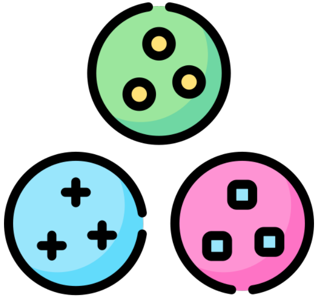
Computer Science

CSC380: Principles of Data Science

Clustering: K Means

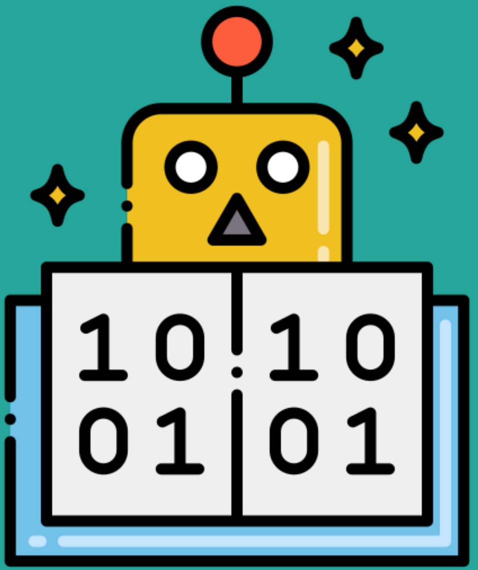


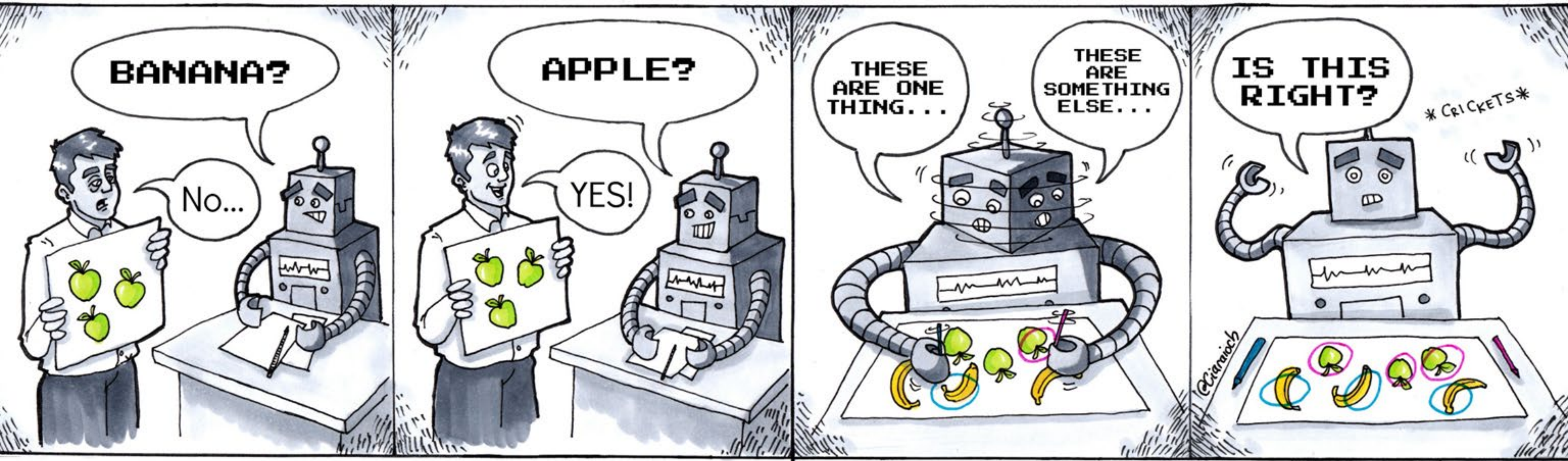
Slides prepared for Lecture in 2021 by Enfa George (TA)

Outline

- Unsupervised Learning
    - Clustering
        - Types of Clustering
            - K Means Intuition
                - Formalising K Means
                - Convergence In K- Means
                - Choosing an Optimum Number Of K
                - K-Means++
                - K-Medoids
                - Assumptions Made by K-Means
            - Application Case
            - How to Use K Means?
        - How can We Improve?

Unsupervised Learning





Supervised Learning

Unsupervised Learning

Clustering

Task 1 : Group These Set of Document into 3 Groups based on meaning

Doc1 : Health , Medicine, Doctor

Doc 2 : Machine Learning, Computer

Doc 3 : Environment, Planet

Doc 4 : Pollution, Climate Crisis

Doc 5 : Covid, Health , Doctor

Task 1 : Group These Set of Document into 3 Groups.

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Task 1 : Group These Set of Document into 3 Groups.

Doc1 : Health , Medicine, Doctor

Doc 5 : Covid, Health , Doctor

Doc 3 : Environment, Planet

Doc 4 : Pollution, Climate Crisis

Doc 2 : Machine Learning, Computer

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering

Image from towardsdatasciencee.com

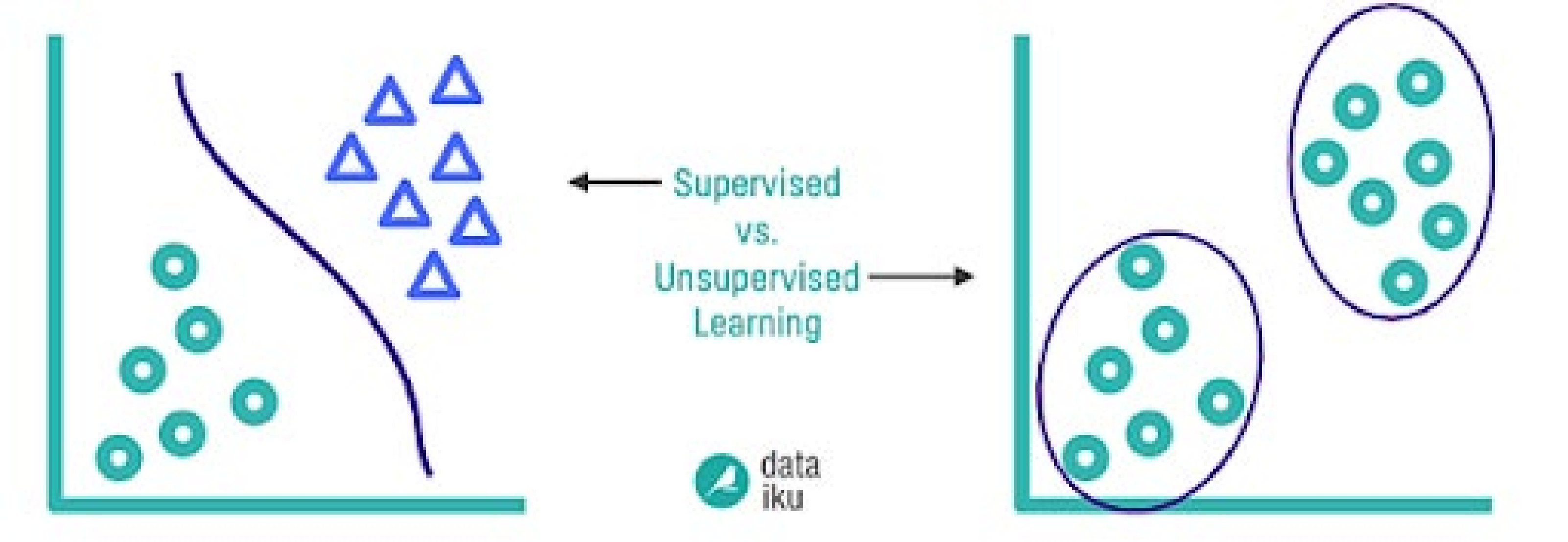
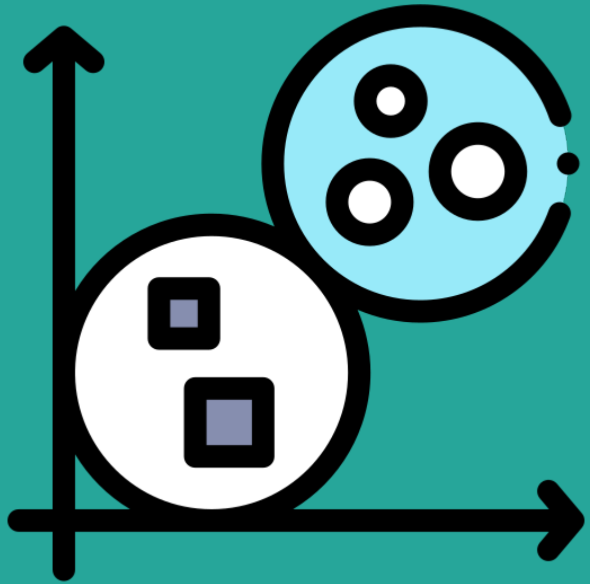


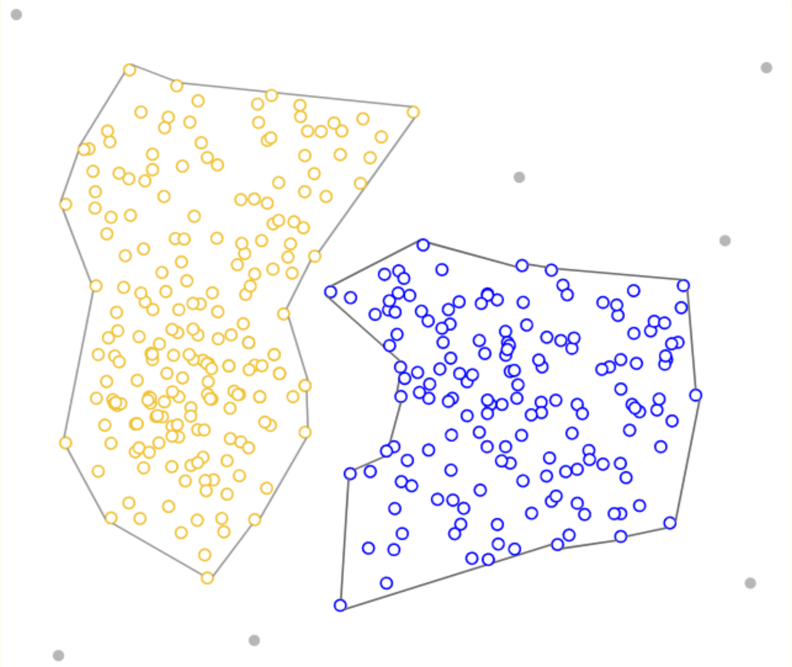
Image from Dataiku

Types of Clustering

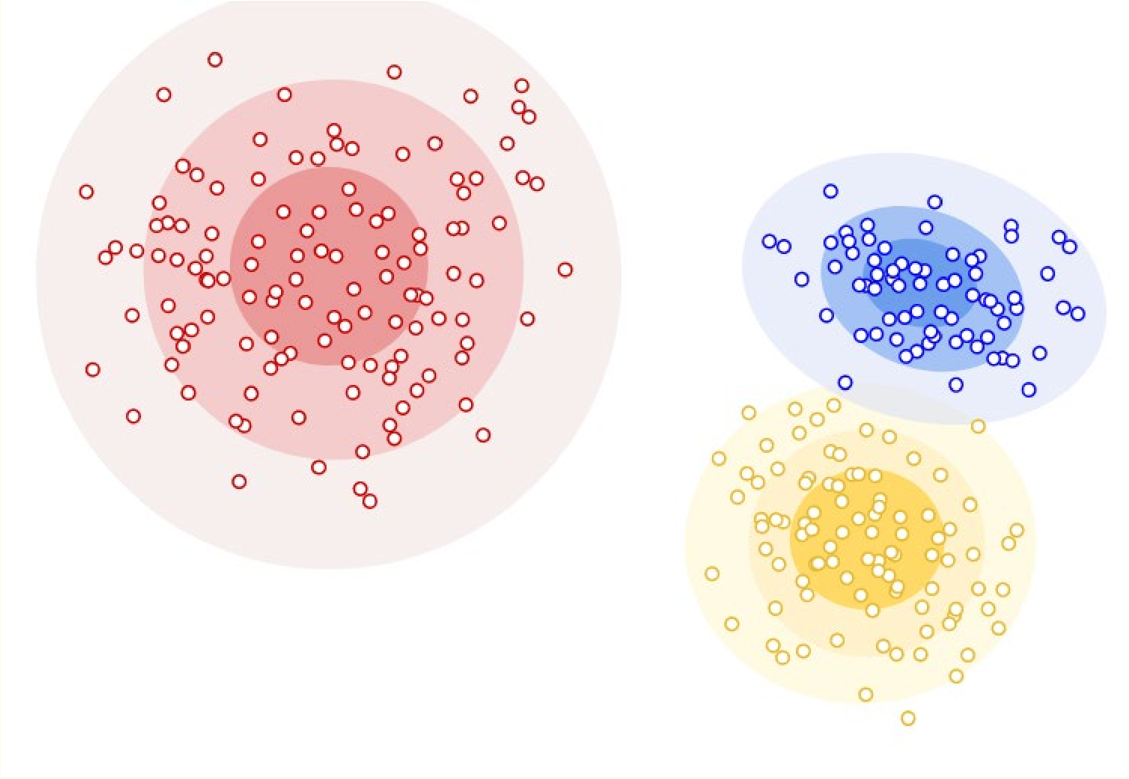


From Clustering in Machine Learning - Google Developers
For a comprehensive List : A Comprehensive Survey of Clustering Algorithms

