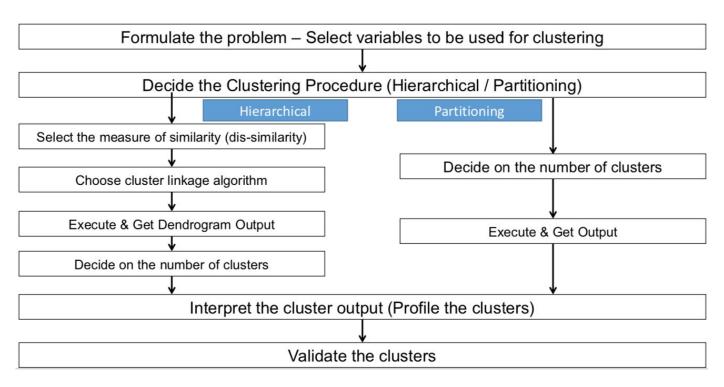
#### Types of Clustering Procedures



Agglomerative: This is a "bottom-up" approach: each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.

Divisive: This is a "top-down" approach: all observations start in one cluster, and splits are performed recursively as one moves down the hierarchy.

# Steps involved in Clustering

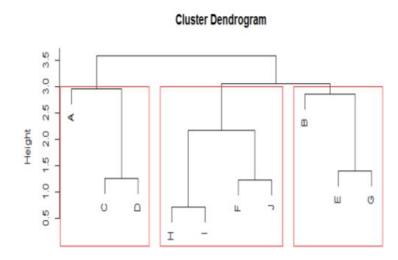


#### Hierarchical Clustering

Hierarchical Clustering is a clustering techniques which seeks to build clusters in a hierarchical tree like structure. This is done in a greedy manner.

Hierarchical clustering makes use of Distance as a measure of similarity

Cluster tree like output is called Dendrogram

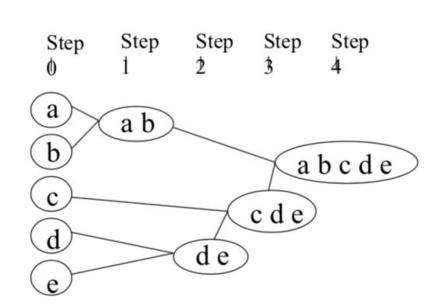


#### Hierarchical Clustering | Agglomerative Clustering Steps

Starts with each record as a cluster of one record each

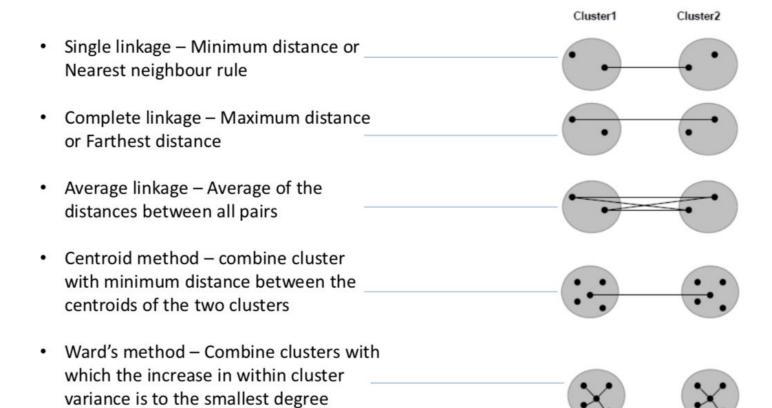
Sequentially merges 2 closest records by distance as a measure of (dis)similarity to form a cluster. This reduces the number of records by 1

Repeat the above step with new cluster and all remaining clusters till we have one big cluster



How do you measure the distance between cluster (a,b) and (c) or the cluster (a,b) and (d,e)?

#### Agglomerative Clustering Linkage Parameter: Between sets of observations



#### Hierarchical Clustering for Retail Customers

Case Study: Indian Retail is a USD 125 Billion Industry. It is extremely important to segment customers and target the appropriate offers. Q Mart has hired you as a Machine Learning Expert to find out the patterns from their shopping purchase data.



