GLOW 2024

Fakultas Informatika
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# UNSUPERVISED LEARNING

## Clustering


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Adapted from Dr. Mahmud Dwi Sulistiyo Slides

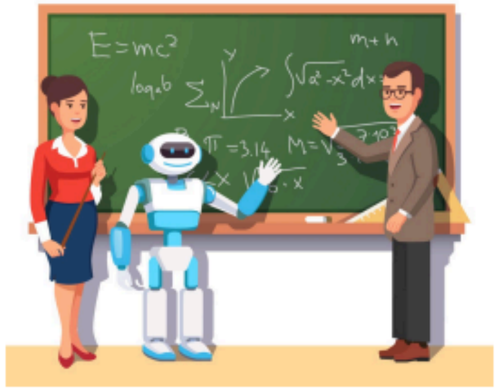
GLOW 2024

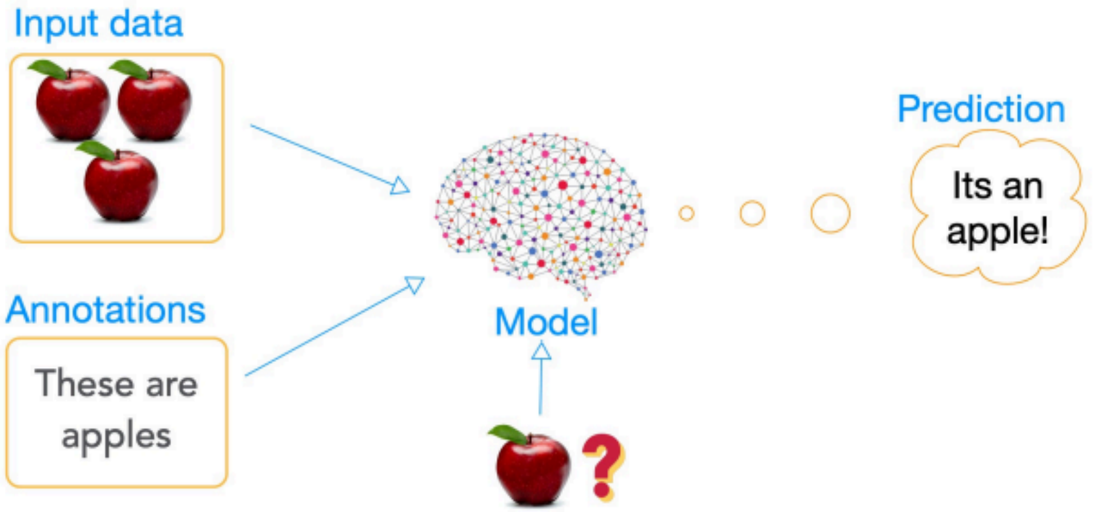
# Outline

- Supervised vs Unsupervised Learning
- Clustering Methods: K-Means & Hierarchical Clustering
- Evaluating Clustering Results
- Implementing Clustering Methods

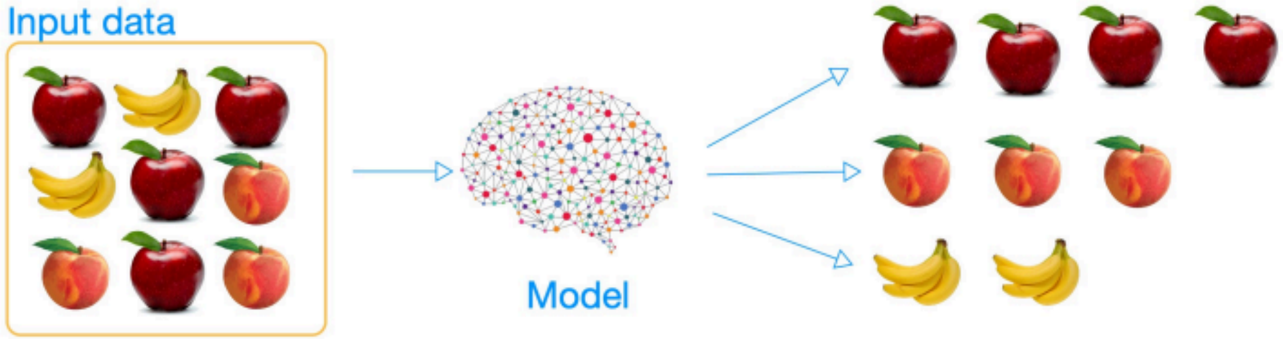
Adapted from Dr. Mahmud Dwi Sulistiyo Slides

**Supervised Learning**
(e.g. Regression, Classification)



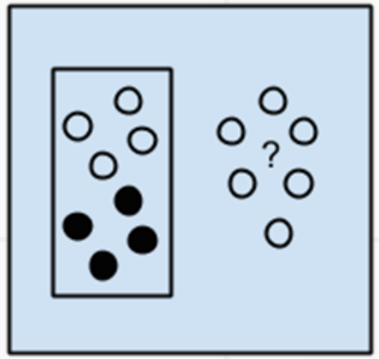



**Unsupervised Learning**
(e.g. Clustering)

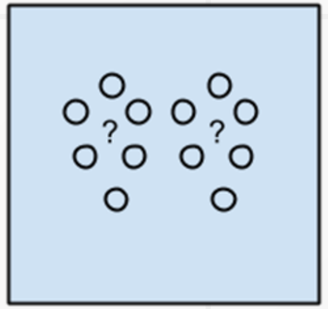


# Supervised VS Unsupervised Learning

- **Supervised**
  - You have labeled data
  - Find a function which can map data to its label
  - discover patterns that relate data attributes with a target (class)
- **Unsupervised**
  - You have unlabeled data
  - Discover the underlying structure of the data
  - Try to understand the data
  - Not predicting anything specific