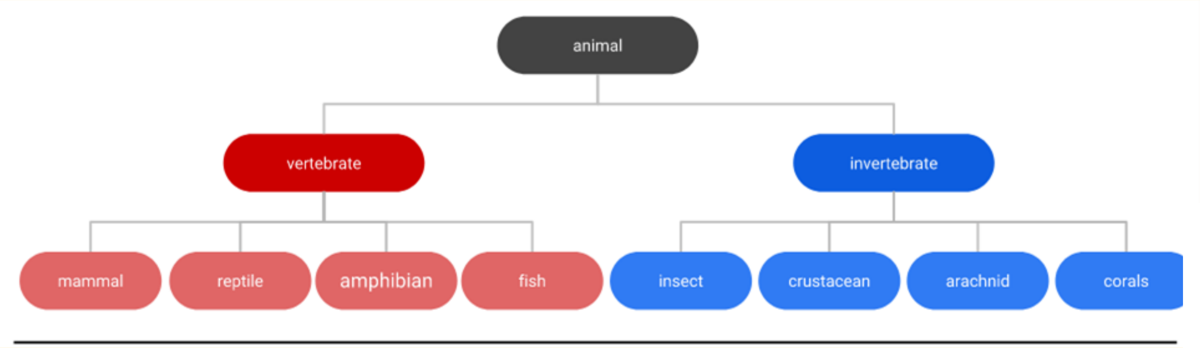
Density Based Clustering

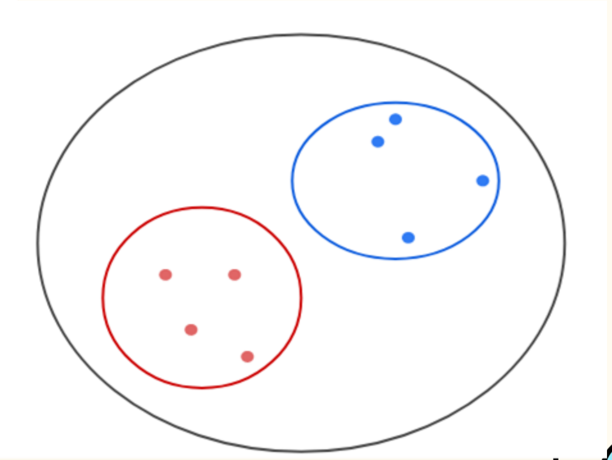


Distribution-based Clustering

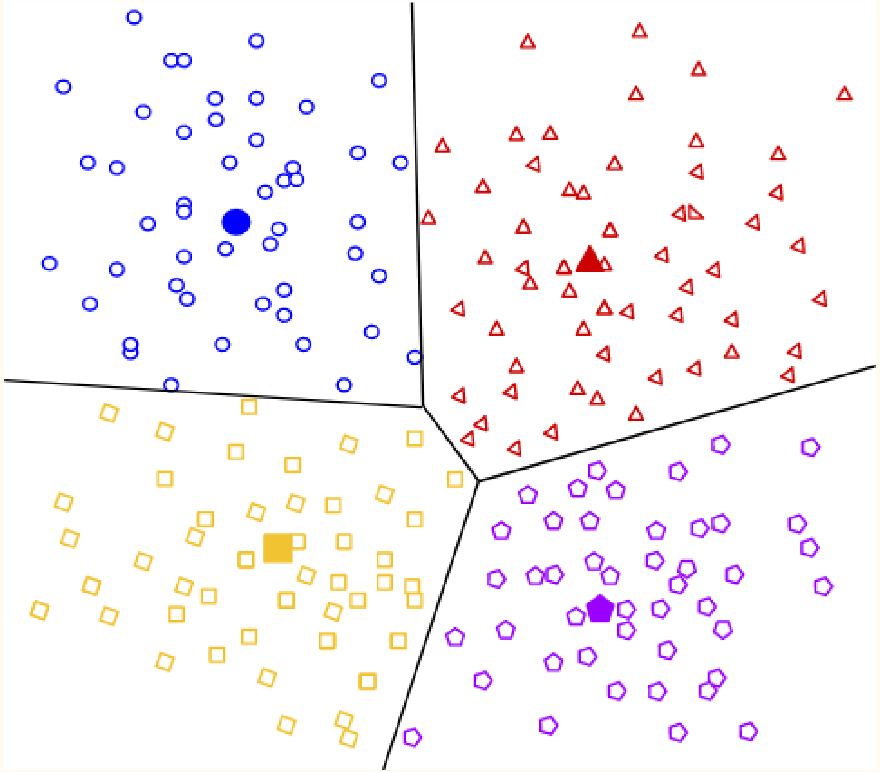


Hierarchical Clustering



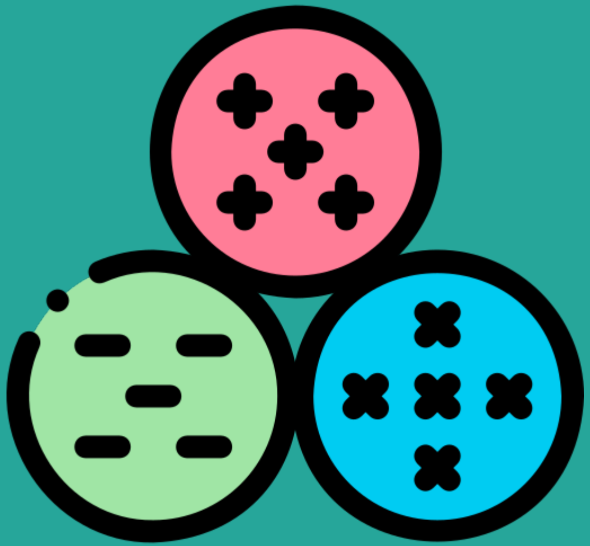


Centroid-based Clustering



One such Centroid Based Clustering Algorithm Is K-Means

K Means Intuition

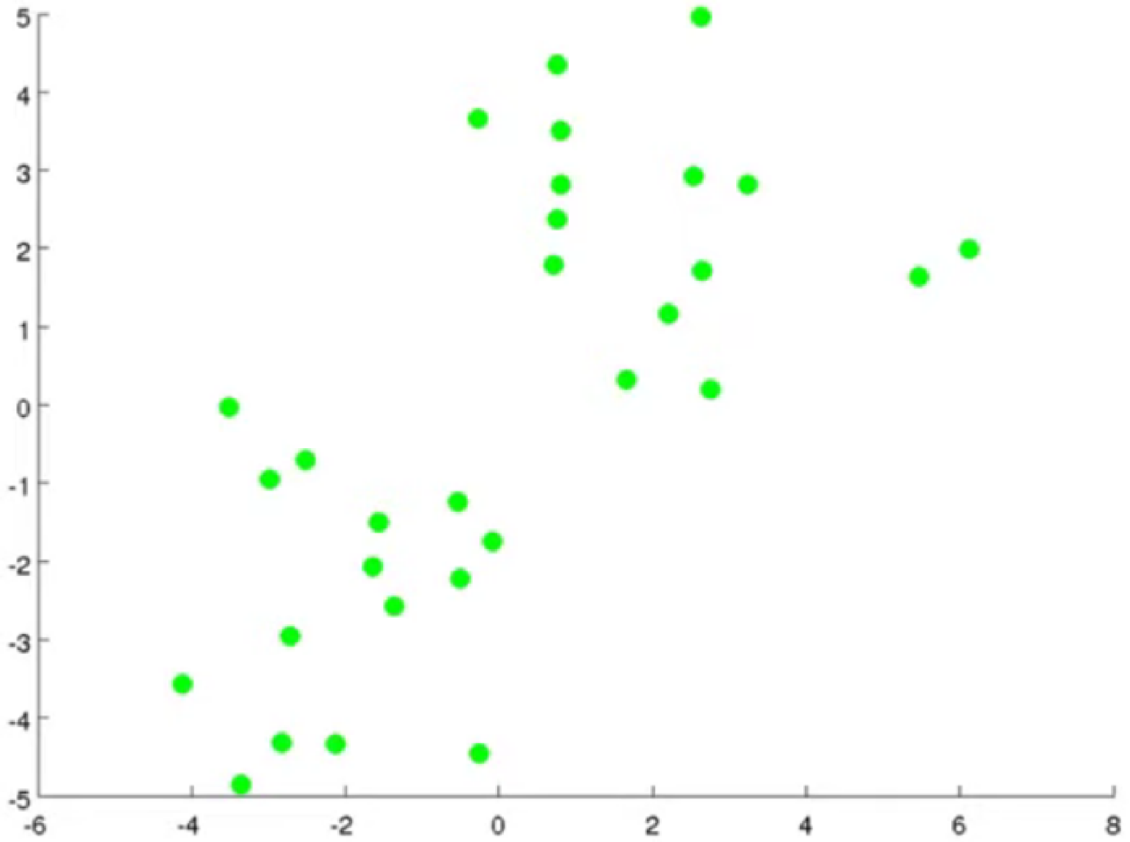


Icons are used from FlatIcon.com

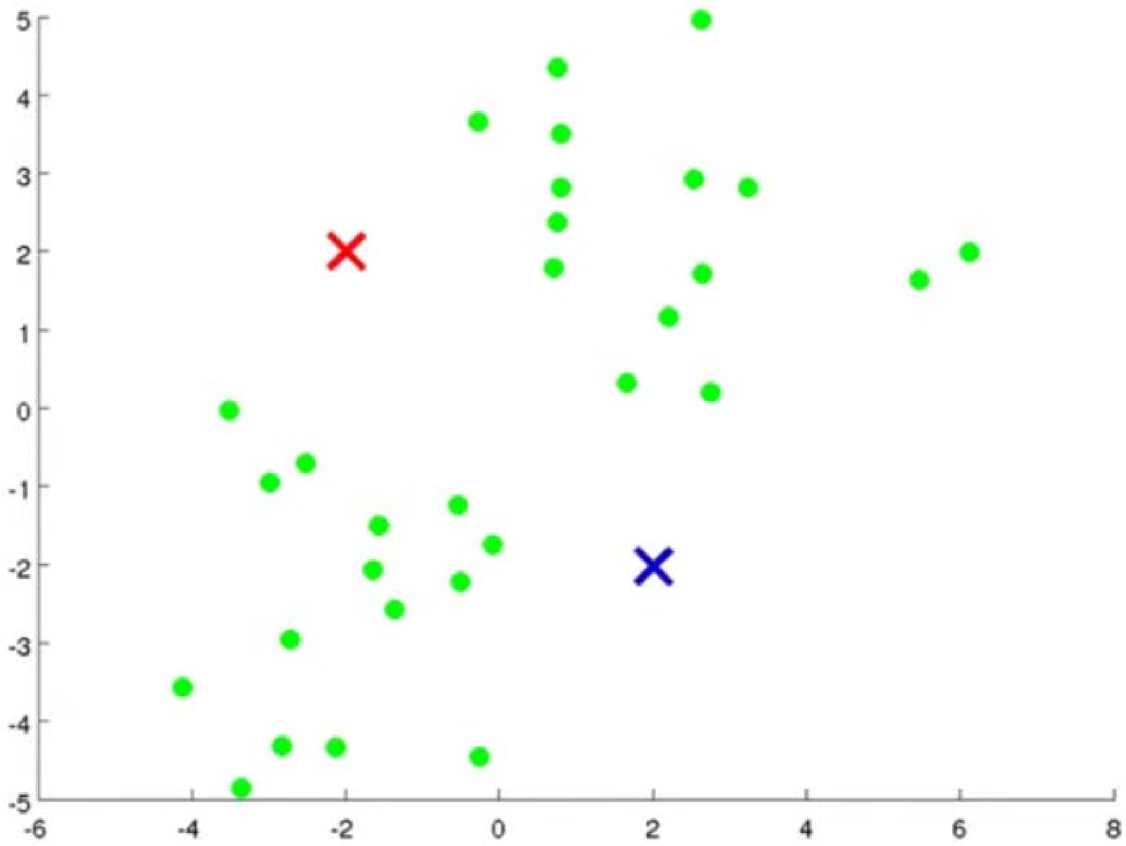