#### Hierarchical Clustering for Retail Customers

Index	Cust_ID	Name	Avg_Mthly_Spend	No_Of_Visits	Apparel_Items	FnV_Items	Staples_Items
9	1	A	10000	2	1	1	0
1	2	В	7000	3	0	10	9
2	3	c	7000	7	1	3	4
3	4	D	6500	5	1	1	4
4	5	E	6000	6	0	12	3
5	6	F	4000	3	0	1	8
6	7	G	2500	5	0	11	2
7	8	н	2500	3	0	1	1
8	9	I	2000	2	0	2	2
9	10	3	1000	4	9	1	7

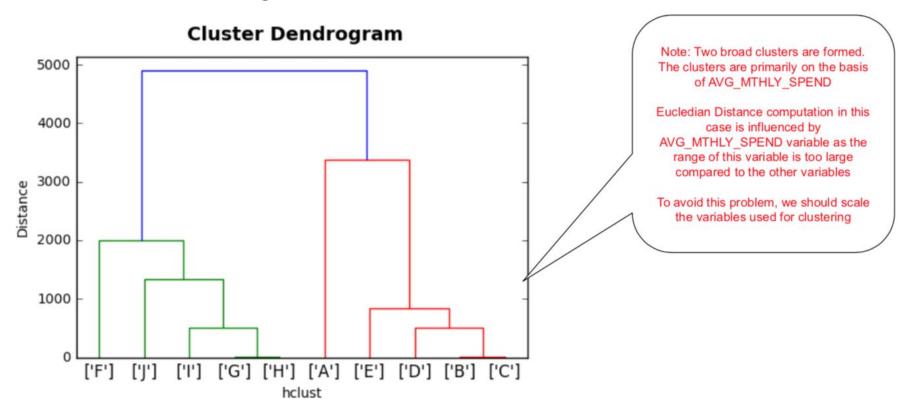
Let us find the clusters in given Retail Customer Spends data

We will use Hierarchical Clustering technique to find clusters on this Dataframe

#### Building the hierarchical clusters (without variable scaling)

```
## Distance Computation
from scipy.spatial.distance import pdist, squareform
pdist ## Ctrl + i
help(pdist)
d_euc = pdist(RCDF.ix[:,2:7], metric = "euclidean")
## Building the Clusters
from scipy.cluster.hierarchy import linkage, dendrogram, cut tree
help(linkage)
clus1 = linkage(d euc, method = "average")
## Displaying the Clusters in Dendrogram
import matplotlib.pyplot as plt
dendrogram(clus1, labels=RCDF[[1]].values.tolist())
plt.xlabel('hclust')
plt.ylabel('Distance')
plt.suptitle('Cluster Dendrogram', fontweight='bold', fontsize=14);
```

#### Cluster Dendrogram



## Scaling the dataset

```
## Hierarchical Clustering with Scaling
from sklearn.preprocessing import scale as scale
## scale function standardizes the values
## Note - The scale function calculates the
## Std. Dev assuming data is Sample
scaled_RCDF = scale(KRCDF.ix[:,2:7])
scaled RCDF
## Note - Here we are scaling taking
## the data as Population
scaled RCDF = KRCDF.ix[:,2:7].apply(
        lambda x: (x- x.mean())/x.std())
scaled RCDF
```

	0	1	2	3	4
0	1.886	-1.240	1.528	-0.741	-1.380
1	0.788	-0.620	-0.655	1.281	1.725
2	0.788	1.861	1.528	-0.292	0.000
3	0.604	0.620	1.528	-0.741	0.000
4	0.421	1.240	-0.655	1.730	-0.345
5	-0.311	-0.620	-0.655	-0.741	1.380
6	-0.861	0.620	-0.655	1.505	-0.690
7	-0.861	-0.620	-0.655	-0.741	-1.035
8	-1.044	-1.240	-0.655	-0.517	-0.690
9	-1.410	0.000	-0.655	-0.741	1.035