Supervised Learning Algorithms



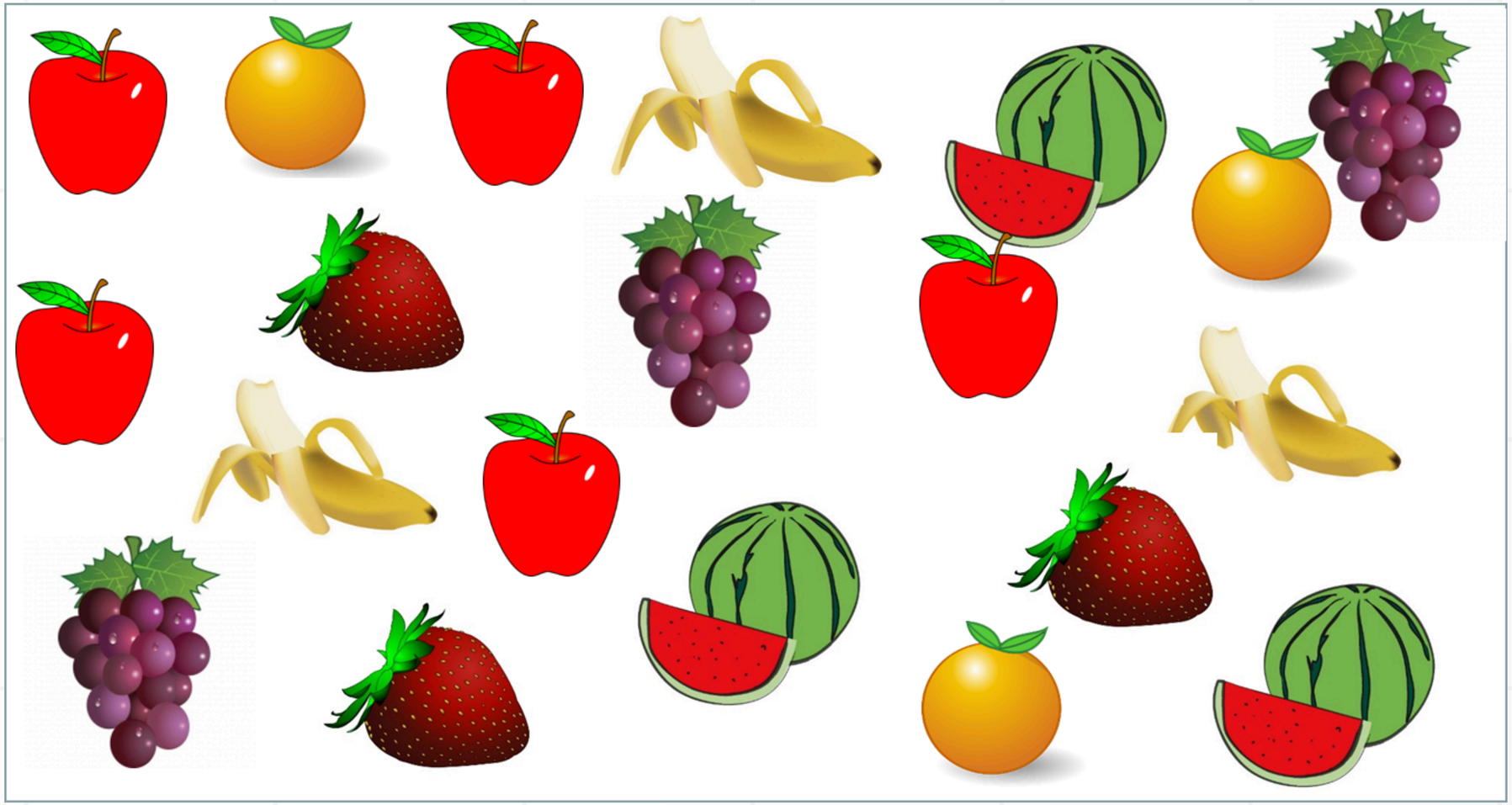

Unsupervised Learning Algorithms

# Clustering

- Grouping data into small groups based on **similarity** such that data in the **same group (cluster)** are as similar as possible and data in different groups are as different as possible.
- Help users **understand the natural grouping or structure in a data set**. Used either as a stand-alone tool to get insight into data distribution or as a preprocessing step for other algorithms.

