COMP 2211 Exploring Artificial Intelligence

K-Means Clustering

Dr. Desmond Tsoi

Department of Computer Science & Engineering
The Hong Kong University of Science and Technology, Hong Kong SAR, China

Problem

- Given the following simplified Mall customers dataset with attributes, age, income (in thousands) and expense score (1-100).

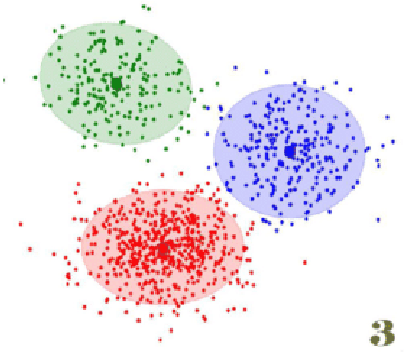
Person	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Age	19	67	35	60	65	49	70	70	57	68	23	65	27	47	57	43	56	40	37	34
Income $\times 1000$	15	19	24	30	38	42	46	49	54	59	62	63	67	71	75	78	79	87	97	103
Expense score 1-100	39	14	35	4	35	52	56	55	51	55	41	52	56	9	5	17	35	13	32	23

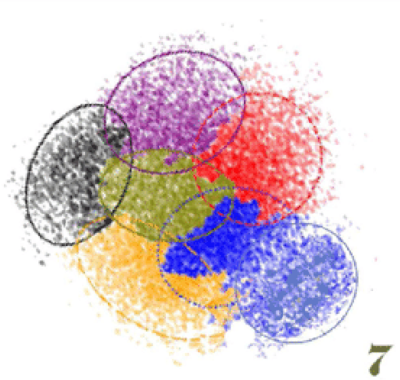
Note: Expense score goes from 1 (low spends) to 100 (high spends).

- Could we cluster the customers based on their characteristics (age, income & expense score) to determine the targeted advertisement and make the marketing budget more efficient?

What is Clustering?

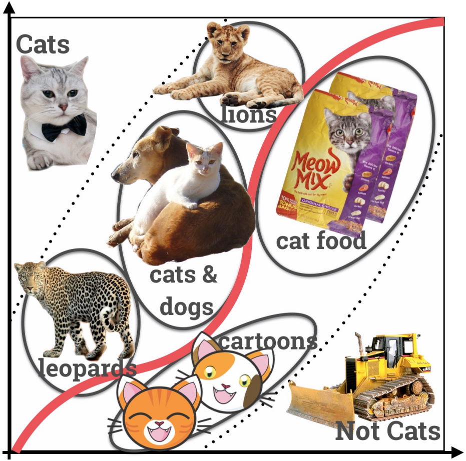
- Clustering is grouping things into "natural" categories when no class label is available.





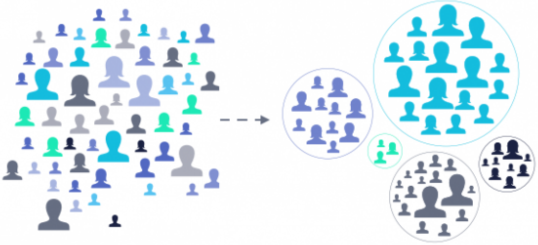
Why Clustering?

- Labeling a large set of data samples can be costly.
- Clustering can be used for finding features that will be useful later for categorization.



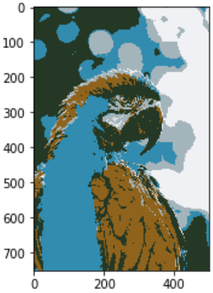
What is Clustering for?

- Group people of similar sizes together to make “small”, “medium”, and “large” T-shirts.
  - Tailor-made for each person: too expensive
  - One-size-fits-all: Does not fit all
- Given a collection of text documents, we want to organize them according to their content similarities
  - To produce a topic hierarchy
- In marketing, segment customers according to their similarities
  - To do targeted marketing

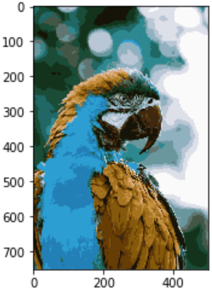


What is Clustering for?