Index	Avg_Mthly_Spend	No_Of_Visits	Apparel_Items	FnV_Items	Staples_Items
0	1.79	-1.18	1.45	-0.703	-1.31
1	0.747	-0.588	-0.621	1.21	1.64
2	0.747	1.77	1.45	-0.277	0
3	0.573	0.588	1.45	-0.703	0
4	0.4	1.18	-0.621	1.64	-0.327
5	-0.295	-0.588	-0.621	-0.703	1.31
6	-0.817	0.588	-0.621	1.43	-0.655
7	-0.817	-0.588	-0.621	-0.703	-0.982
8	-0.99	-1.18	-0.621	-0.49	-0.655
9	-1.34	0	-0.621	-0.703	0.982

#### Understanding the Distance Calculation

```
import numpy as np
print(np.round(squareform(d_euc).tolist(),3))
        4.482 3.596 2.648 4.499 4.195 4.615 3.58 3.725 4.796]
  4.482 0.
               4.045 3.66 2.843 2.327
                                        3.184 3.798
                                                    3.578 3.127]
  3.596 4.045 0. 1.332 3.08 3.772 3.567 3.861 4.273 3.785]
              1.332 0. 3.377 3.007 3.526 3.085 3.386 3.206]
  2.648 3.66
  4.499 2.843 3.08 3.377 0. 3.617 1.483 3.419 3.67 3.592]
  4.195 2.327 3.772 3.007 3.617 0.
                                       3.343 2.477 2.293 1.308]
  4.615 3.184 3.567 3.526 1.483 3.343 0. 2.589 2.754 2.951]
  3.58 3.798 3.861 3.085 3.419 2.477 2.589 0.
                                                    0.767 2.23 1
  3.725 3.578
              4.273 3.386 3.67 2.293 2.754 0.767 0.
                                                          2.168]
 4.796
        3.127
               3.785 3.206 3.592 1.308
                                       2.951 2.23
                                                    2.168
distance = clus2[:,2]
distance
array([ 0.76660834, 1.30817103, 1.33188797, 1.48252699, 2.29187962,
     3.01368978, 3.12171991, 3.23053961, 3.78685213])
```



4.80

3.13

3.79

3.206]

3.59

1.31

2.95

2.23

2.17

0.00

#### Profiling the clusters

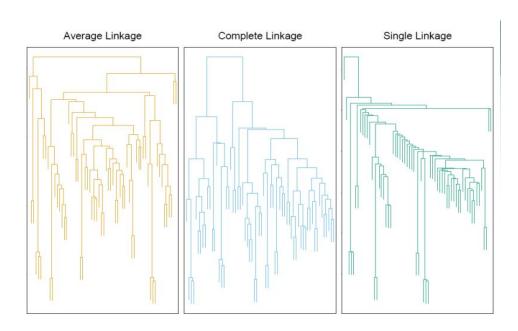
```
## Profiling Step
RCDF['Clusters'] = cut_tree(clus2, 3)
clus_profile = RCDF.ix[:,2:8].groupby(['Clusters'], as_index=False).mean()
clus_profile
```

Index	Clusters	Avg_Mthly_Spend	No_Of_Visits	Apparel_Items	FnV_Items	Staples_Items
0	0	7833	4.667	1	1.667	2.667
1	1	5167	4.667	0	11	4.667
2	2	2375	3	0	1.25	4.5

#### Scaling the data yields different dendrogram!

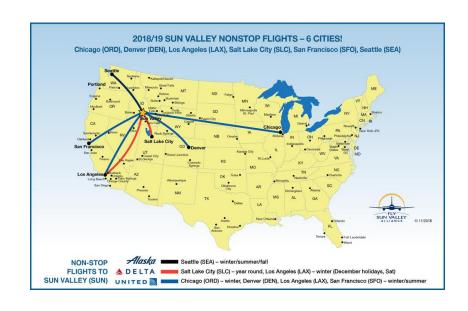
In Class exercise, see how the dendrogram changes (tuning) with different linkages or with different distances?