Basic Steps

- Assign Cluster Centroids

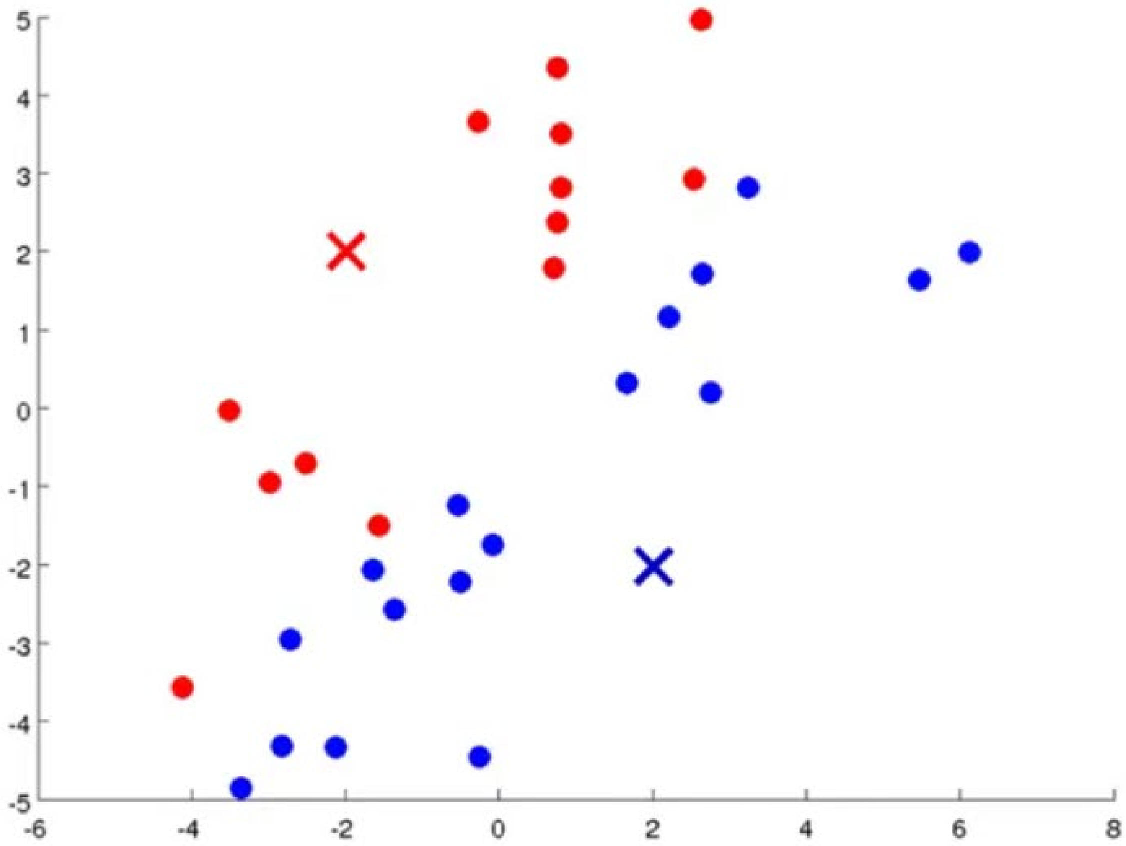
- Until Convergence :
  - Cluster Assignment Step
  - Re-assigning Centroid Step



Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2



Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2



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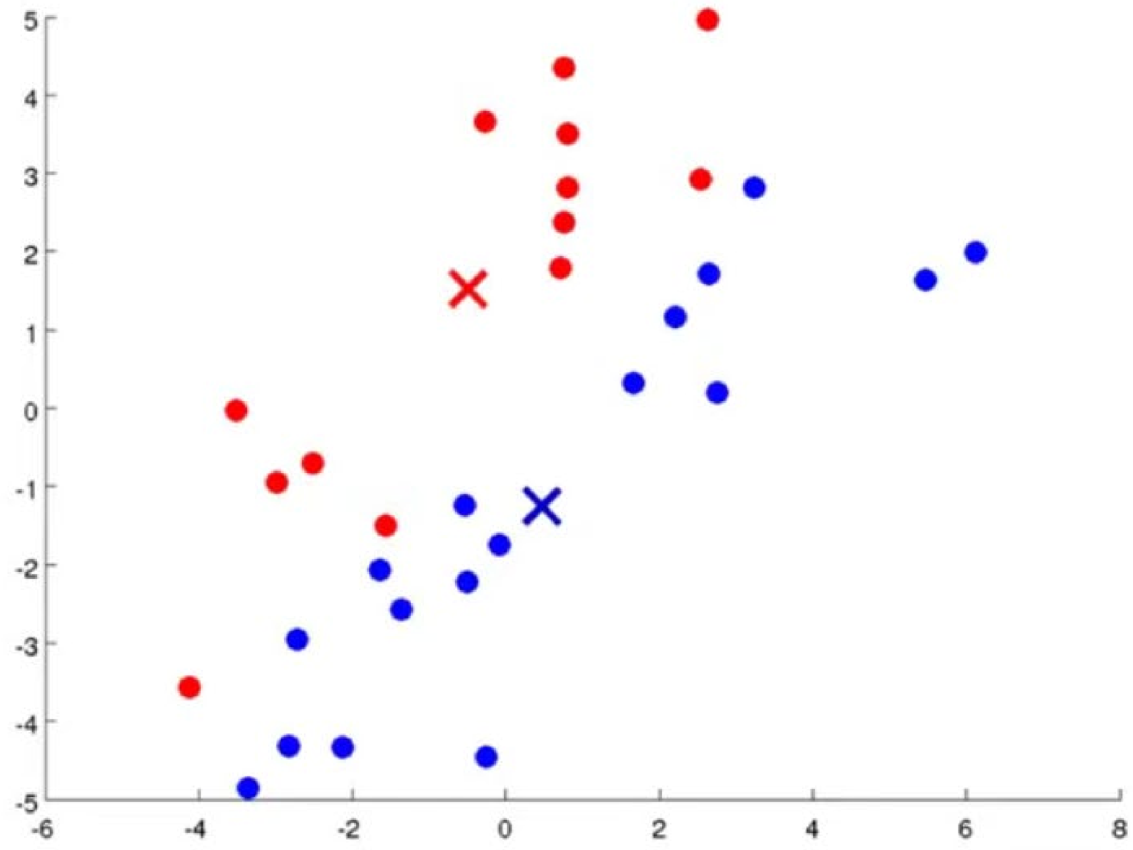
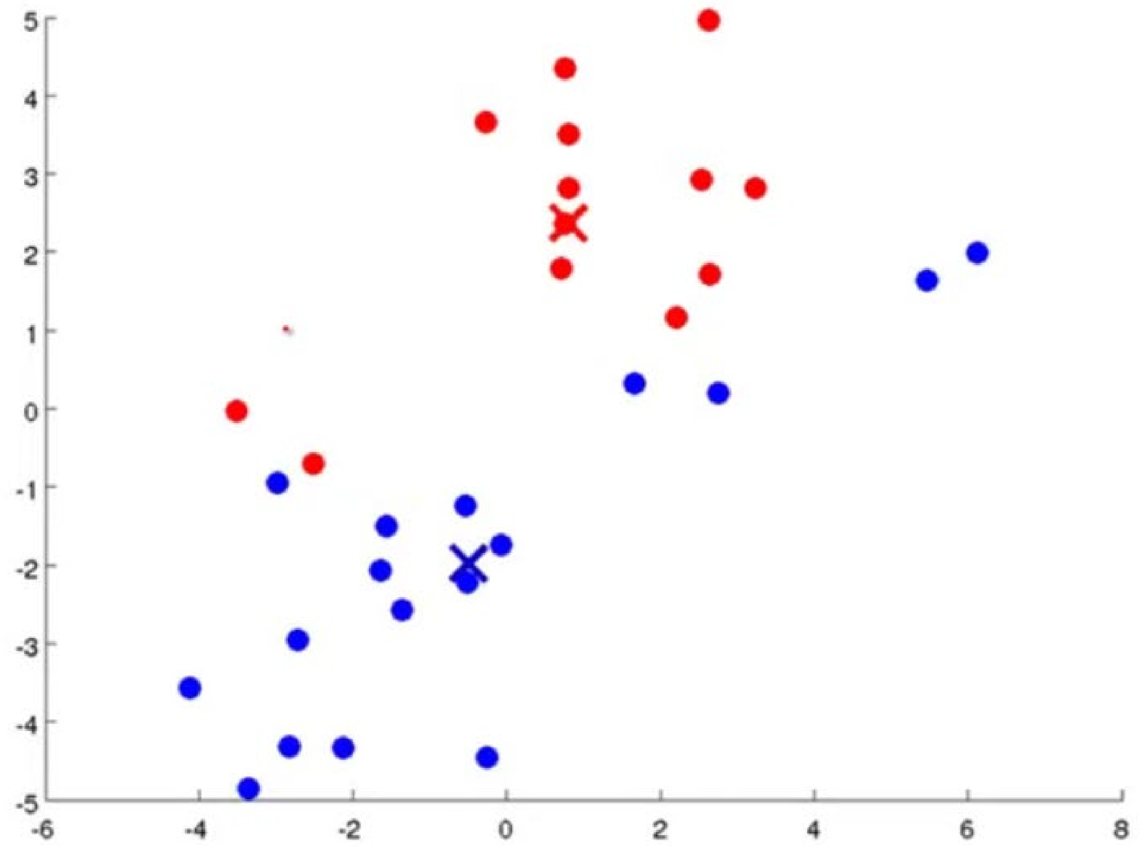
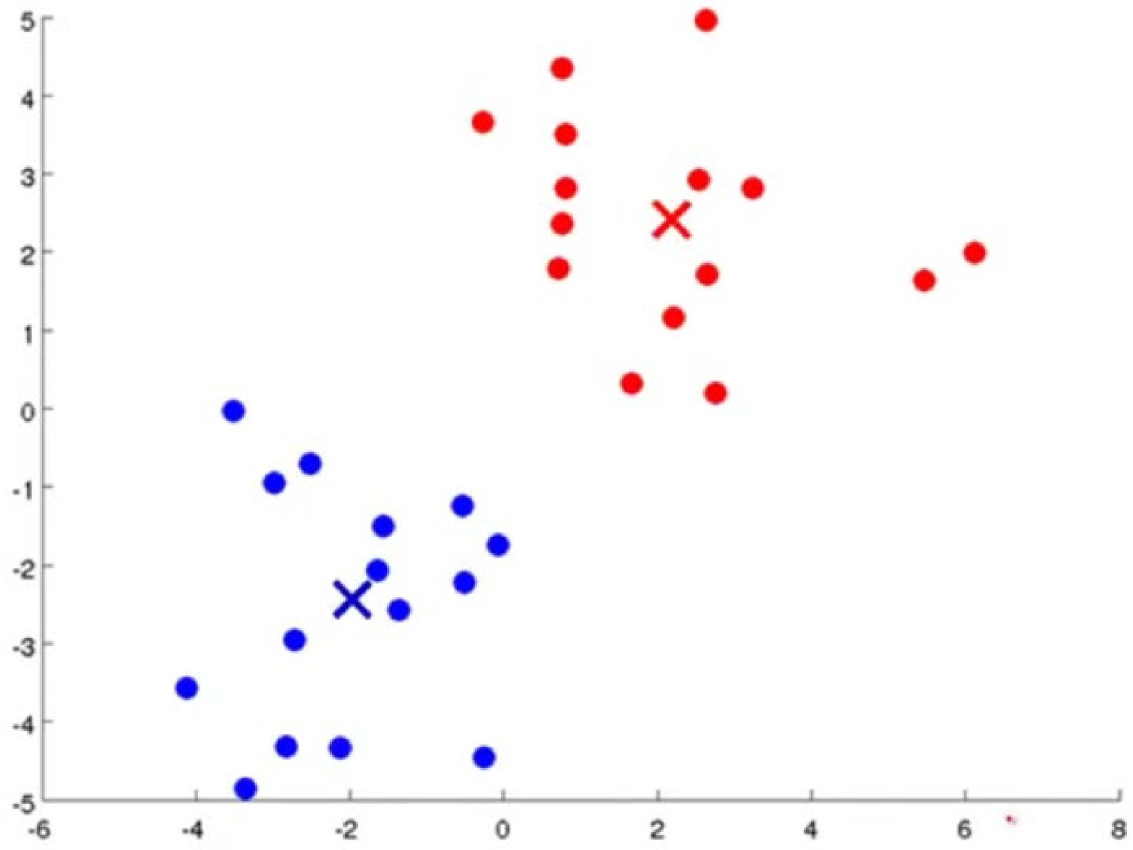