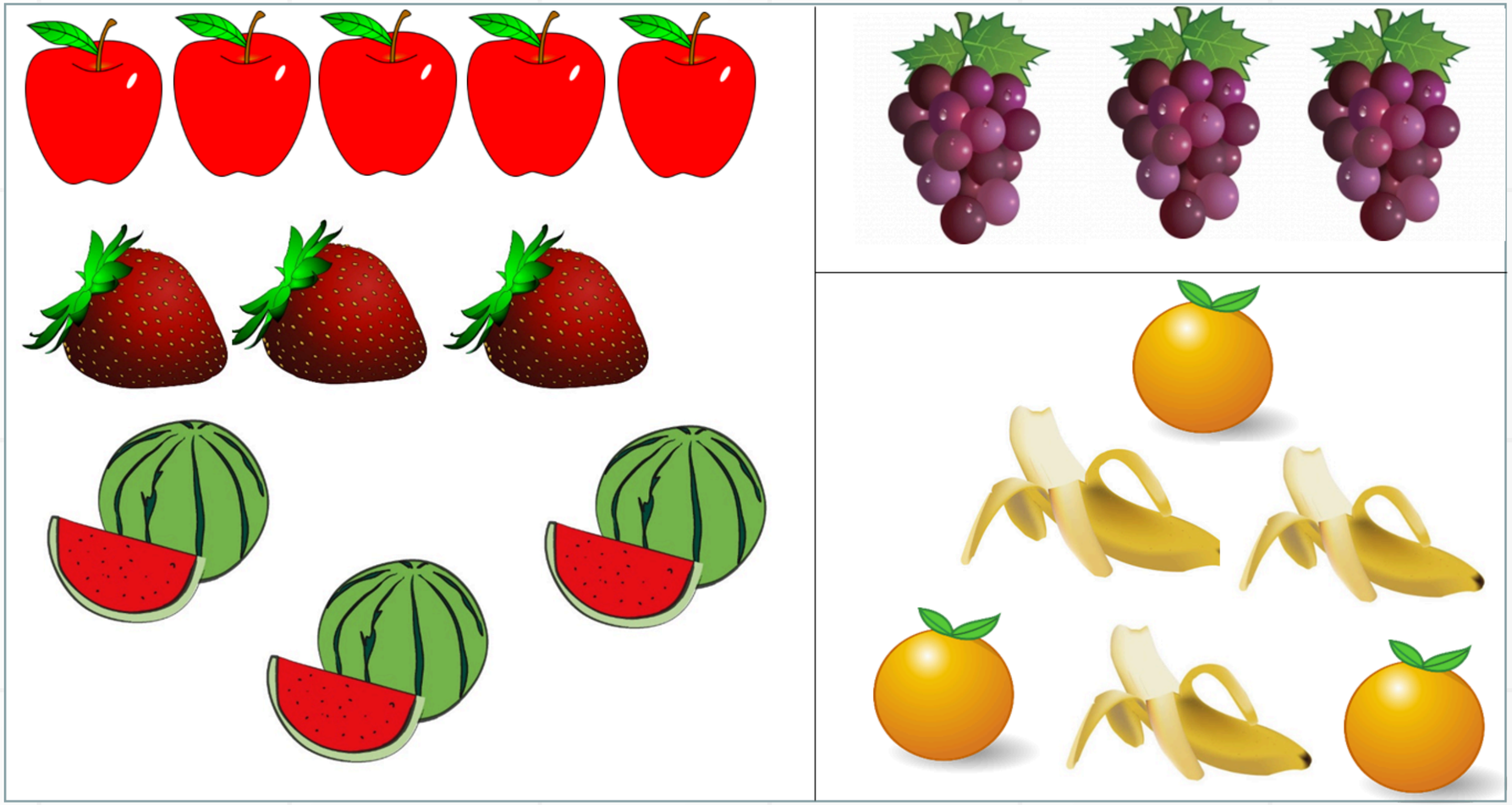
# Clustering

- Example: How do we want to group these fruits?