Complexity can increase based on tuning!



#### Case Study

Indigo is trying to setup a new operations in the USA. They have hired you as a data scientist to understand where might be the optimal locations to setup their operations



## Example of agglomerative clustering

	BOS	NY	DC	МІА	СНІ	SEA	SF	LA	DEN
BOS	0	206	429	1504	963	2976	3095	2979	1949
NY	206	0	233	1308	802	2815	2934	2786	1771
DC	429	233	0	1075	671	2684	2799	2631	1616
МІА	1504	1308	1075	0	1329	3273	3053	2687	2037
сні	963	802	671	1329	0	2013	2142	2054	996
SEA	2976	2815	2684	3273	2013	0	808	1131	1307
SF	3095	2934	2799	3053	2142	808	0	379	1235
LA	2979	2786	2631	2687	2054	1131	379	0	1059
DEN	1949	1771	1616	2037	996	1307	1235	1059	0

At each iteration, pick two data points that have least distance between them. Add the points into a cluster

	BOS/NY	DC	MIA	CHI	SEA	SF	LA	DEN
BOS/NY	0	233	1308	802	2815	2934	2786	1771
DC	233	0	1075	671	2684	2799	2631	1616
МІА	1308	1075	0	1329	3273	3053	2687	2037
СНІ	802	671	1329	0	2013	2142	2054	996
SEA	2815	2684	3273	2013	0	808	1131	1307
SF	2934	2799	3053	2142	808	0	379	1235
LA	2786	2631	2687	2054	1131	379	0	1059
DEN	1771	1616	2037	996	1307	1235	1059	0

Note how we update distances between other clusters. The lower distance is picked. Distance between BOS to DC was 429, now set to 233. Distance from BOS to MIA was 1504, now set to 1308. Averaging may also be used instead of taking distance to the closest point.

	BOS/NY/DC	МІА	СНІ	SEA	SF	LA	DEN
BOS/NY/DC	0	1075	671	2684	2799	2631	1616
МІА	1075	0	1329	3273	3053	2687	2037
CHI	671	1329	0	2013	2142	2054	996
SEA	2684	3273	2013	0	808	1131	1307
SF	2799	3053	2142	808	0	379	1235
LA	2631	2687	2054	1131	379	0	1059
DEN	1616	2037	996	1307	1235	1059	0

Note how creation of SF/LA cluster has changed distances

	BOS/NY/DC	МПА	CHI	SEA	SF	LA	DEN
BOS/NY/DC	0	1075	671	2684	2799	2631	1616
MIA	1075	0	1329	3273	3053	2687	2037
CHI	671	1329	0	2013	2142	2054	996
SEA	2684	3273	2013	0	808	1131	1307
SF	2799	3053	2142	808	0	379	1235
LA	2631	2687	2054	1131	379	0	1059
DEN	1616	2037	996	1307	1235	1059	0

	BOS/	МІА	СНІ	SEA	SF/LA	DEN
	NY/DC					
BOS/NY/DC	0	1075	671	2684	2631	1616
МІА	1075	0	1329	3273	2687	2037
СНІ	671	1329	0	2013	2054	996
SEA	2684	3273	2013	0	808	1307
SF/LA	2631	2687	2054	808	0	1059
DEN	1616	2037	996	1307	1059	0

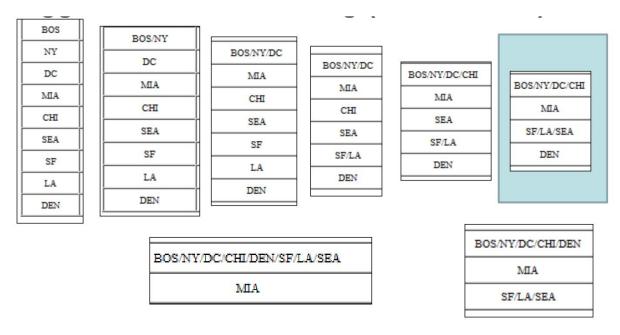
	BOS/NY/DC/	МІА	SEA	SF/LA	DEN
	CHI				
BOS/NY/DC/CHI	0	1075	2013	2054	996
МІА	1075	0	3273	2687	203
SEA	2013	3273	0	808	1307
SF/LA	2054	2687	808	0	1059
DEN	996	2037	1307	1059	0