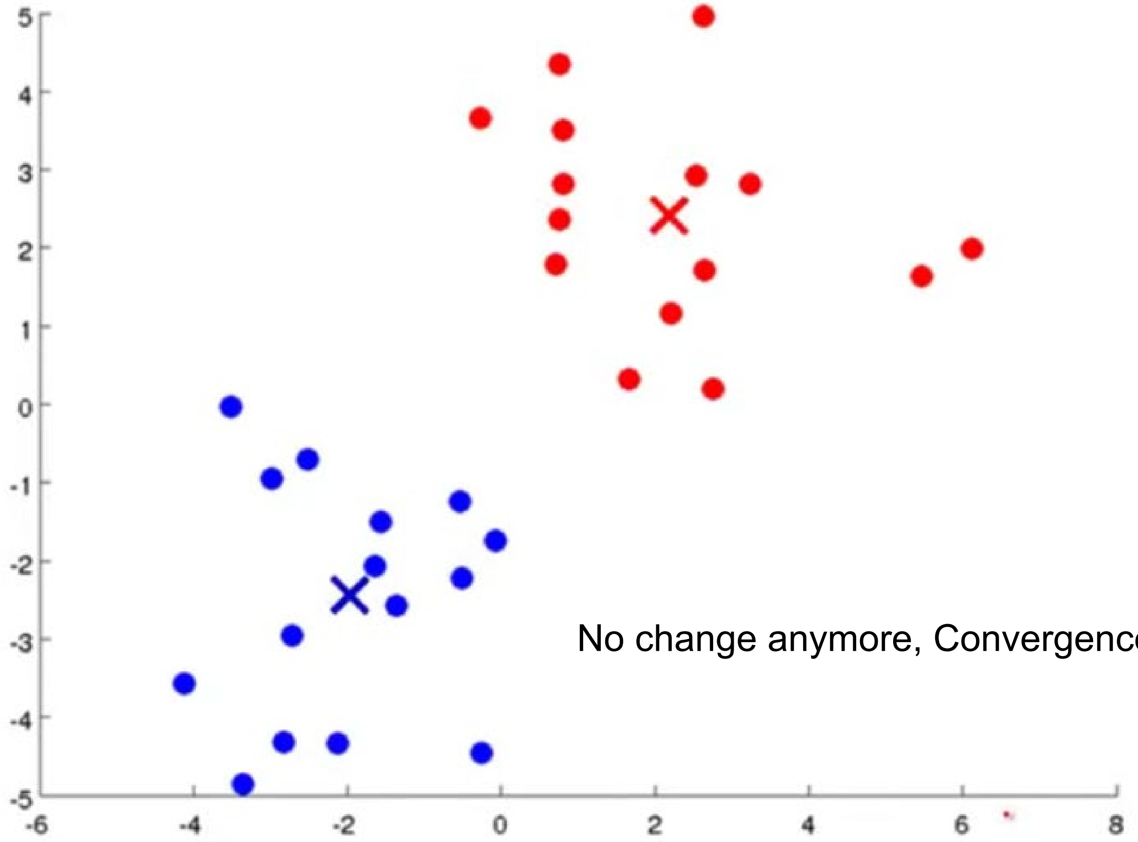
Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2



Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2



Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2



No change anymore, Convergence!

Slides from Andrew Ng | Machine Learning Coursera Lecture 13.2

Basic Steps

- Assign Cluster Centroids
- Until Convergence :
  - Cluster Assignment Step
  - Re-assigning Centroid Step

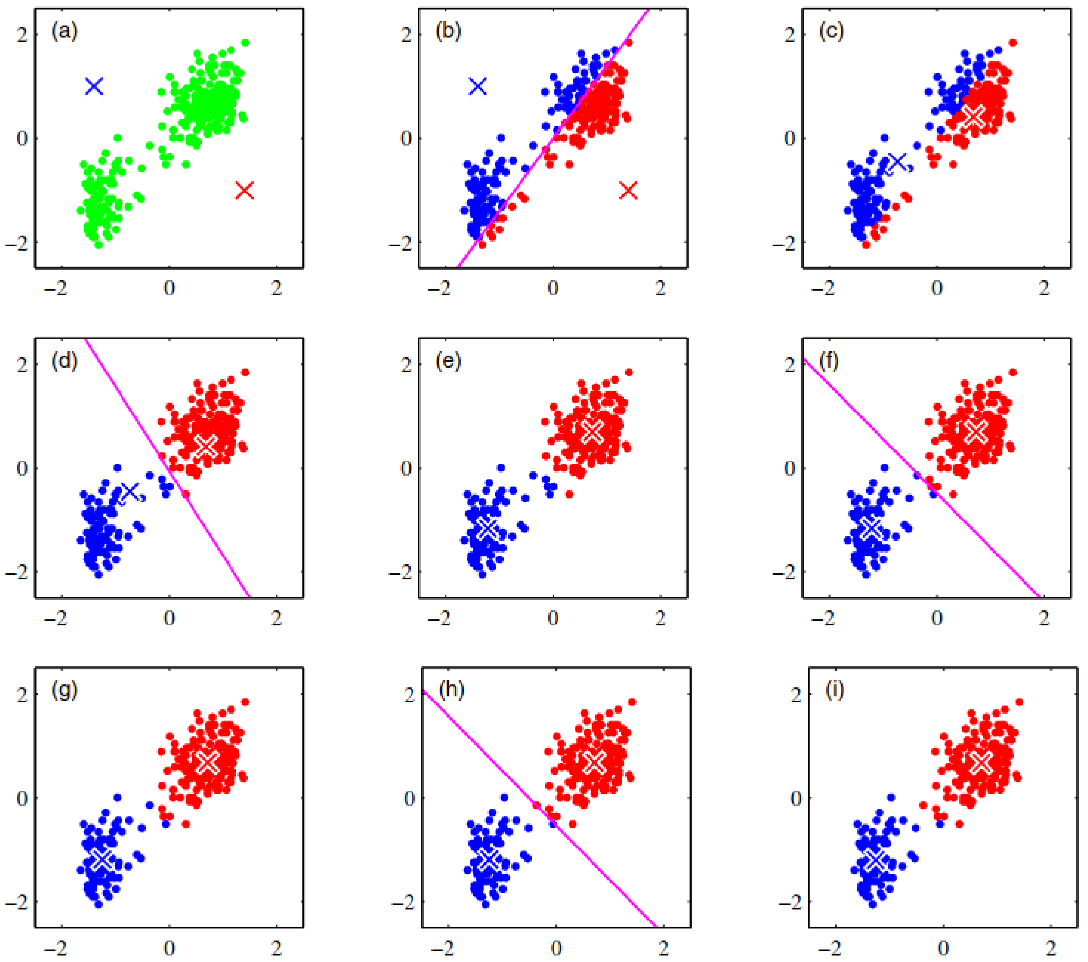
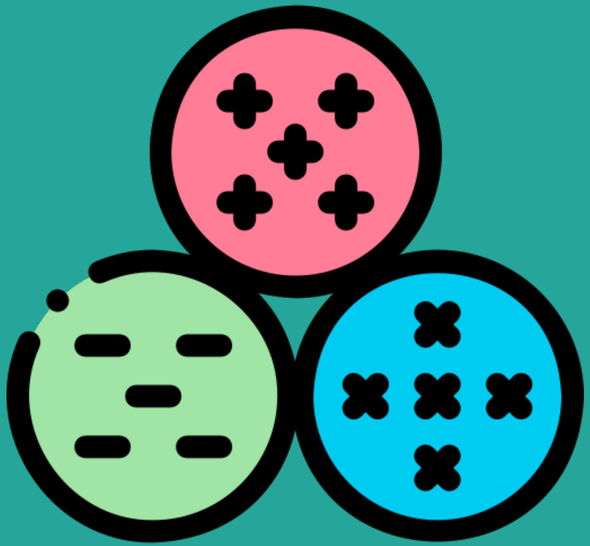


Fig 9.1 from Bishop - Pattern Recognition And Machine Learning

K Means Formalisation



What is a Cluster?

A group of data points whose inter-point distances are small compared with the distances to points outside of the cluster.

Clustering?

Consider a set of D-dimensional vectors μ_k, where $k = 1, \ldots, K$, in which μ_k is a prototype associated with the kth cluster.

Clustering?

The goal of Clustering is then to find an assignment of data points to clusters, as well as a set of vectors $\{\mu_k\}$, such that the sum of the squares of the distances of each data point to its closest vector μk, is a minimum.

First we choose some initial values for the μ_k

Step1 : Assignment of data points to clusters

- 1-of-K coding scheme

For each data point x_n, we introduce a corresponding set of binary indicator variables $r_{nk} \in \{ 0, 1\}$, where $k = 1 , . . . , K$ describing which of the K clusters the data point xn is assigned to, so that if data point x_n is assigned to cluster k then $r_{nk} = 1$, and $r_{nj} = 0$ for $j = k$.

Objective function - Distortion Measure

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

Step 2 : Assign Cluster to Each Point.