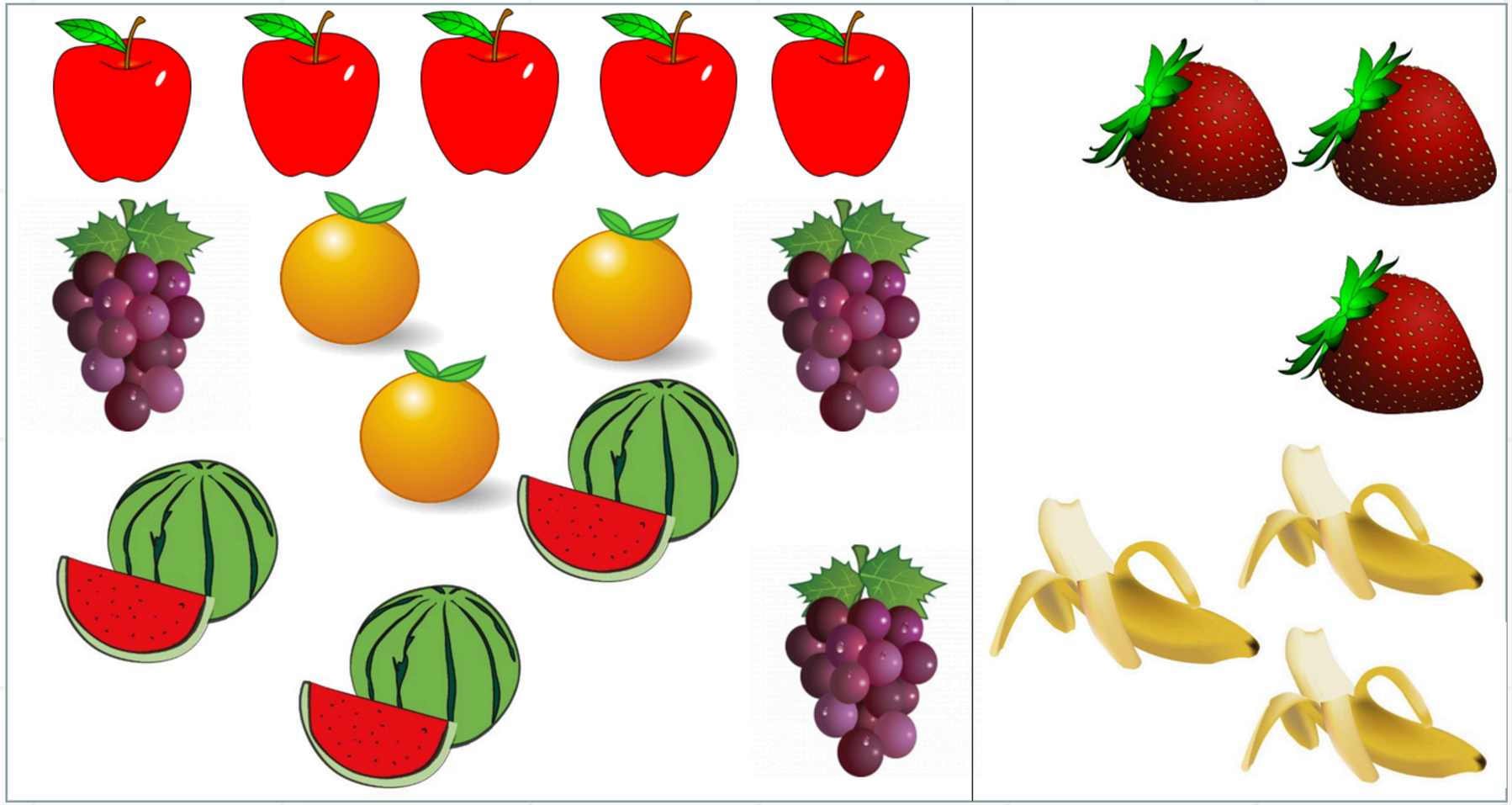
# Clustering

- a) Grouping based on colour



# Clustering

- a) Grouping based on shape



# Clustering

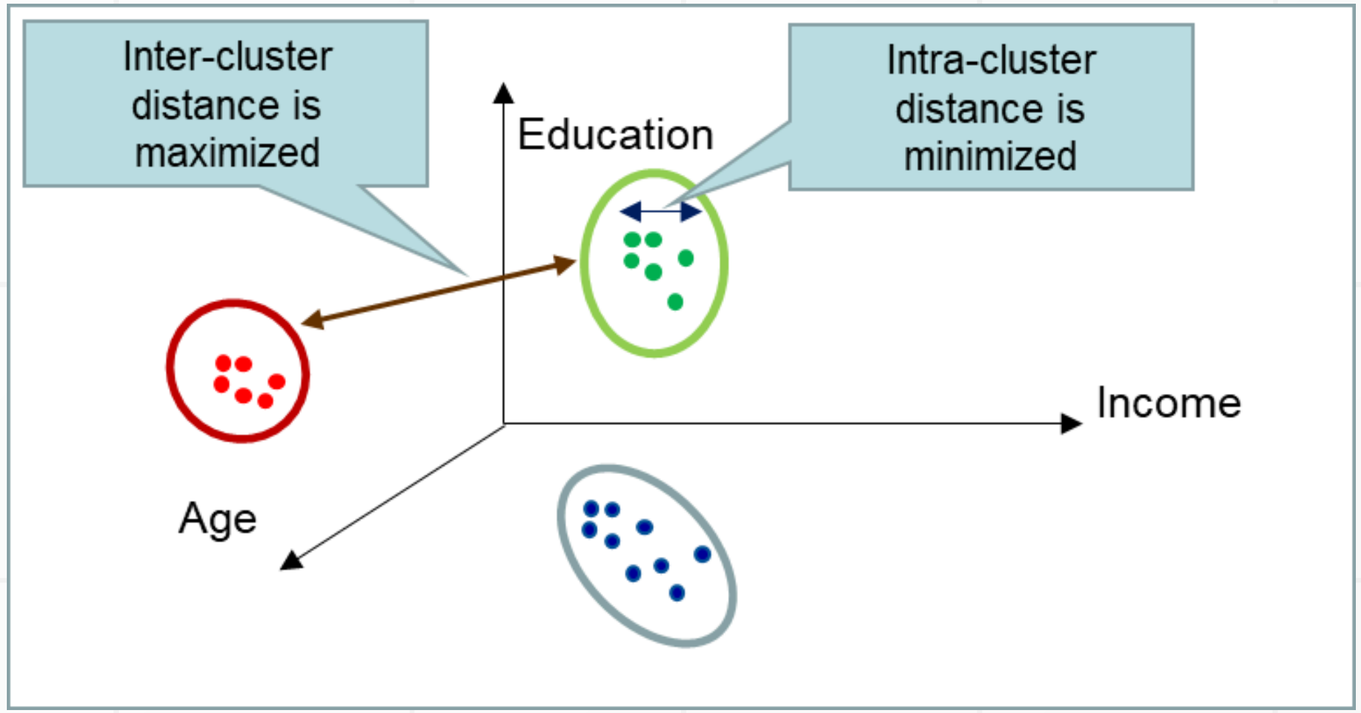
- Any other ways/approaches to group these fruits?
  - Based on size
  - Based on weight
  - Based on locality/origin

# Clustering

- Other examples:
  - Cluster customers based on their purchase histories, so that a targeted marketing program can be developed
  - Cluster products based on the sets of customers who purchased them
  - Cluster documents based on similar words
  - Cluster DNA sequences based on edit distance

# Clustering

- Good clustering method will produce high quality clusters with:
  - High intra-cluster similarity
  - Low inter-cluster similarity



# Clustering

- The quality of a clustering result depends on
  - the similarity measure used
  - implementation of the similarity measure
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

# Steps to Perform Clustering

**Step 1:**
**Formulate the problem – Decide on the clustering variable**

**Step 2:**
**Decide on the clustering procedure**

**Step 3:**
**Decide on the number of clusters**

**Step 4:**
**Validate and Interpret cluster solution**

# Steps to Perform Clustering

## Step 1:
## Formulate the problem – Decide on the clustering variable

- The objective of this step is:
  - To select variables that could provide a clear-cut **differentiation between segments/groups** regarding a specific managerial objective
- Types and examples of clustering variables:

| | General | Specific |
|---|---|---|
| **Observable (directly measurable)** | Cultural, geographic, demographic, socio-economic | User status, usage frequency, store and brand loyalty |
| **Unobservable (inferred)** | Psychographics, values, personality, lifestyle | Benefits, perceptions, attitudes, intentions, preferences |