- Image segmentation
  - To partition a digital image into multiple image segments, also known as image regions.



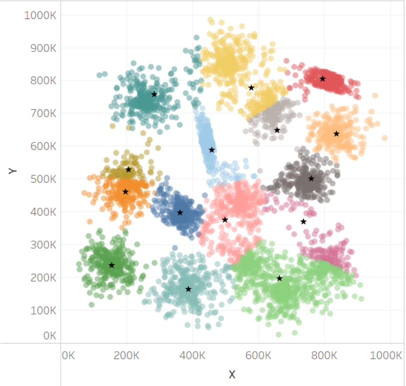
k = 5



k = 20

K-Means Clustering

- K-Means clustering is an unsupervised learning algorithm.
- There is no labeled data for this clustering, unlike supervised learning.
- It performs the division of data into non-overlapping clusters that share similarities and are dissimilar to the data belonging to another cluster.
- The term 'K' is a number telling the system how many clusters you need to create. For example, if K = 3 refers to three clusters.

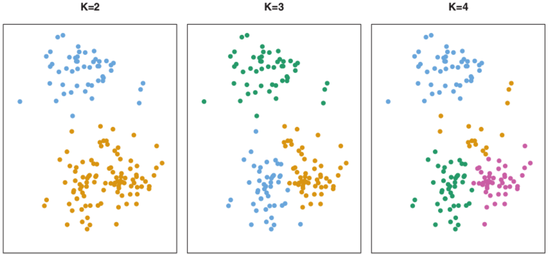


K-Means Clustering

- Let the set of data points

$$\mathbf{D} = \{\mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}, \ldots, \mathbf{x_n}\}$$

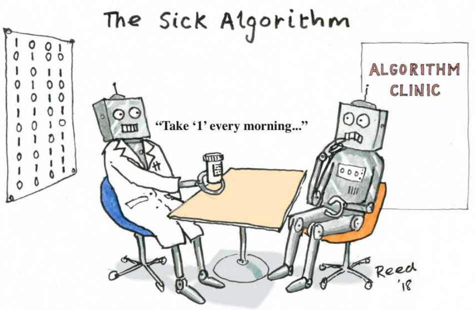
  where $\mathbf{x_i} = (x_{i1}, x_{i2}, \ldots, x_{id})$ is the i^{th} data point, and d is the number of dimensions.
- To perform K-means clustering, we must first specify the desired number of clusters K.
- The K-Means algorithm partitions the given data points into K non-overlapped clusters:
  - Each cluster has a cluster center, called centroid



K-means Algorithm

Given K, the K-Means algorithm works as follows:

1. Choose K (random) data points (seeds) to be the initial centroids (cluster centers)
2. Find the distances between each data point in our training set with the K centroids
3. Assign each data point to the closest centroid according to the distance found
4. Re-compute the centroids using the current cluster memberships
5. If a convergence criterion is NOT met, repeat steps 2 to 4



Example

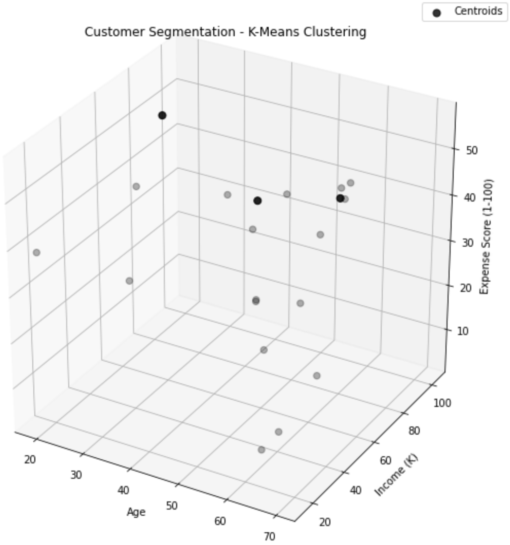
- Let's perform K-Means Clustering on the following simplified Mall customers dataset with attributes, age, income (in thousands) and expense score (1-100).