We minimize J with respect to the r_{nk}, keeping the μ_k fixed

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$

Step 3 : Reassignment of Centroids

We minimize J with respect to the μ_k, keeping rnk fixed.

function J is a quadratic function of $\boldsymbol{\mu}_k$, and it can be minimized by setting its derivative with respect to $\boldsymbol{\mu}_k$ to zero giving

$$2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) = 0 \tag{9.3}$$

which we can easily solve for $\boldsymbol{\mu}_k$ to give

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}. \tag{9.4}$$

This simply means -

μ_k equal to the mean of all of the data points x_n assigned to cluster k

This simply means -

μ_k equal to the mean of all of the data points xn assigned to cluster k

Hence the name K Means

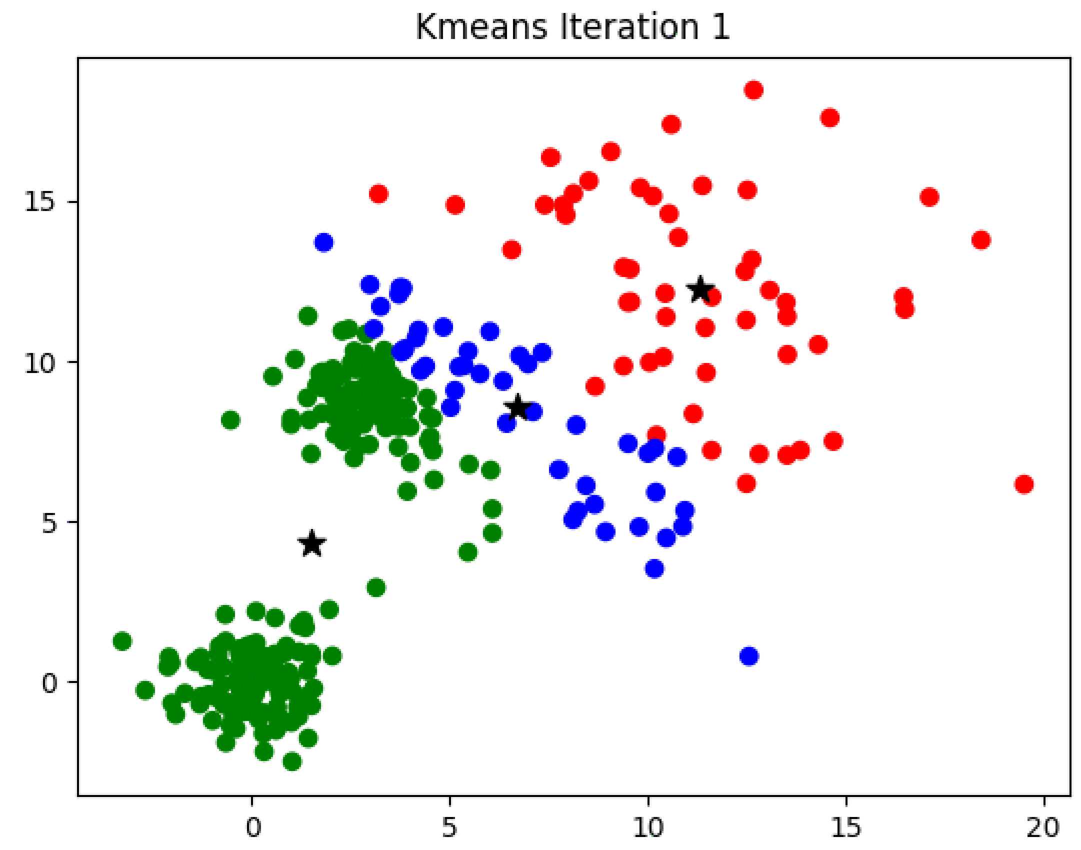


Image from [Floydhub]

K-means algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

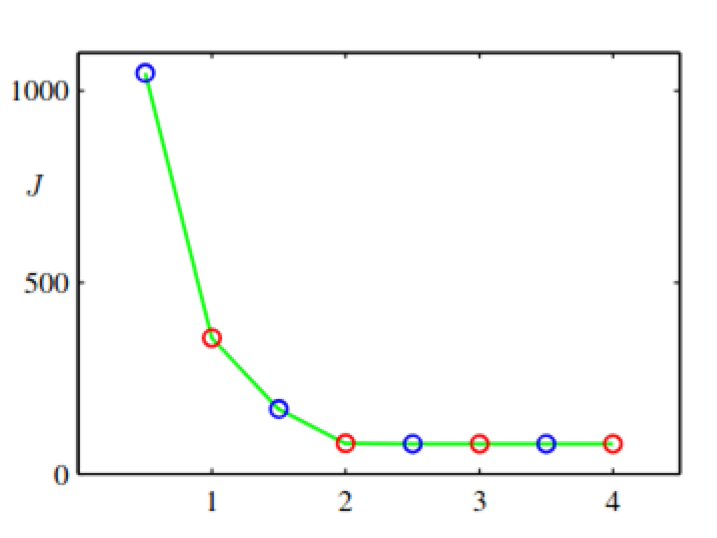
μ_k := average (mean) of points assigned to cluster k

}

Convergence In K-Means

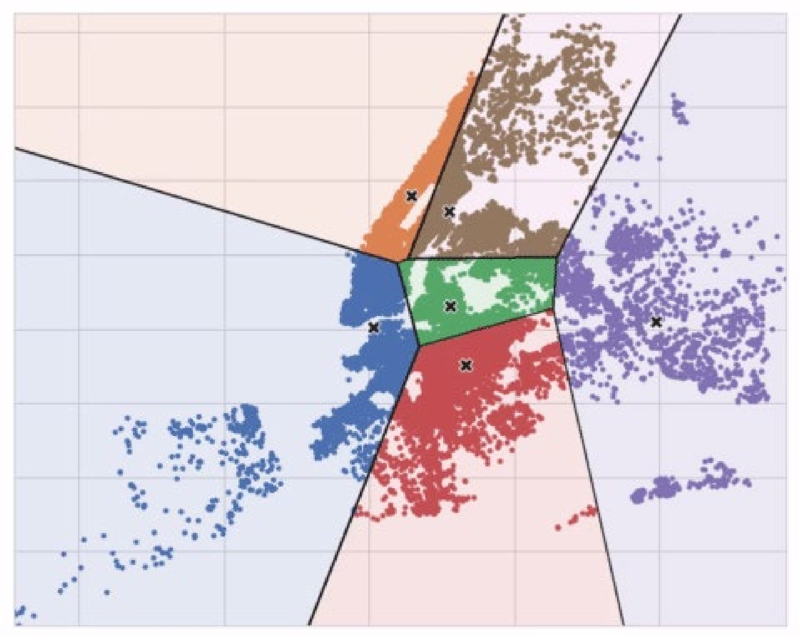
Promise of Convergence

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$



Plot of the cost function J given by (9.1) after each E step (blue points) and M step (red points) of the K-means algorithm for the example shown in Figure 9.1.

Iterating until Convergence



Animation from Kaggle

But,

It may converge to a local rather than global minimum of J.

Local optima

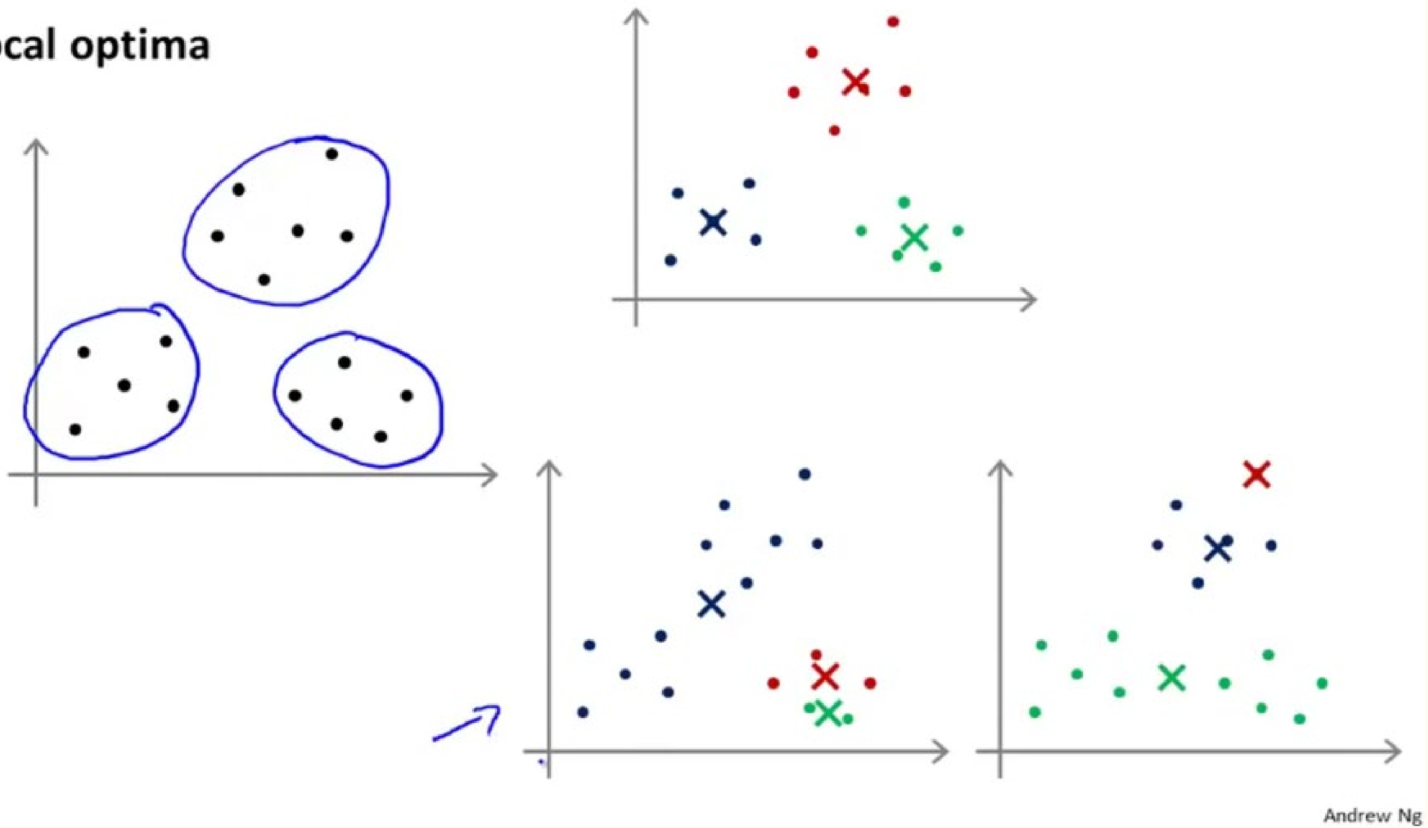


Image from Andrew NG Coursera Machine Learning Course

A cluster Has Just One Point?

Why ?

A cluster Has Just One Point?

Why ?

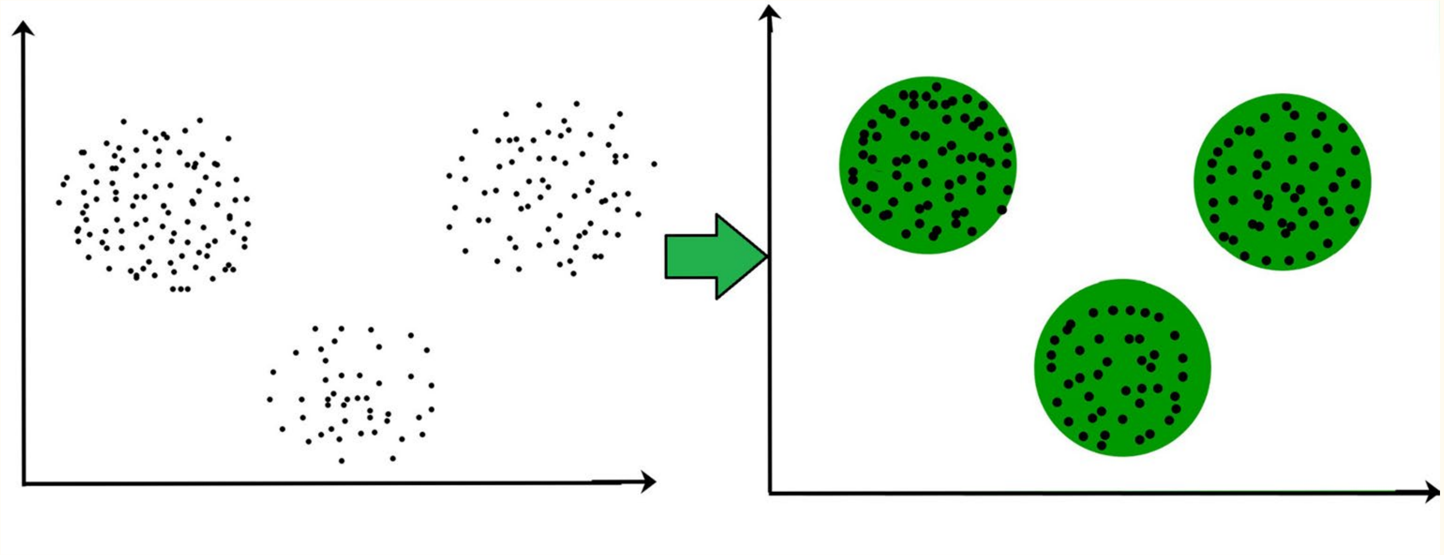
What to Do?