# Steps to Perform Clustering

**Step 2:**
**Decide on the clustering procedure**

**Option 1:**
**Hierarchical methods**

**Option 2:**
**Partitioning methods**

# Steps to Perform Clustering

## 1. Hierarchical methods

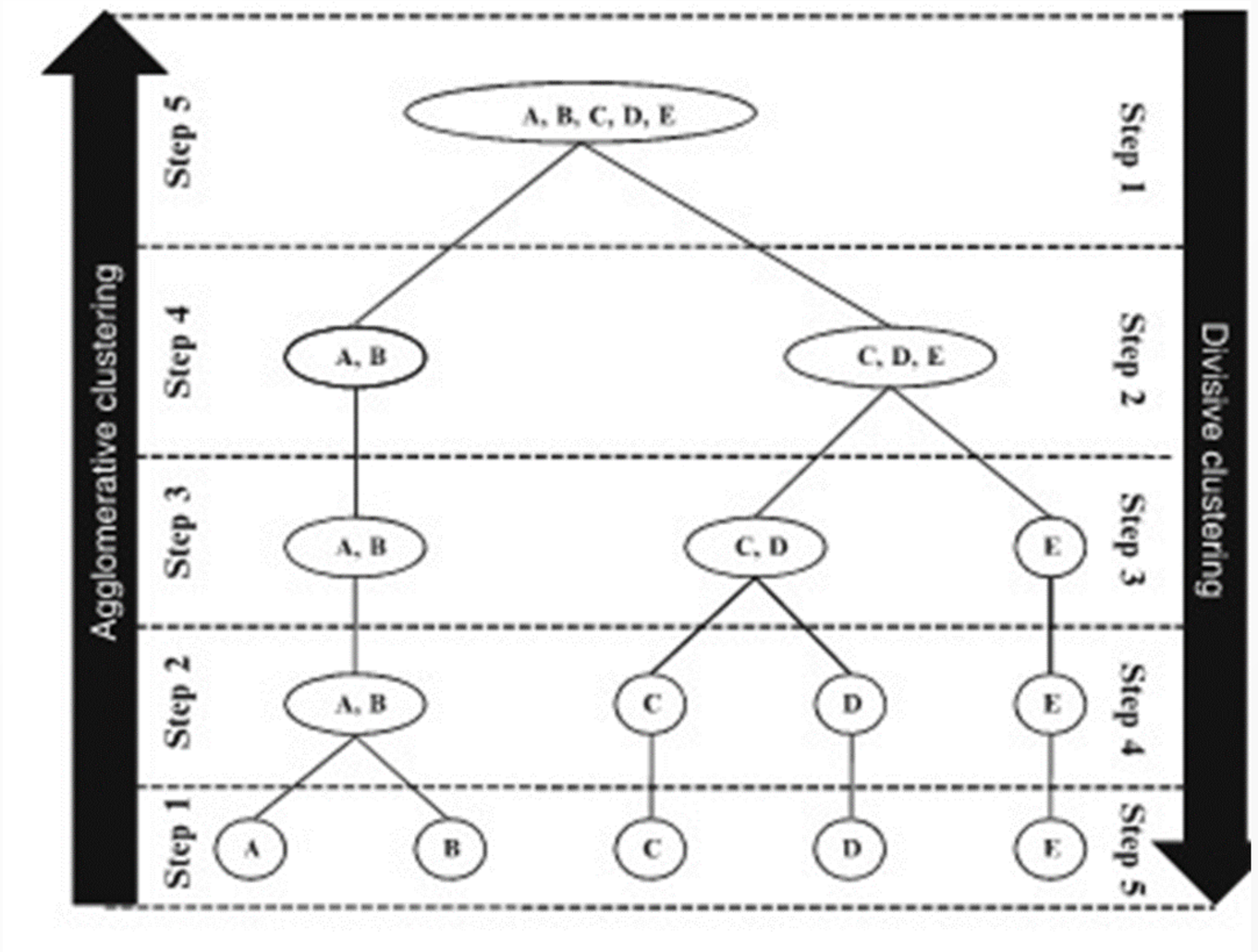
### Agglomerative

Each object starts with their own separate cluster. Then, two ‘closest’ (most similar) cluster is combined and repeatedly performed until all objects become in one cluster

### Divisive

All objects start in the same cluster, and gradually split up until each object becomes in individual cluster