Person	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Age	19	67	35	60	65	49	70	70	57	68	23	65	27	47	57	43	56	40	37	34
Income $\times$1000	15	19	24	30	38	42	46	49	54	59	62	63	67	71	75	78	79	87	97	103
Expense score 1-100	39	14	35	4	35	52	56	55	51	55	41	52	56	9	5	17	35	13	32	23

Note: Expense score goes from 1 (low spends) to 100 (high spends).

Step 1: Randomly Pick 3 Data Points as Initial Centriods

- 1st centroid: (70, 46, 56)
- 2nd centroid: (27, 67, 56)
- 3rd centroid: (37, 97, 32)



Step 2: Find the Distances Between Each Data Point with the 3 Centroids

- 1st centroid: (70, 46, 56)
- 2nd centroid: (27, 67, 56)
- 3rd centroid: (37, 97, 32)

Assume Euclidean distance is used.

Person	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Age	19	67	35	60	65	49	70	70	57	68	23	65	27	47	57	43	56	40	37	34
Income $\times$1000	15	19	24	30	38	42	46	49	54	59	62	63	67	71	75	78	79	87	97	103
Expense score 1-100	39	14	35	4	35	52	56	55	51	55	41	52	56	9	5	17	35	13	32	23
DC1	62	50	46	55	23	22	0	3	16	13	52	18	48	58	60	57	42	67	65	75
DC2	55	75	49	72	52	34	48	47	33	42	16	38	0	51	60	44	38	49	40	49
DC3	84	86	73	76	65	60	65	63	51	54	39	48	40	36	40	25	26	22	0	11

where DC1, DC2, DC3 are the distances between the data points and 1st centroid, 2nd centroid, and 3rd centroid, respectively.

Step 3: Assign Each Data Point to the Closest Centroid

- 1st centroid: (70, 46, 56)
- 2nd centroid: (27, 67, 56)
- 3rd centroid: (37, 97, 32)

Person	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Age	19	67	35	60	65	49	70	70	57	68	23	65	27	47	57	43	56	40	37	34
Income $\times 1000$	15	19	24	30	38	42	46	49	54	59	62	63	67	71	75	78	79	87	97	103
Expense score 1-100	39	14	35	4	35	52	56	55	51	55	41	52	56	9	5	17	35	13	32	23
DC1	62	50	46	55	23	22	0	3	16	13	52	18	48	58	60	57	42	67	65	75
DC2	55	75	49	72	52	34	48	47	33	42	16	38	0	51	60	44	38	49	40	49
DC3	84	86	73	76	65	60	65	63	51	54	39	48	40	36	40	25	26	22	0	11
Cluster	2	1	1	1	1	1	1	1	1	1	2	1	2	3	3	3	3	3	3	3

where DC1, DC2, DC3 are the distances between the data points and 1st centroid, 2nd centroid, and 3rd centroid, respectively.

Step 4: Re-compute the Centroids Using the Current Cluster Memberships

Person	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Age	19	67	35	60	65	49	70	70	57	68	23	65	27	47	57	43	56	40	37	34
Income $\times 1000$	15	19	24	30	38	42	46	49	54	59	62	63	67	71	75	78	79	87	97	103
Expense score 1-100	39	14	35	4	35	52	56	55	51	55	41	52	56	9	5	17	35	13	32	23
DC1	62	50	46	55	23	22	0	3	16	13	52	18	48	58	60	57	42	67	65	75
DC2	55	75	49	72	52	34	48	47	33	42	16	38	0	51	60	44	38	49	40	49
DC3	84	86	73	76	65	60	65	63	51	54	39	48	40	36	40	25	26	22	0	11
Cluster	2	1	1	1	1	1	1	1	1	1	2	1	2	3	3	3	3	3	3	3

- New 1st centroid:

$$x_1 = (67 + 35 + 60 + 65 + 49 + 70 + 70 + 57 + 68 + 65)/10 = 60.6$$
$$x_2 = (19 + 24 + 30 + 38 + 42 + 46 + 49 + 54 + 59 + 63)/10 = 42.4$$
$$x_3 = (14 + 35 + 4 + 35 + 52 + 56 + 55 + 51 + 55 + 52)/10 = 40.9$$