Choosing The Number Of K

How to Choose Number of K?

- Most common approach is Visualise, and then pick manually

Most common approach is Visualise, and then pick manually



How to Choose Number of K?

The Elbow Method

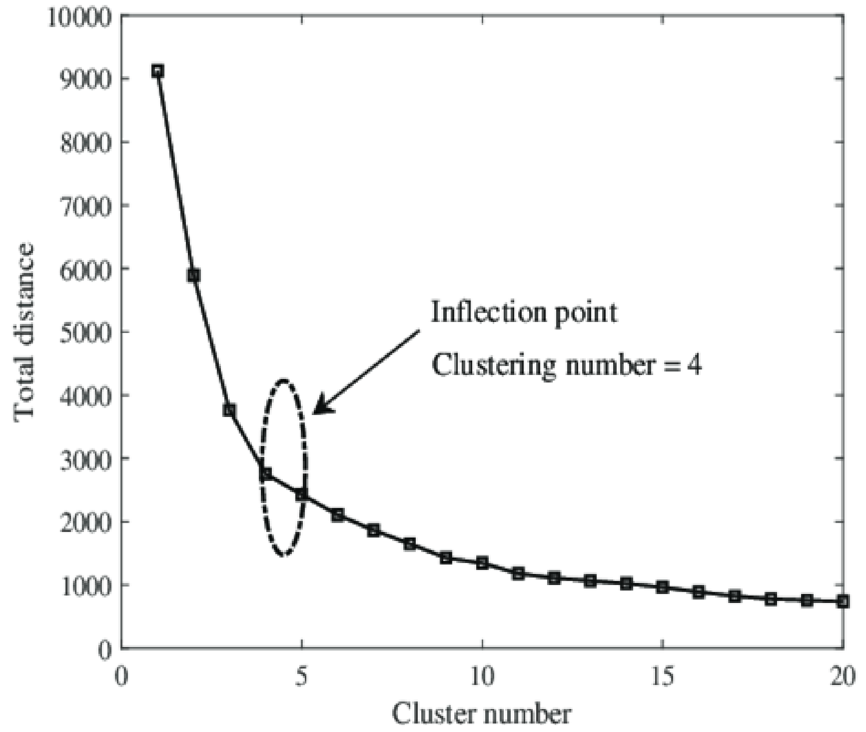


Image Source

How to Choose Number of K?

But sometimes it doesn't work

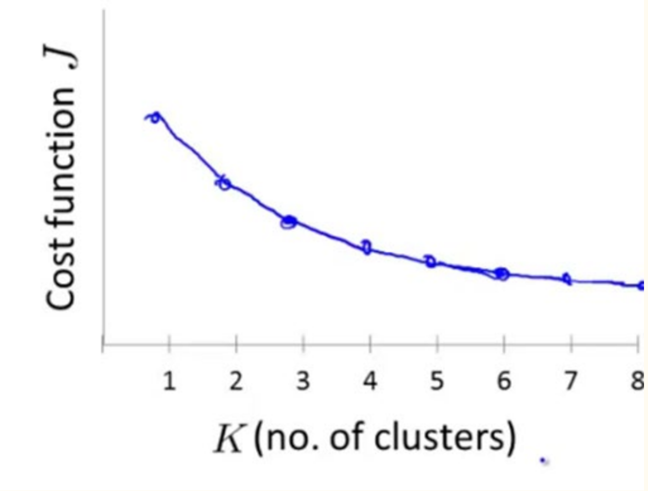


Image Source : Andrew NG Machine Learning

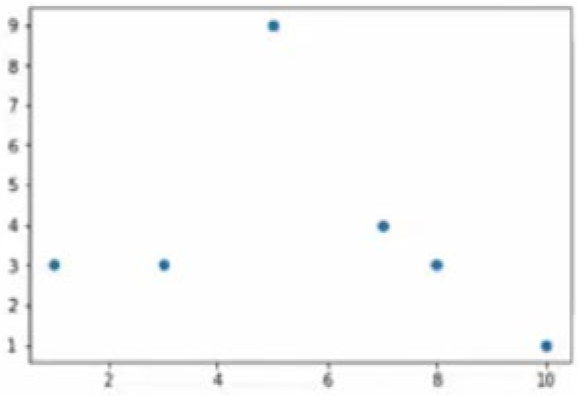
KMeans ++

Is there a way to start Smarter?

From Sara Jensen’s Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.
We begin by randomly selecting (7,4) to be a cluster center.

x	$\min(d(x, z_i)^2)$
(7,4)	
(8,3)	
(5,9)	
(3,3)	
(1,3)	
(10,1)	



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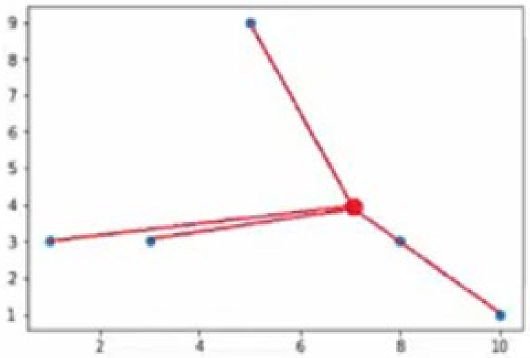
We begin by randomly selecting (7,4) to be a cluster center.

x	$\min(d(x,z_i)^2)$
(7,4)	-
(8,3)	2
(5,9)	29
(3,3)	17
(1,3)	37
(10,1)	18



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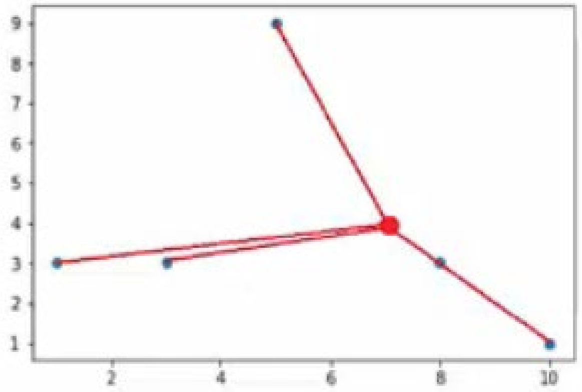
We begin by randomly selecting (7,4) to be a cluster center.

x	prob
(7,4)	-
(8,3)	2/103
(5,9)	29/103
(3,3)	17/103
(1,3)	37/103
(10,1)	18/103

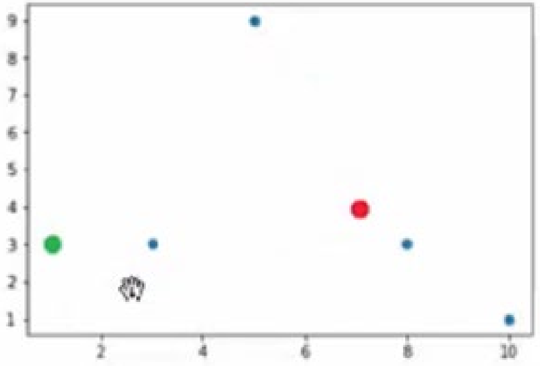


From Sara Jensen's Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.

We add (1,3) to the list of cluster centers.

x	$\min(d(x, z_i)^2)$
(7,4)	-
(8,3)	
(5,9)	
(3,3)	
(1,3)	-
(10,1)	

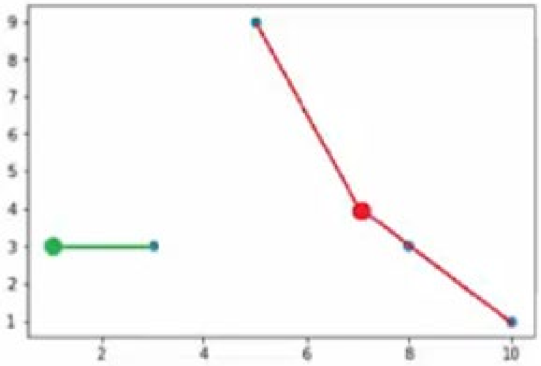


From Sara Jensen's Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.

We add (1,3) to the list of cluster centers.

x	$\min(d(x, z_i)^2)$
(7,4)	-
(8,3)	2
(5,9)	29
(3,3)	4
(1,3)	-
(10,1)	18

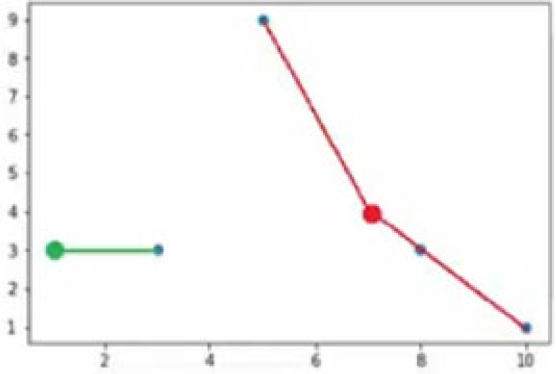


From Sara Jensen's Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.

We add (1,3) to the list of cluster centers.

x	prob
(7,4)	-
(8,3)	2/55
(5,9)	29/55
(3,3)	4/55
(1,3)	-
(10,1)	18/55

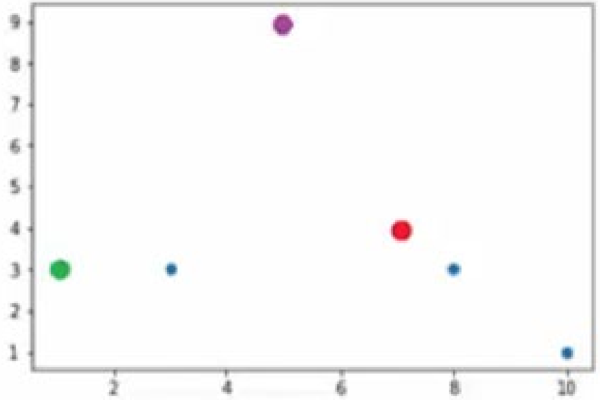


From Sara Jensen's Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.

We add (5,9) to the list of cluster centers.