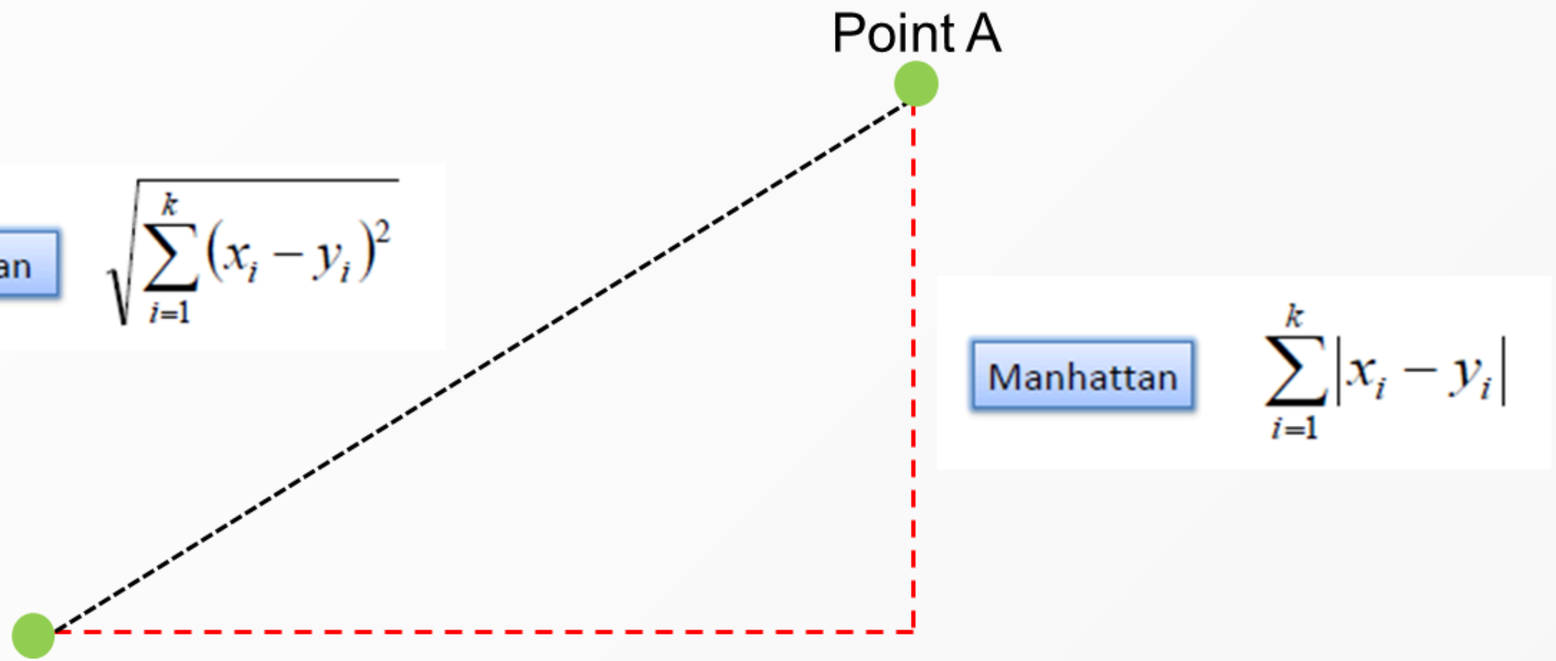
# Steps to Perform Clustering



# Steps to Perform Clustering

- Steps in **hierarchical methods**:

1. Measure of similarity/dissimilarity
    - Euclidean distance
    - Manhattan distance

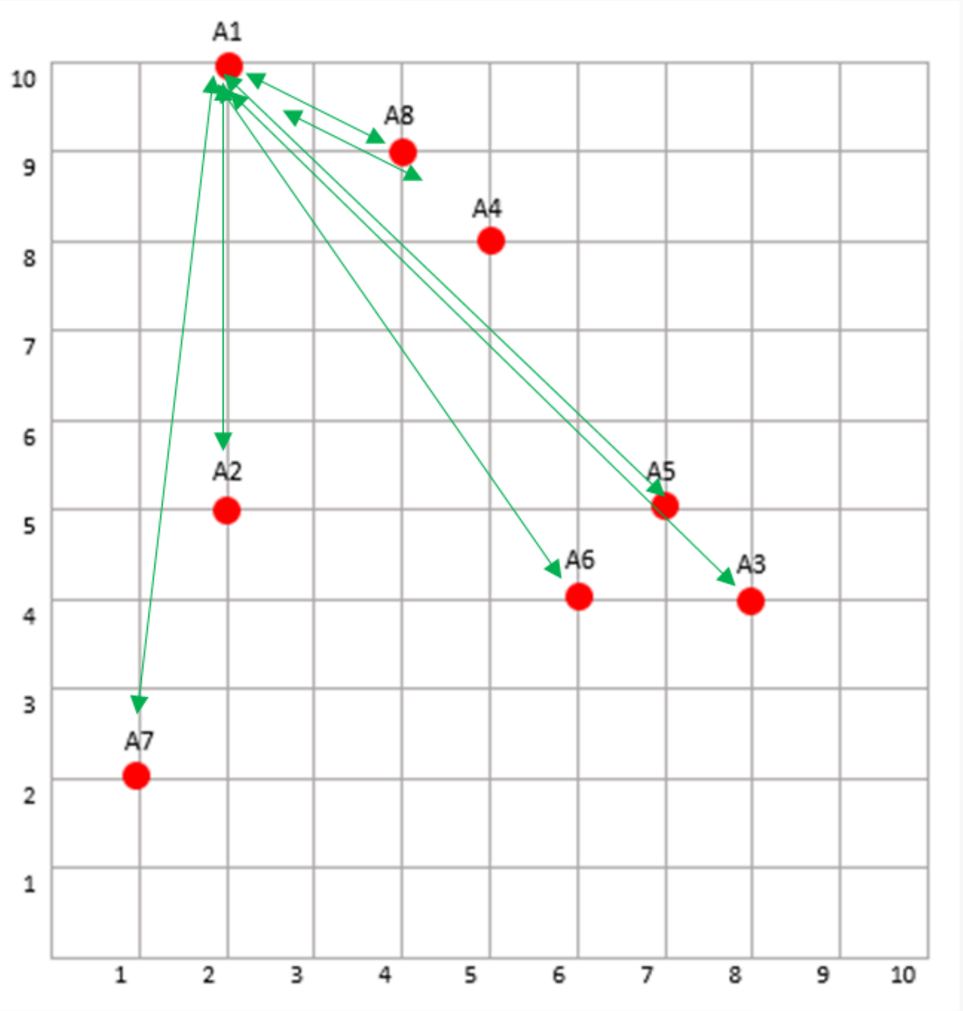


# Steps to Perform Clustering

- Let's do some exercises:

Calculate the Euclidean distance for the following data sets:

A1 = (2,10)
A2 = (2,5)
A3 = (8,4)
A4 = (5,8)
A5 = (7,5)
A6 = (6,4)
A7 = (1,2)
A8 = (4,9)