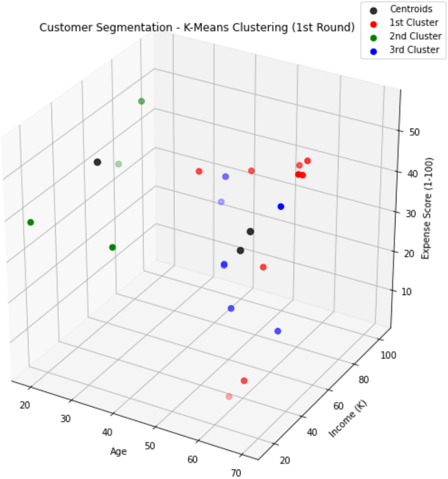
- New 2nd centroid:

$$x_1 = (19 + 23 + 27)/3 = 23$$
$$x_2 = (15 + 62 + 67)/3 = 48$$
$$x_3 = (39 + 41 + 56)/3 = 45.33$$

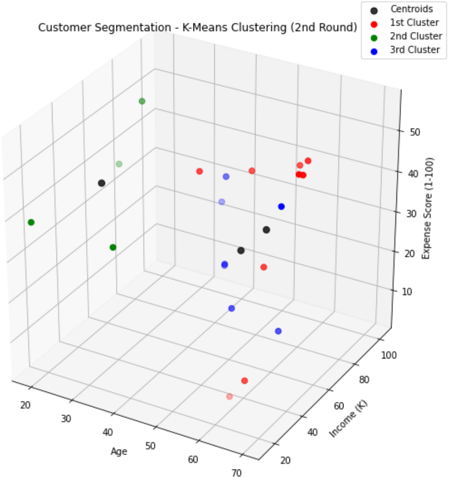
- New 3rd centroid:

$$x_1 = (47 + 57 + 43 + 56 + 40 + 37 + 34)/7 = 44.86$$
$$x_2 = (71 + 75 + 78 + 79 + 87 + 97 + 103)/7 = 84.29$$
$$x_3 = (9 + 5 + 17 + 35 + 13 + 32 + 23)/7 = 19.14$$

The 1st and the 2nd Round

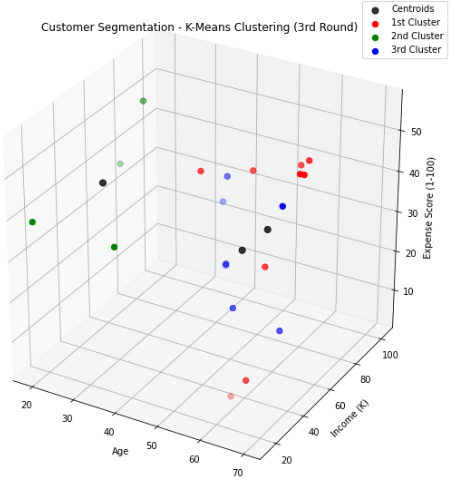


1st centroid: (70, 46, 56)
2nd centroid: (27, 67, 56)
3rd centroid: (37, 97, 32)

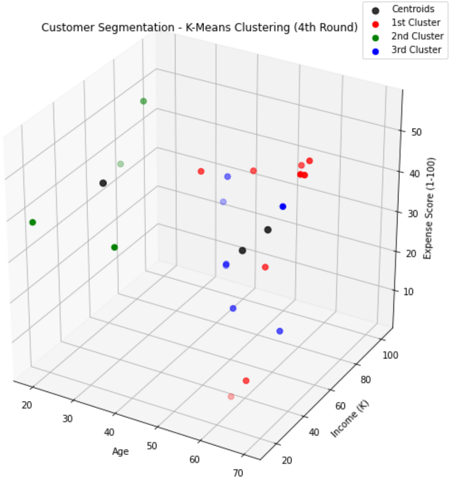


1st centroid: (60.6, 42.4, 40.9)
2nd centroid: (23, 48, 45.3)
3rd centroid: (44.9, 84.3, 19.1)

The 3rd and the 4th Round



1st centroid: (63.4, 44.4, 41.6)
2nd centroid: (26, 42, 42.8)
3rd centroid: (44.9, 84.3, 19.1)



1st centroid: (63.4, 44.4, 41.6)
2nd centroid: (26, 42, 42.8)
3rd centroid: (44.9, 84.3, 19.1)

Conclusion

- Cluster 1:
  The average age is 63 years old, the average annual income is \$44K, and the average expense score is 42 of 100.
- Cluster 2:
  The average age is 26 years old, the average annual income is \$42K, and the average expense score is 43 of 100.
- Cluster 3:
  The average age is 45 years old, the average annual income is \$84K, and the average expense score is 19 of 100.