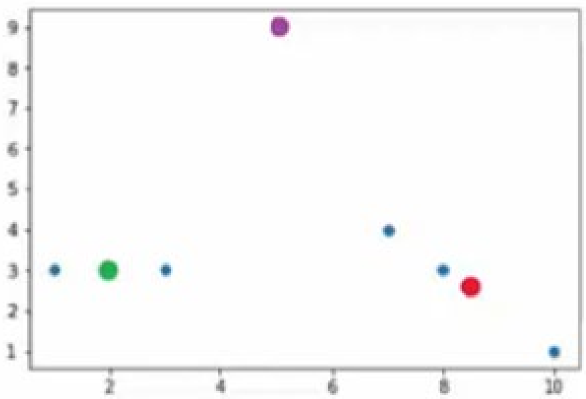
x	prob
(7,4)	-
(8,3)	
(5,9)	-
(3,3)	
(1,3)	-
(10,1)	



From Sara Jensen’s Youtube Channel

Suppose we have the small dataset [(7,4),(8,3),(5,9),(3,3),(1,3),(10,1)] to which we wish to assign 3 clusters.
We now run k-means with initialized centers (7,4),(1,3), and (5,9).

x	prob
(7,4)	-
(8,3)	
(5,9)	-
(3,3)	
(1,3)	-
(10,1)	



K Medoids

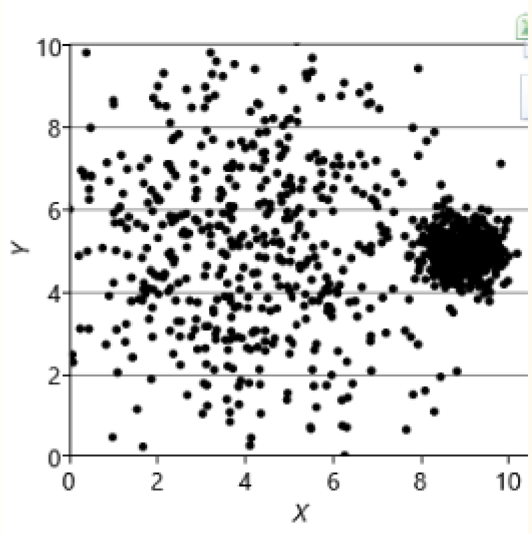
- The issue with Squared Euclidean Distance
    - Type of Data
    - Reaction to Outliers
- How can we generalise better?

K-medoids algorithm

$$\widetilde{J} = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$

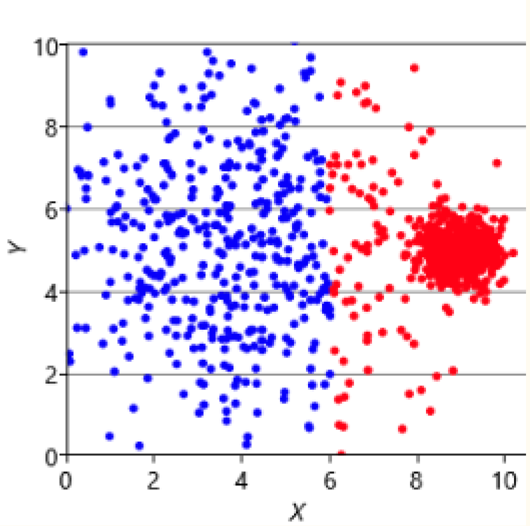
Assumptions made by K Means

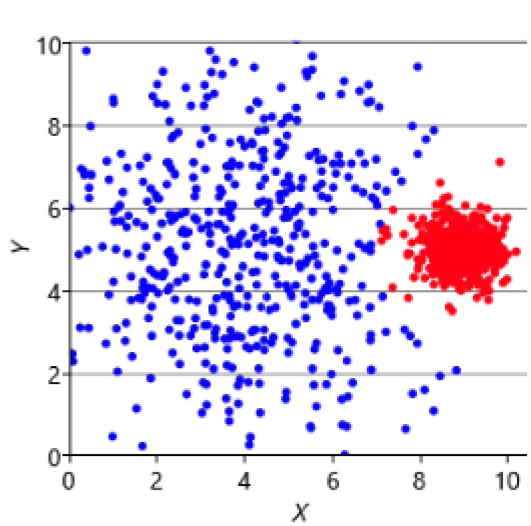
Based onmlbmlbook

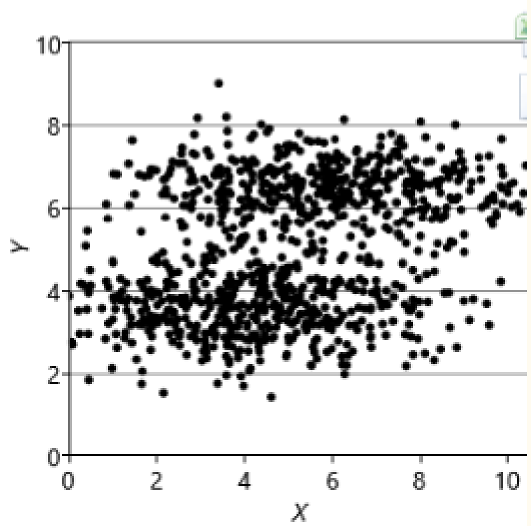


10
8
6
4
2
0
Y
0
2
4
6
8
10
X

1. All clusters are the same size.(Area not Cardinality)

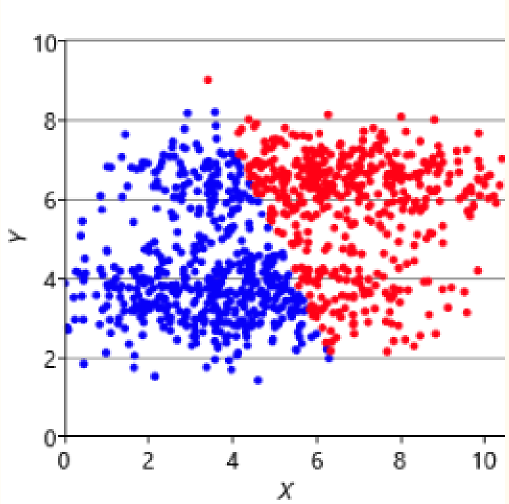


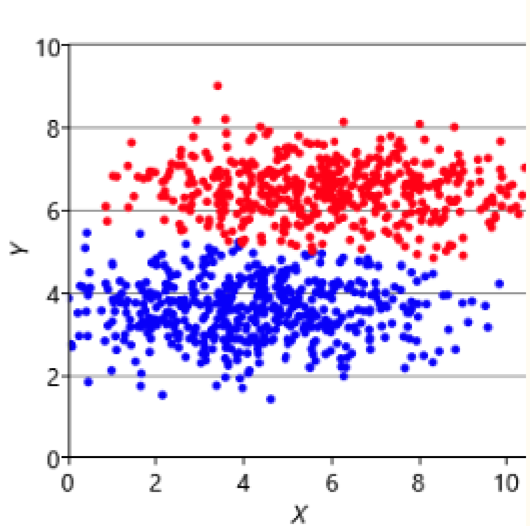


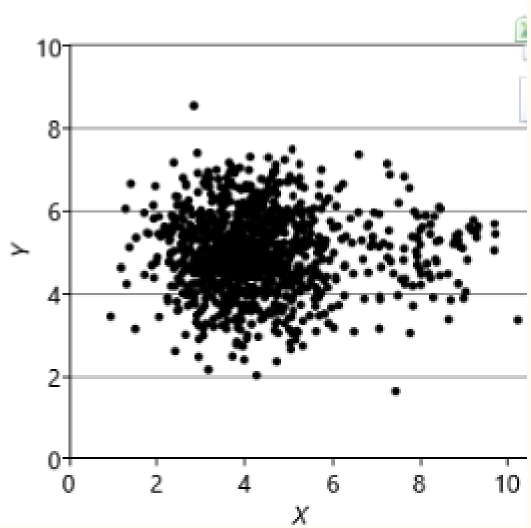


10
8
6
4
2
0
y
0
2
4
6
8
10
X

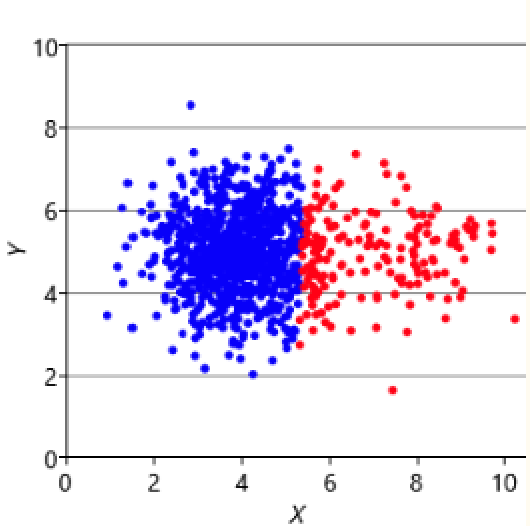
2. Clusters have the same extent in every direction.

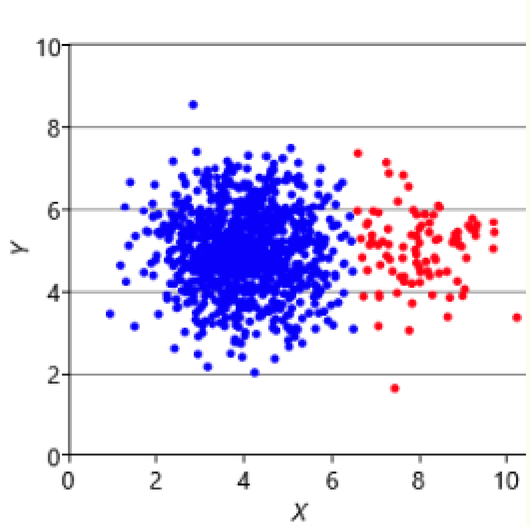


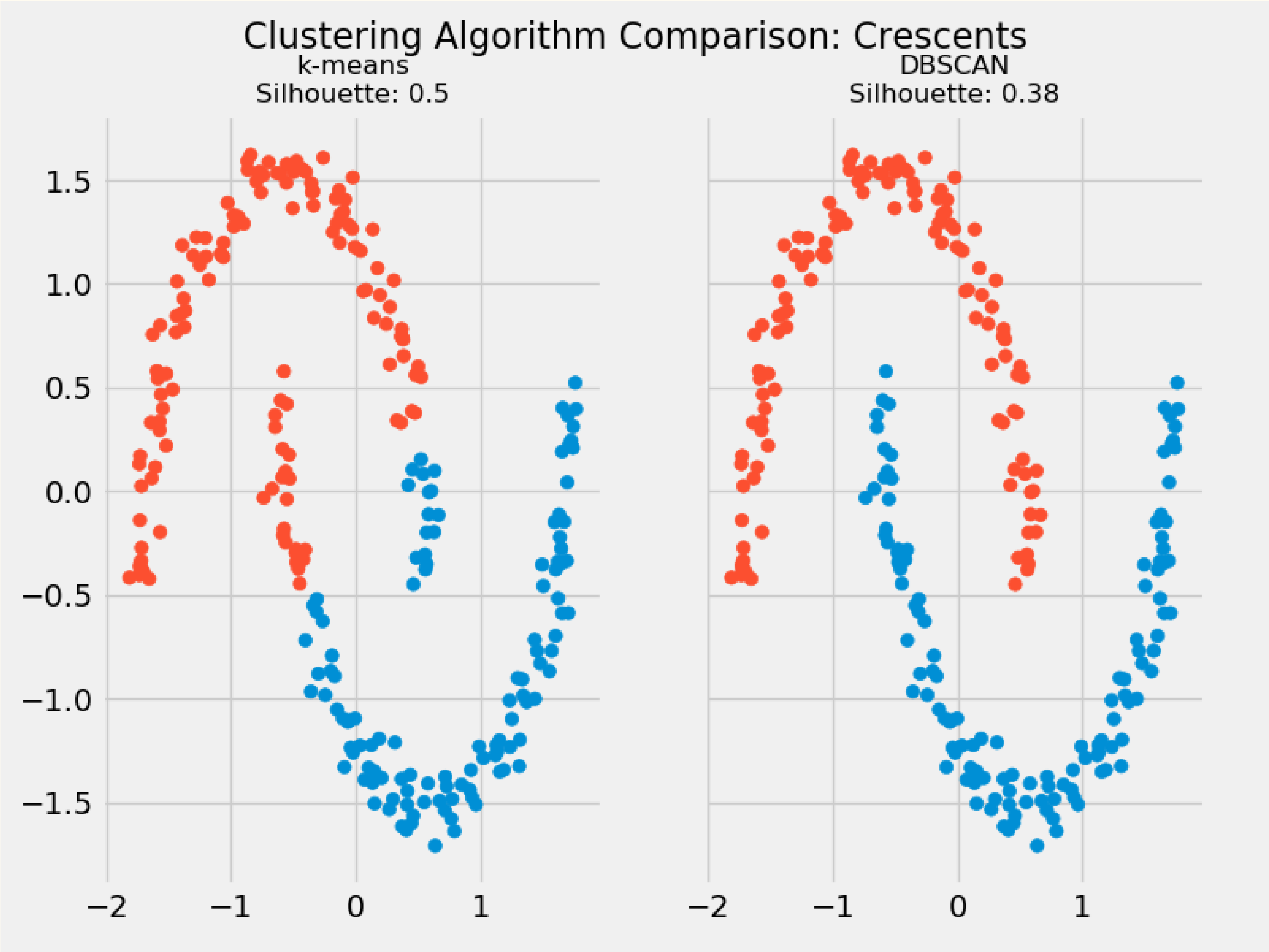



10
8
6
4
2
0
Y
0
2
4
6
8
10
X

3. Clusters have similar numbers of points assigned to them.






Clustering Algorithm Comparison: Crescents
k-means
Silhouette: 0.5
DBSCAN
Silhouette: 0.38
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2
−1
0
1
−2
−1
0
1

Application Case:

Image Segmentation and Compression

What is Segmentation?