	BOS/NY/DC/CHI	MIA	SF/LA/SEA	DEN
BOS/NY/DC/CHI	0	1075	2013	996
MIA	1075	0	2687	2037
SF/LA/SEA	2054	2687	0	1059
DEN	996	2037	1059	0

	BOS/NY /DC/CHI/DEN	МІА	SF/LA/SEA
BOS/NY/DC/CHI/DEN	0	1075	1059
MIA	1075	0	2687
SF/LA/SEA	1059	2687	0

	BOS/NY /DC/CHI /DEN/SF /LA/SEA	МІА
BOS/NY/DC/CHI/DEN/SF/LA/SEA	0	1075
MIA	1075	0

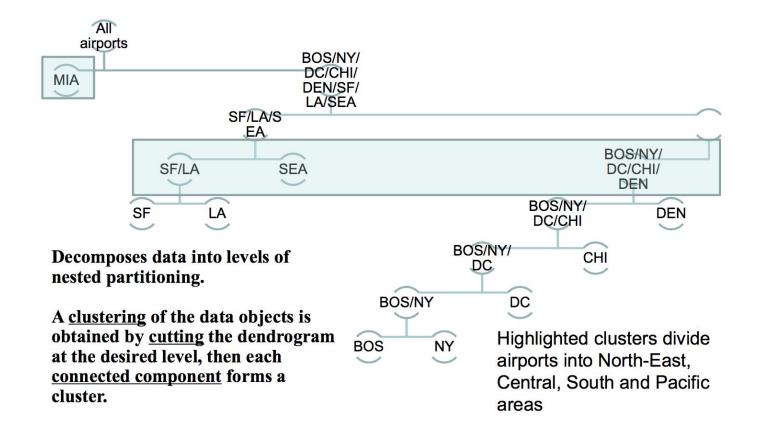
#### Agglomerative clustering (Hierarchical)



Typically, a particular "level" of the hierarchy is selected to be your clustering result

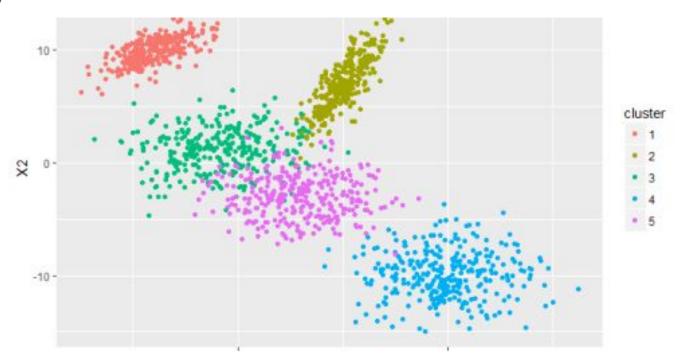
Highlighted clusters divide airports into North-East, Central, South and Pacific areas

## Agglomerative clustering (Hierarchical)



# Partitioning Clustering

K Means Clustering



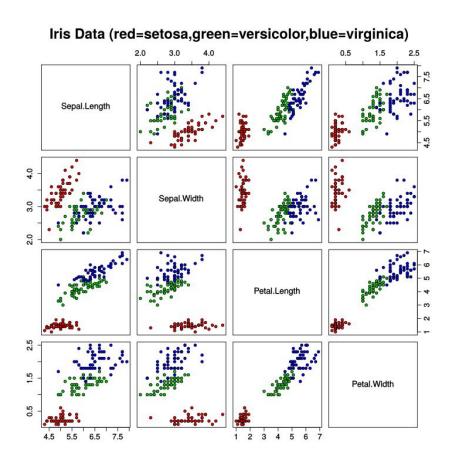
## K Means Clustering

K-Means is the most used, non-hierarchical clustering technique

It is not based on Distance

It is based on within cluster Variation, in other words Squared Distance from the Centre of the Cluster