K-Means Clustering Implementation using Scikit-Learn

```python
# Import the required libraries
import numpy as np
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt

# Unlabled training data
data = np.array([[19, 15, 39], [67, 19, 14], [35, 24, 35], [60, 30, 4], [65, 38, 35],
                 [49, 42, 52], [70, 46, 56], [70, 49, 55], [57, 54, 51], [68, 59, 55],
                 [23, 62, 41], [65, 63, 52], [27, 67, 56], [47, 71, 9],  [57, 75, 5],
                 [43, 78, 17], [56, 79, 35], [40, 87, 13], [37, 97, 32], [34, 103, 23]])

# Initial centroids
init_centroids = np.array([[70, 46, 56], [27, 67, 56], [37, 97, 32]])

# Create a KMeans object by specifying
# - Number of clusters (n_clusters) = 3, initial centroids (init) = init_centroids
# - Number of time the k-means algorithm will be run with different centroid seeds (n_init) = 1
# - Maximum number of iterations of the k-means algorithm for a single run (max_iter) = 4
kmeans = KMeans(n_clusters=3, init=init_centroids, n_init=1, max_iter = 4)
```

K-Means Clustering Implementation using Scikit-Learn

```
kmeans.fit(data)                     # Compute k-means clustering
labels = kmeans.predict(data)        # Predict the closest cluster each sample in data belongs to
centroids = kmeans.cluster_centers_ # Get resulting centroids
fig = plt.figure(figsize = (10,10)) # Figure width = 10 inches, height = 10 inches
ax = fig.gca(projection='3d')        # Defining 3D axes so that we can plot 3D data into it

# Get boolean arrays representing entries with labels = 0, 1, and 2
a = np.array(labels == 0); b = np.array(labels == 1); c = np.array(labels == 2)

# Plot centroids with color = black, size = 50 units, transparency = 20%, and put label "Centroids"
ax.scatter(centroids[:,0], centroids[:,1], centroids[:,2],
           c="black", s=50, alpha=0.8, label="Centroids")
# Plot data in the different clusters (1st in red, 2nd in green, 3rd blue)
ax.scatter(data[a,0], data[a,1], data[a,2], c="red", s=40, label="1st Cluster")
ax.scatter(data[b,0], data[b,1], data[b,2], c="green", s=40, label="2nd Cluster")
ax.scatter(data[c,0], data[c,1], data[c,2], c="blue", s=40, label="3rd Cluster")
ax.legend() # Show legend

ax.set_xlabel("Age")                   # Put x-axis label "Age"
ax.set_ylabel("Income (K)")            # Put y-axis label "Income (K)"
ax.set_zlabel("Expense Score (1-100)") # Put z-axis label "Expense Score (1-100)"
ax.set_title("Customer Segmentation - K-Means Clustering") # Put figure title
```

K-Means Stopping Criterion

- No/Minimum re-assignments of data points to different clusters, or
- No/Minimum change of centroids, or
- Minimum decrease in the sum of squared error (SSE) between successive iteration

$$SSE = \sum_{j=1}^{k} \sum_{\mathbf{x} \in C_j} dist(\mathbf{x}, \mathbf{m_j})^2$$

where

- C_j is the jth cluster
- $\mathbf{m_j}$ is the centroid of cluster C_j
- dist($\mathbf{x}$, $\mathbf{m_j}$) is the distance between data point $\mathbf{x}$ and centroid $\mathbf{m_j}$

Common Questions

1. How to choose K?

   Answer: The following methods are used to find the optimal value of K for K-Means Clustering.