# Steps to Perform Clustering

- Euclidean distance matrix

| | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 3.6 | 7.1 | 7.2 | 8.1 | 2.2 |
| A2 | | 0 | 6.1 | 4.2 | 5 | 4.1 | 3.1 | 4.5 |
| A3 | | | 0 | 5 | 1.4 | 1.4 | 7.2 | 6.4 |
| A4 | | | | 0 | 3.6 | 4.1 | 7.2 | 1.4 |
| A5 | | | | | 0 | 1.4 | 6.7 | 5 |
| A6 | | | | | | 0 | 5.4 | 5.4 |
| A7 | | | | | | | 0 | 7.6 |
| A8 | | | | | | | | 0 |

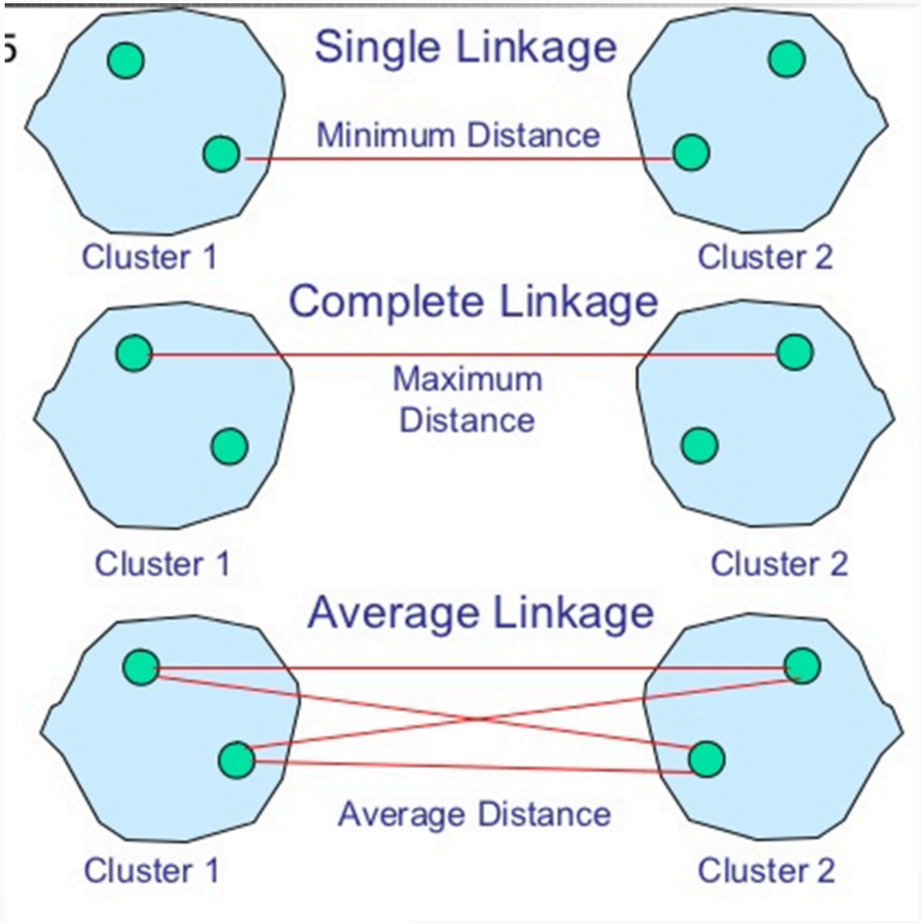
# Steps to Perform Clustering

2. Choose clustering algorithm

- **Single linkage**
  - The distance between two objects is defined to be the smallest distance possible between them.
  - If both objects are clusters, the distance between the two closest members are used.
- **Complete linkage**
  - This method is much like the single linkage, but instead of using the minimum of the distances, we use the maximum distance
- **Average linkage**
  - The distance between two clusters is defined as the average distance between all pairs of the two clusters' members