The algorithm aims at segmenting data such that within cluster variation is reduced (WSS)



#### K Means Algorithm

#### Steps

```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=4)
kmeans.fit(X)
y_kmeans = kmeans.predict(X)
```

- Assume K Centroids (for K Clusters)
- 2. Compute Euclidean distance of each objects with these Centroids
- 3. Assign the objects to clusters with shortest distance
- 4. Compute the new centroid (mean) of each cluster based on the objects assigned to each clusters. The K number of means obtained will become the new centroids for each cluster
- 5. Repeat step 2 to 4 till there is convergence

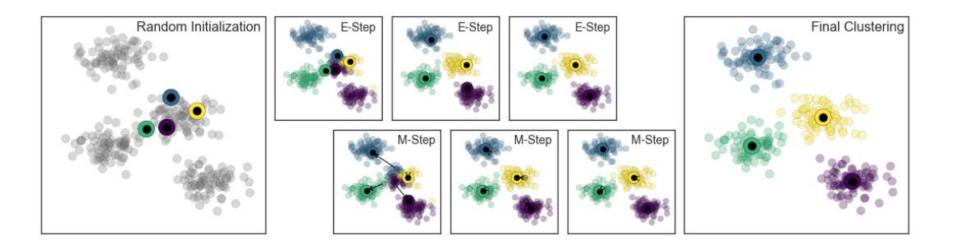
  a) i.e. there is no movement of objects from one cluster to another

  b) Or threshold number of iterations have occurred

## K Means Algorithm (Expectation Maximization)

E-Step: assign points to the nearest cluster center

M-Step: set the cluster centers to the mean



#### K-means advantages

K-means is superior technique compared to Hierarchical technique as it is less impacted by outliers

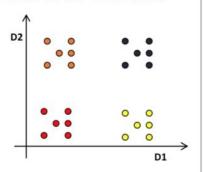
Computationally it is more faster compared to Hierarchical

Preferable to use on interval or ratio-scaled data as it uses Euclidean distance... desirable to avoid using on ordinal data

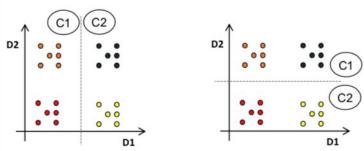
Challenge – Number of clusters are to be predefined and to be provided as input to the process

## Why find optimal No. of Clusters?

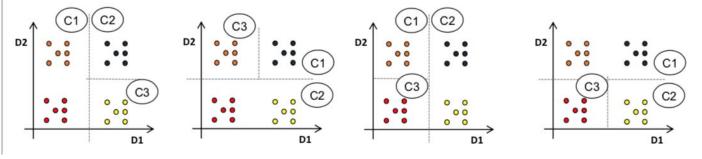
#### Data to be clustered



■ Two Clusters – 2 possible solution



■ Three Clusters – Multiple possible solution



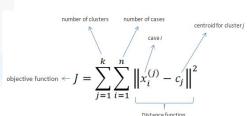
## Retail Customer Data Case Study

As a Machine Learning
Engineer, you are asked to
find out the patterns in the
data using any unsupervised
techniques

	Cust_ID	Name	Avg_Mthly_Spend	No_Of_Visits	Apparel_Items	FnV_Items	Staples_Items
0	1	Α	10000	2	1	1	0
1	2	В	7000	3	0	10	9
2	3	С	7000	7	1	3	4
3	4	D	6500	5	1	1	4
4	5	Е	6000	6	0	12	3
5	6	F	4000	3	0	1	8
6	7	G	2500	5	0	11	2
7	8	Н	2500	3	0	1	1
8	9	1	2000	2	0	2	2
9	10	J	1000	4	0	1	7