   - Elbow method
   - Silhouette method

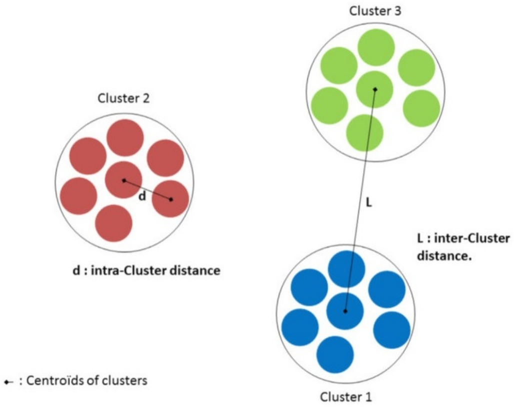
   These methods will be discussed in advanced level machine learning courses.

2. What distance metric should be used for K-Means?

   Answer: It depends on your data. Normally, K-Means uses Euclidean distance.

Clustering Quality

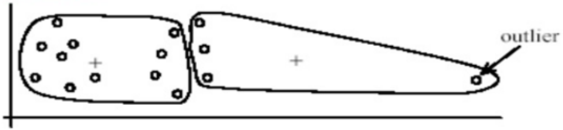
- High quality clustering
  - Maximizes inter-clusters distance (Isolation)
    (i.e., distance between clusters)
  - Minimizes intra-clusters distance (Compactness)
    (i.e., distance between data points in the same cluster)



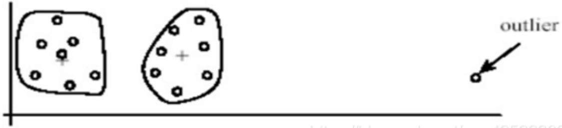
The quality of a clustering result depends on the algorithm, the distance function, and the application.

Weaknesses of K-Means

- It is sensitive to outliers
  - Outliers are data points that are very far away from other data points
  - Outliers could be errors in the data recording or some special data points with very different values
  - Desirable and undesirable clustering with outliers



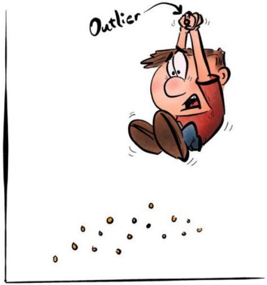
Undesirable clustering



Desirable clustering

How to Deal with Outliers?

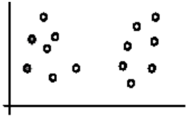
- Remove some data points in the clustering process that are much further away from the centroids than other data points.
  - To be safe, we may want to monitor these possible outliers over a few iterations and then decide to remove them.
- Perform random sampling. Since in sampling, we only choose a small subset of the data points, the chance of select an outlier is very small.
  - Assign the rest of the data points to the clusters by distance or similarity comparison, or classification.



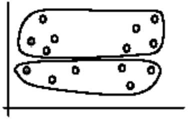
Weaknesses of K-Means

- The algorithm is sensitive to initial seeds.

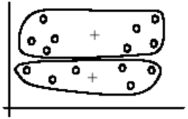
If we use seeds that are not-so-good:
not-so-good results



(A). Random selection of seeds (centroids)

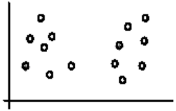


(B). Iteration 1

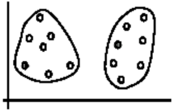


(C). Iteration 2

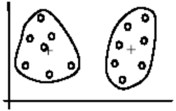
If we use different seeds:
good results



(A). Random selection of k seeds (centroids)



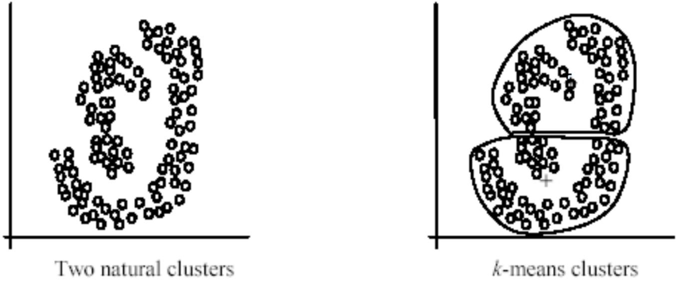
(B). Iteration 1



(C). Iteration 2

Weaknesses of K-Means

- The K-Means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).