Segmentation is to partition an image into regions each of which has a reasonably homogeneous visual appearance or which corresponds to objects or parts of objects

Original image

$K = 10$

Original image

$K = 3$

Original image

$K = 2$

How to Use?

sklearn.cluster.KMeans

class sklearn.cluster.KMeans(*n_clusters=8*, ***, *init='k-means++'*, *n_init=10*, *max_iter=300*, *tol=0.0001*, *verbose=0*, *random_state=None*, *copy_x=True*, *algorithm='auto'*) [source]

```
>>> from sklearn.cluster import KMeans
>>> import numpy as np
>>> X = np.array([[1, 2], [1, 4], [1, 0],
...               [10, 2], [10, 4], [10, 0]])
>>> kmeans = KMeans(n_clusters=2, random_state=0).fit(X)
>>> kmeans.labels_
array([1, 1, 1, 0, 0, 0], dtype=int32)
>>> kmeans.predict([[0, 0], [12, 3]])
array([1, 0], dtype=int32)
>>> kmeans.cluster_centers_
array([[10.,  2.],
       [ 1.,  2.]])
```

```python
# Importing the dataset
dataset = pd.read_csv('../input/Mall_Customers.csv',index_col='CustomerID')
```

```python
dataset.head()
```

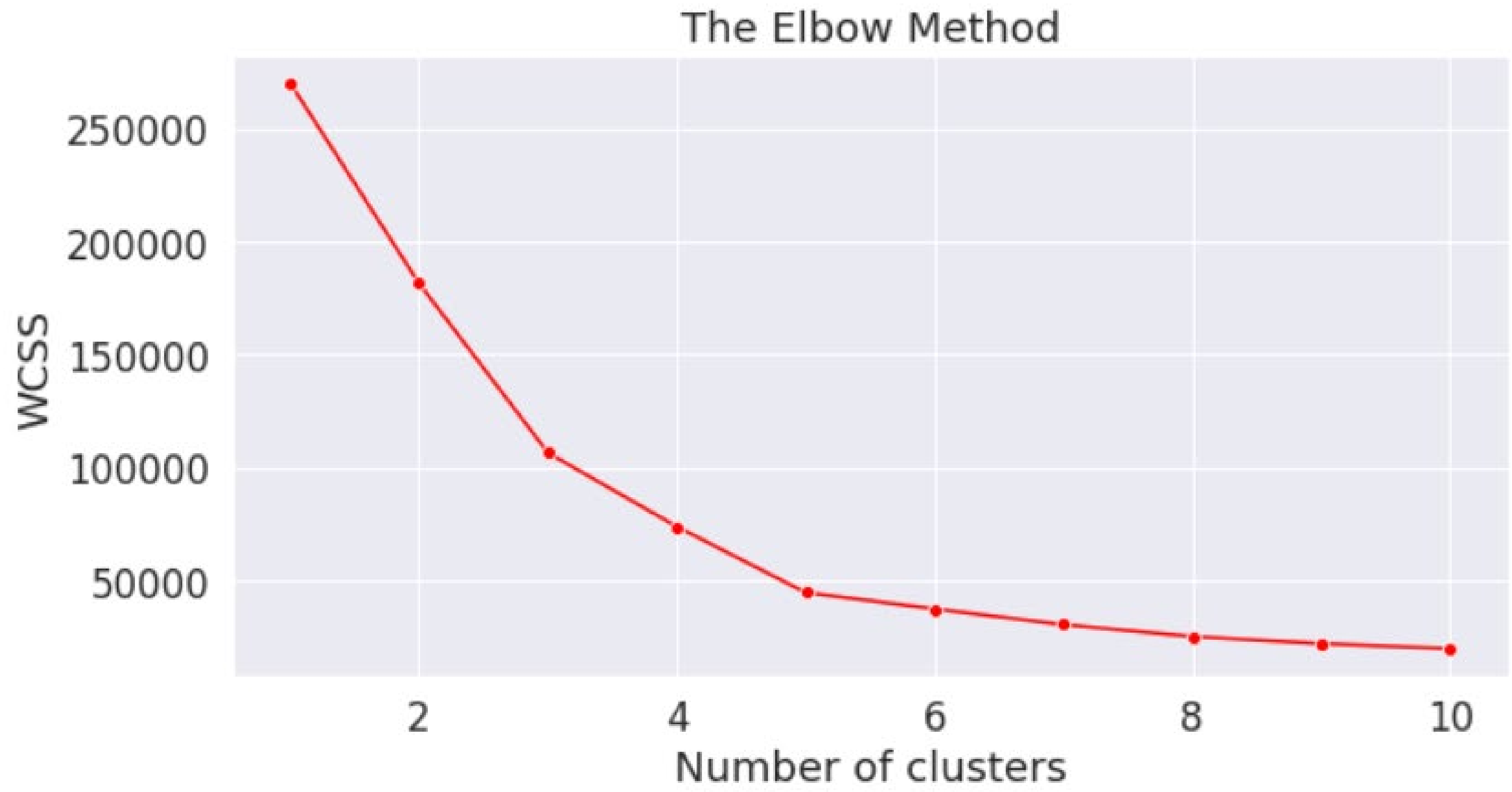
	Genre	Age	Annual_Income_(k$)	Spending_Score
CustomerID				
1	Male	19	15	39
2	Male	21	15	81
3	Female	20	16	6
4	Female	23	16	77
5	Female	31	17	40

Step by Step KMeans Explained in Detail

```python
# Using the elbow method to find the optimal number of clusters
from sklearn.cluster import KMeans
wcss = []
for i in range(1, 11):
    kmeans = KMeans(n_clusters = i, init = 'k-means++', random_state = 42)
    kmeans.fit(X)
    # inertia method returns wcss for that model
    wcss.append(kmeans.inertia_)
```

```python
plt.figure(figsize=(10,5))
sns.lineplot(range(1, 11), wcss,marker='o',color='red')
plt.title('The Elbow Method')
plt.xlabel('Number of clusters')
plt.ylabel('WCSS')
plt.show()
```

Step by Step KMeans Explained in Detail



Step by Step KMeans Explained in Detail

```python
# Fitting K-Means to the dataset
kmeans = KMeans(n_clusters = 5, init = 'k-means++', random_state = 42)
y_kmeans = kmeans.fit_predict(X)
```

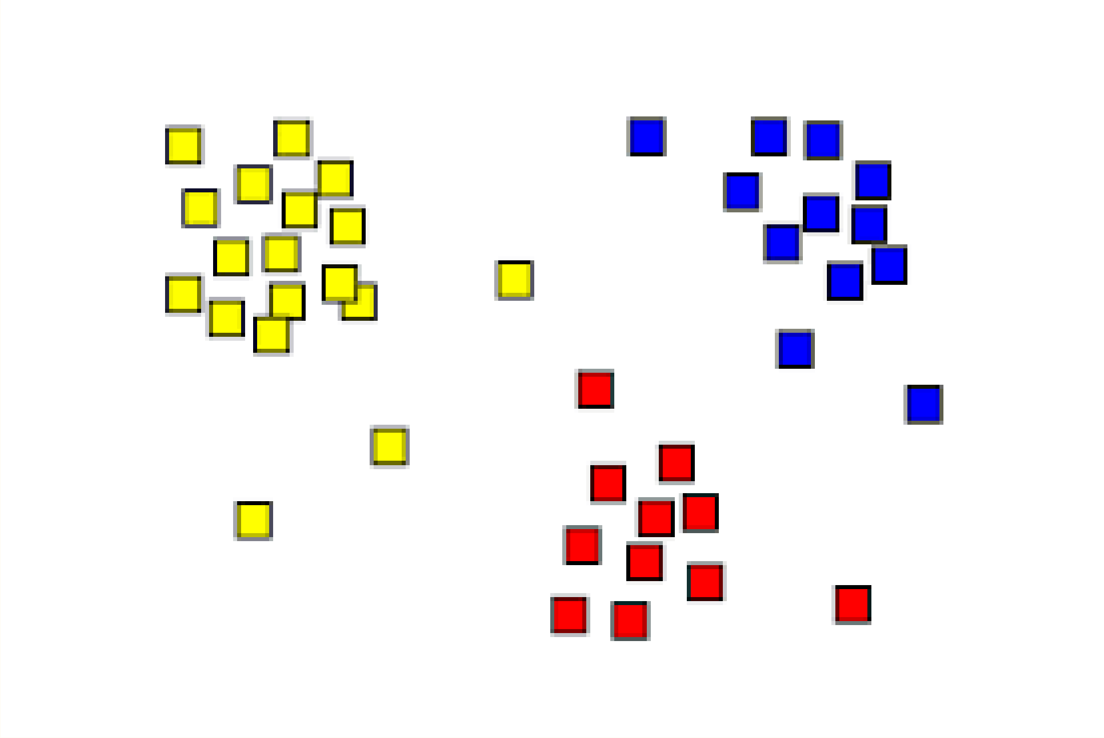
Step by Step KMeans Explained in Detail

```
# Visualising the clusters
plt.figure(figsize=(15,7))
sns.scatterplot(X[y_kmeans == 0, 0], X[y_kmeans == 0, 1], color = 'yellow', label = 'Cluster 1',s=50)
sns.scatterplot(X[y_kmeans == 1, 0], X[y_kmeans == 1, 1], color = 'blue', label = 'Cluster 2',s=50)
sns.scatterplot(X[y_kmeans == 2, 0], X[y_kmeans == 2, 1], color = 'green', label = 'Cluster 3',s=50)
sns.scatterplot(X[y_kmeans == 3, 0], X[y_kmeans == 3, 1], color = 'grey', label = 'Cluster 4',s=50)
sns.scatterplot(X[y_kmeans == 4, 0], X[y_kmeans == 4, 1], color = 'orange', label = 'Cluster 5',s=50)
sns.scatterplot(kmeans.cluster_centers_[:, 0], kmeans.cluster_centers_[:, 1], color = 'red',
                label = 'Centroids',s=300,marker=',')
plt.grid(False)
plt.title('Clusters of customers')
plt.xlabel('Annual Income (k$)')
plt.ylabel('Spending Score (1-100)')
plt.legend()
plt.show()
```

Step by Step KMeans Explained in Detail

Step by Step KMeans Explained in Detail

What Can We improve Further?



Each Data Point is assigned to just One Cluster ie Hard Assignment.

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Question : Is this the most optimum way to look at the problem?

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Soft Assignments?

References

- Google Developers - Clustering in Machine Learning
- KMeans++ - Sara Jensen
- Pattern Recognition and Machine Learning- Christopher Bishop
- Mlb - MLBook - How to Read a Model?

All icons used in the slides are fromflaticon.com