#### WSS of Clusters (In Class Exercise: 10min Python)

```
## Identify the optimal number of clusters
# elbow method
cluster range = range( 1, 10 )
cluster wss = []
for num clusters in cluster range:
    clusters = KMeans( num clusters )
    clusters.fit(scaled RCDF)
    cluster wss.append( clusters.inertia )
from collections import OrderedDict
clusters df = pd.DataFrame( OrderedDict (
        {"num clusters": cluster range,
        "cluster_wss": cluster wss }
clusters df[0:10]
```



## Optimal No. of Clusters: (In Class Exercise: 10min Python)

```
plt.figure(figsize=(12,6))
plt.xlabel('Number of Clusters')
plt.ylabel('Within Sum of Squares')
plt.xticks(np.arange(min(clusters df.num clusters),
                        max(clusters df.num clusters)+1,
                        1.0))
                                                Optimal number of clusters
plt.plot( clusters df.num clusters,
          clusters df.cluster wss,
          marker = "o")
                                               100
                                              Total With
```

#### Profiling the Clusters: (In Class Exercise: 10 min Python)

```
## Profiling the clusters
clusterer = KMeans(n clusters=2, random state=10)
cluster labels = clusterer.fit predict(scaled RCDF)
cluster labels
KRCDF['Clusters'] = cluster labels
clus profile = KRCDF.iloc[:,2:8].groupby(['Clusters'],
                       as index=False).mean()
clus profile
```

	Clusters	Avg_Mthly_Spend	No_Of_Visits	Apparel_Items	FnV_Items	Staples_Items
0	0	7833.333333	4.666667	1.0	1.666667	2.666667
1	1	3571.428571	3.714286	0.0	5.428571	4.571429

### **K Means Limitations**

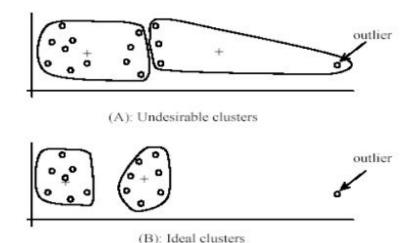
- 1. What is clusters are not clearly separable?
- 2. Applicable to data where "mean" is well-defined

  Restricts applicability to only Euclidean spaces i.e. if categorical attributes present (e.g. Marital Status, Gender), "mean" not meaningful

**K-Medoids (a minor variant)**: Choose most centrally located point within the cluster as representative (This step is more computationally intensive)

Sensitivity to outliers in data – Detect and remove outliers before clustering – K-Medians is relatively more robust to outliers

### **K Means Limitations**



Sensitivity to outliers in data

Detect and remove outliers before clustering

K-Medians is relatively more robust to outliers and because a medoid is less influenced by outliers or other extreme values than a mean

Works efficiently for small data sets but does not scale well for large data sets

## **Evaluation of Cluster Quality**

Extrinsic Evaluation - Given Ground Truth Data

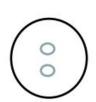
 $AlgoPrecision = \sum_{i} \frac{|c_{i}|}{n} \max_{j} Precision(C_{i}, L_{j})$ 

Precision 
$$(C_i, L_j) = \frac{|C_i \cap L_j|}{|C_i|}$$

Discovered (C)



Precision = 3/3 Recall = 3/4



Truth (L)

 $AlgoRecall = \sum_{i} \frac{|L_i|}{n} \max_{i} Recall (C_j, L_i)$ 

$$Recall (C_j, L_i) = \frac{|c_j \cap L_i|}{|L_i|}$$

$$F = \sum_{i} \frac{|L_i|}{n} \max_{j} \{F(C_j, L_i)\}$$

$$F(C_j, L_i) = \frac{2 \times Recall(C_j, L_i) \times Precision(C_i, L_j)}{Recall(C_j, L_i) + Precision(C_i, L_j)}$$