Pros and Cons

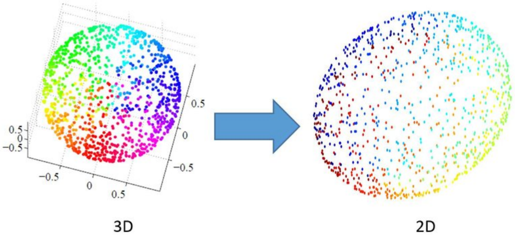
- Pros:
  - Easy to understand and implement
  - It is efficient, given K and the number of iterations is small
- Cons:
  - It is only applicable if the mean is defined.
    For categorical data, K-mode is used, i.e., the centroid is represent by most frequent values
  - The user needs to specify K
  - It is sensitive to outliers

Summary

- Despite weaknesses, K-Means is still the most popular algorithm due to its simplicity, efficiency and other clustering algorithms have their own lists of weaknesses.
- No clear evidence that any other clustering algorithm performs better in general, although they may be more suitable for some specific types of data or applications.
- Comparing different clustering algorithms is a difficult task. No one knows the correct clusters.

Remark: Dimension Reduction using PCA

- Principal Component Analysis (PCA) is one of the easiest, most intuitive and most frequently used methods for dimensionality reduction, projecting data onto its orthogonal feature subspace.
    - The main idea of PCA is to reduce the dimensionality of a data set consisting of many variables correlated with each other, while retaining the variation present in the dataset, up to the maximum extent.
- It is a common practice to apply PCA before K-Means clustering is performed.
- It is believed that it improves the clustering results in practice (noise reduction).



Practice Problem

- Given 4 types of medicines and each has two attributes (weight and pH index).
- Group these medicines into $K = 2$ group using K-Means clustering.

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4

- Use (1, 1) and (2, 1) as the initial centroids (i.e., seeds) and performing K-Means Clustering until there is no re-assignments of data points to different clusters.

Step 1: Use the 2 Given Data Points as Initial Centriods
Step 2: Find the Distances Between Each Data Point with the 2 Centroids

- 1st centroid: (1, 1)
- 2nd centroid: (2, 1)

Assume Euclidean distance is used.

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	1	0	2.8	4.2

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 3: Assign Each Data Point to the Closest Centroid

- 1st centroid: (1, 1)
- 2nd centroid: (2, 1)

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	1	0	2.8	4.2
Cluster	1	2	2	2

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 4: Re-compute the Centroids Using the Current Cluster Memberships

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	1	0	2.8	4.2
Cluster	1	2	2	2

- New 1st centroid:

$$x_1 = 1$$
$$x_2 = 1$$

- New 2nd centroid:

$$x_1 = (2 + 4 + 5)/3 = 3.67$$
$$x_2 = (1 + 3 + 4)/3 = 2.67$$

Step 5: Find the Distance Between Each Data Point with the 2 Centroids

- 1st centroid: (1, 1)
- 2nd centroid: (3.67, 2.67)

Assume Euclidean distance is used.

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	3.1	2.4	0.5	1.9

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 6: Assign Each Data Point to the Closest Centroid

- 1st centroid: (1, 1)
- 2nd centroid: (3.67, 2.67)

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	3.1	2.4	0.5	1.9
Cluster	1	1	2	2

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 7: Re-compute the Centroids Using the Current Cluster Memberships

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	3.1	2.4	0.5	1.9
Cluster	1	1	2	2

- New 1st centroid:

$$x_1 = (1+2)/2 = 1.5$$
$$x_2 = (1+1)/2 = 1$$

- New 2nd centroid:

$$x_1 = (4+5)/2 = 4.5$$
$$x_2 = (3+4)/2 = 3.5$$

Step 8: Find the Distance Between Each Data Point with the 2 Centroids

- 1st centroid: (1.5, 1)
- 2nd centroid: (4.5, 3.5)

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0.5	0.5	3.2	4.6
DC2	4.3	2.4	0.5	1.9

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 9: Assign Each Data Point to the Closest Centroid

- 1st centroid: (1.5, 1)
- 2nd centroid: (4.5, 3.5)

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0.5	0.5	3.2	4.6
DC2	4.3	2.4	0.5	1.9
Cluster	1	1	2	2

where DC1, DC2 are the distances between the data points and 1st centroid, and 2nd centroid, respectively.

Step 7: Re-compute the Centroids Using the Current Cluster Memberships

Medicine	A	B	C	D
Weight Index	1	2	4	5
pH Index	1	1	3	4
DC1	0	1	3.6	5
DC2	3.1	2.4	0.5	1.9
Cluster	1	1	2	2

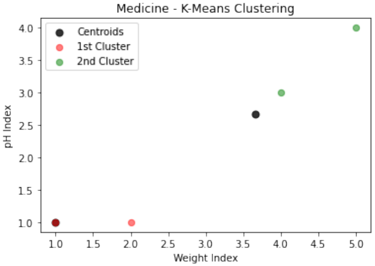
- New 1st centroid:

$$x_1 = (1+2)/2 = 1.5$$
$$x_2 = (1+1)/2 = 1$$

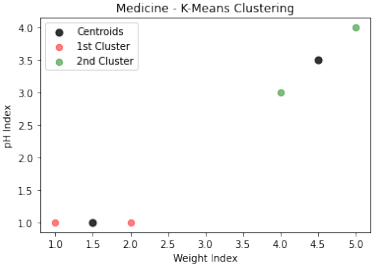
- New 2nd centroid:

$$x_1 = (4+5)/2 = 4.5$$
$$x_2 = (3+4)/2 = 3.5$$

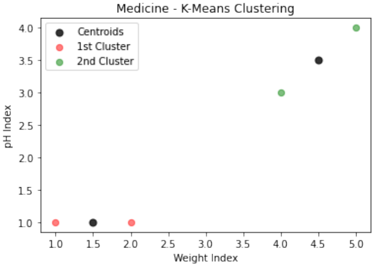
The 1st, the 2nd, and the 3rd Round



1st centroid: (1, 1)
2nd centroid: (3.67, 2.67)



1st centroid: (1.5, 1)
2nd centroid: (4.5, 3.5)



1st centroid: (1.5, 1)
2nd centroid: (4.5, 3.5)

Conclusion

- Cluster 1:
  The average weight index is 1.5, and the average pH index is 1.
- Cluster 2:
  The average weight index is 4.5, and the average pH index is 3.5.

K-Means Clustering Implementation using Scikit-Learn

```
# Import the required libraries
import numpy as np
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt

# Unlabled training data
data = np.array([[1,1], [2,1], [4,3], [5,4]])

# Initial centroids
init_centroids = np.array([[1,1], [2,1]])

# Create a KMeans object by specifying
# - Number of clusters (n_clusters) = 2, initial centroids (init) = init_centroids
# - Number of time the k-means algorithm will be run with different centroid seeds (n_init) = 1
# - Maximum number of iterations of the k-means algorithm for a single run (max_iter) = 3
kmeans = KMeans(n_clusters=2, init=init_centroids, n_init=1, max_iter = 3)
```

K-Means Clustering Implementation using Scikit-Learn

```
kmeans.fit(data)                     # Compute k-means clustering
labels = kmeans.predict(data)        # Predict the closest cluster each sample in data belongs to
centroids = kmeans.cluster_centers_  # Get resulting centroids
fig, ax = plt.subplots()             # Defining 2D axes so that we can plot 2D data into it

# Get boolean arrays representing entries with labels = 0 and 1
a = np.array(labels == 0); b = np.array(labels == 1)

# Plot centroids with color = black, size = 50 units, transparency = 20%, and put label "Centroids"
ax.scatter(centroids[:,0], centroids[:,1], c="black", s=50, alpha=0.8, label="Centroids")
# Plot data in the different clusters (1st in red, 2nd in green) with transparency = 50%
ax.scatter(data[a,0], data[a,1], c="red", s=40, alpha=0.5, label="1st Cluster")
ax.scatter(data[b,0], data[b,1], c="green", s=40, alpha=0.5, label="2nd Cluster")
ax.legend() # Show legend

ax.set_xlabel("Weight Index")                    # Put x-axis label "Weight Index"
ax.set_ylabel("pH Index")                        # Put y-axis label "pH Index"
ax.set_title("Medicine - K-Means Clustering")    # Put figure title
```

That's all!

Any questions?