## **Evaluation of Cluster Quality**

Intrinsic Evaluation

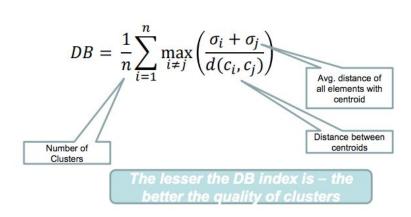
When no gold standard data is available

Develop measures for some general goodness criterion

E.g. Good clusters should high intra-cluster similarity and low inter cluster

similarity Davies-Bouldin (DB) Index

To check the stability of the clusters take a random sample of 95% of records. Compute the clusters. If the clusters formed are very similar to the original, then the clusters are fine



## Next steps after clustering

Clustering provides you with clusters in the given dataset

Clustering does not provide you rules to classify future records

To be able to classify future records you may do the following

**Build Discriminant Model on Clustered Data** 

Build Classification Tree Model on Clustered Data

https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-t o-know-a36d136ef68

#### K-means versus Hierarchical

K-means produces a single partitioning

K-means needs the number of clusters to be specified

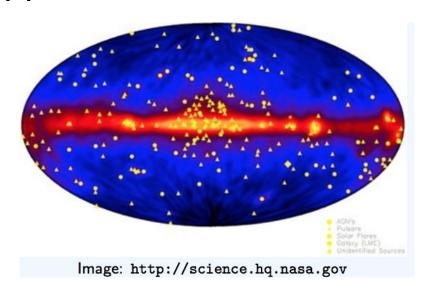
K-means is usually more efficient run-time wise

Hierarchical Clustering can give different partitions depending on the level-of-resolution we are looking at

Hierarchical clustering doesn't need the number of clusters to be specified

Hierarchical clustering can be slow (has to make several merge/Split decisions)

## Clustering applications - Astrostatistics



#### THREE TYPES OF GAMMA-RAY BURSTS

Soma Mukherjee, 1,2,3 Eric D. Feigelson, 4 Gutti Jogesh Babu, 5 Fionn Murtagh, 6,7 Chris Fraley, 8 and Adrian Raftery 8

Received 1998 February 9; accepted 1998 June 25

#### "One" schematic for addressing problems in machine learning...

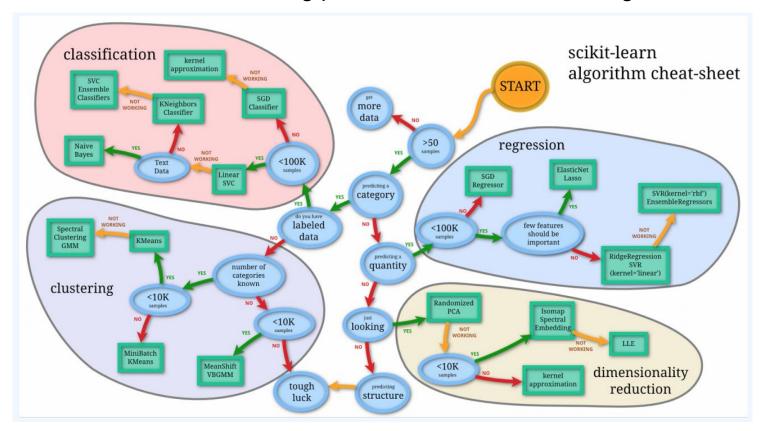


Image: Andy's Computer Vision and Machine Learning Blog http://peekaboo-vision.blogspot.com

## Summary

Introduced the paradigm of "Unsupervised Learning" – The task of discovering intrinsic patterns from data without any supervision

Depending on the specific objective to be optimized and assumptions made about data, there are many clustering algorithms proposed in literature

Some clustering algorithms we discussed:

Agglomerative Clustering - Case Study & Worked out Example K-Means - Worked out Example

Practical issues while using the above algorithms. We also studied the notion of cluster evaluation

#### References

References

Chapter 9: Cluster Analysis (<a href="http://www.springer.com">http://www.springer.com</a>)

Google search: "www.springer.com cluster analysis chapter 9"

http://sites.stat.psu.edu/~ajw13/stat505/fa06/19\_cluster/09\_cluster\_wards.html •

https://home.deib.polimi.it/matteucc/Clustering/tutorial\_html/

# Thank you! Questions