# Steps to Perform Clustering

## 2. Choose clustering algorithm



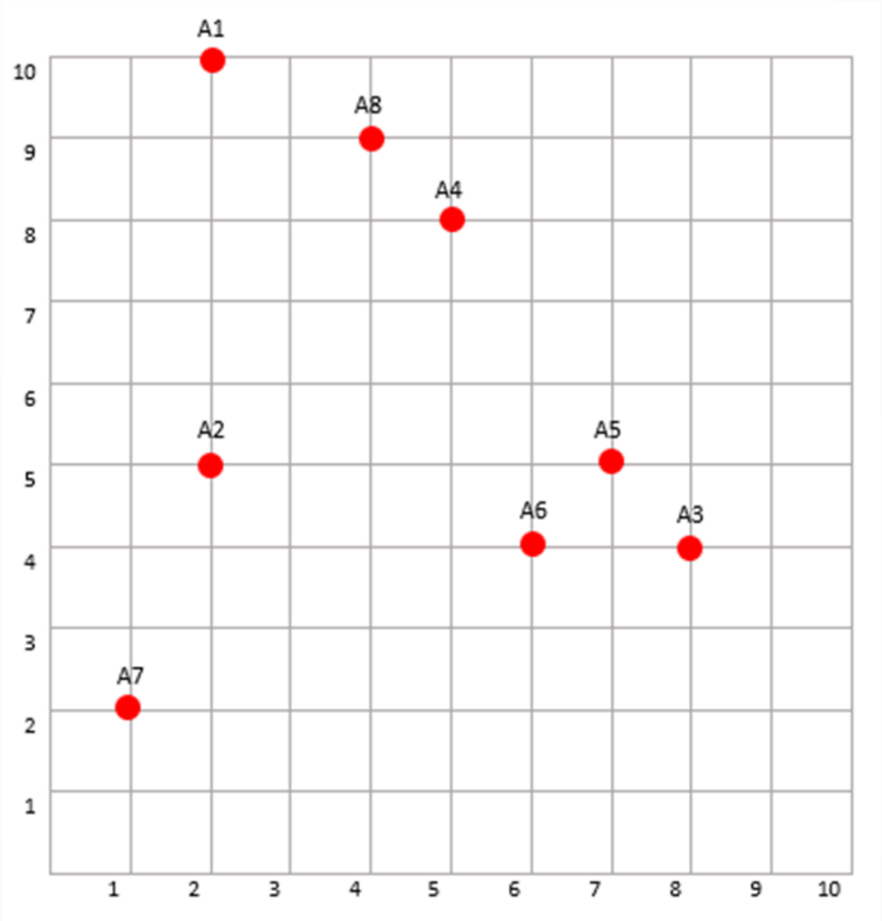
# Steps to Perform Clustering

2. Perform hierarchical clustering using single link algorithms for the sample datasets

| | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 3.6 | 7.1 | 7.2 | 8.1 | 2.2 |
| A2 | | 0 | 6.1 | 4.2 | 5 | 4.1 | 3.1 | 4.5 |
| A3 | | | 0 | 5 | 1.4 | 1.4 | 7.2 | 6.4 |
| A4 | | | | 0 | 3.6 | 4.1 | 7.2 | 1.4 |
| A5 | | | | | 0 | 1.4 | 6.7 | 5 |
| A6 | | | | | | 0 | 5.4 | 5.4 |
| A7 | | | | | | | 0 | 7.6 |
| A8 | | | | | | | | 0 |

# Steps to Perform Clustering

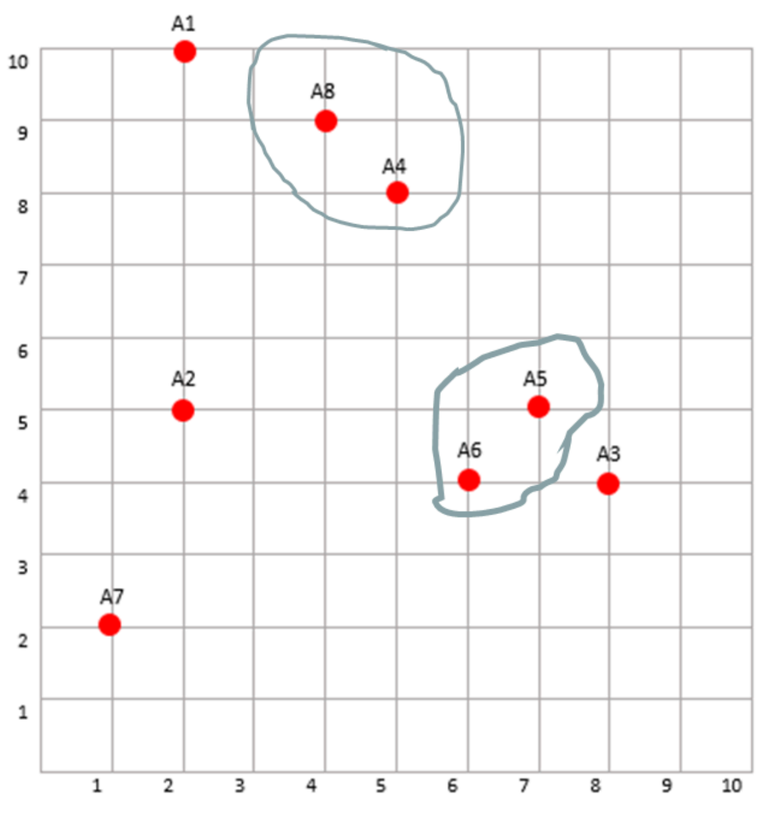
## Initial state – 8 clusters



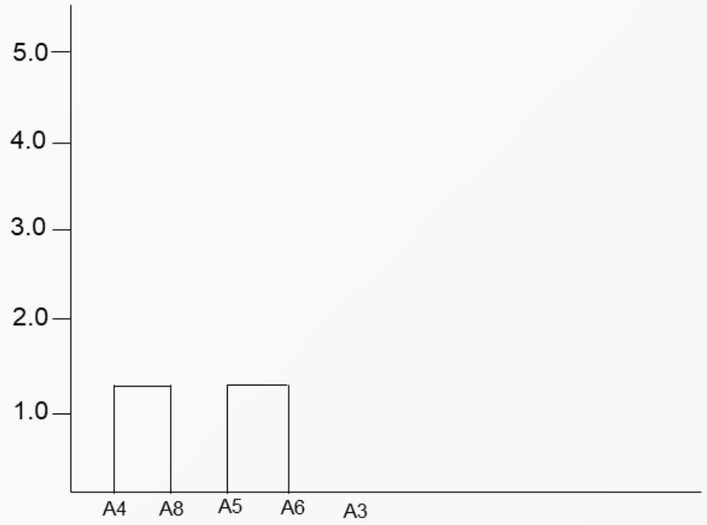

| | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 3.6 | 7.1 | 7.2 | 8.1 | 2.2 |
| A2 | | 0 | 6.1 | 4.2 | 5 | 4.1 | 3.1 | 4.5 |
| A3 | | | 0 | 5 | 1.4 | 1.4 | 7.2 | 6.4 |
| A4 | | | | 0 | 3.6 | 4.1 | 7.2 | 1.4 |
| A5 | | | | | 0 | 1.4 | 6.7 | 5 |
| A6 | | | | | | 0 | 5.4 | 5.4 |
| A7 | | | | | | | 0 | 7.6 |
| A8 | | | | | | | | 0 |

# Steps to Perform Clustering

## 1st clustering cycle



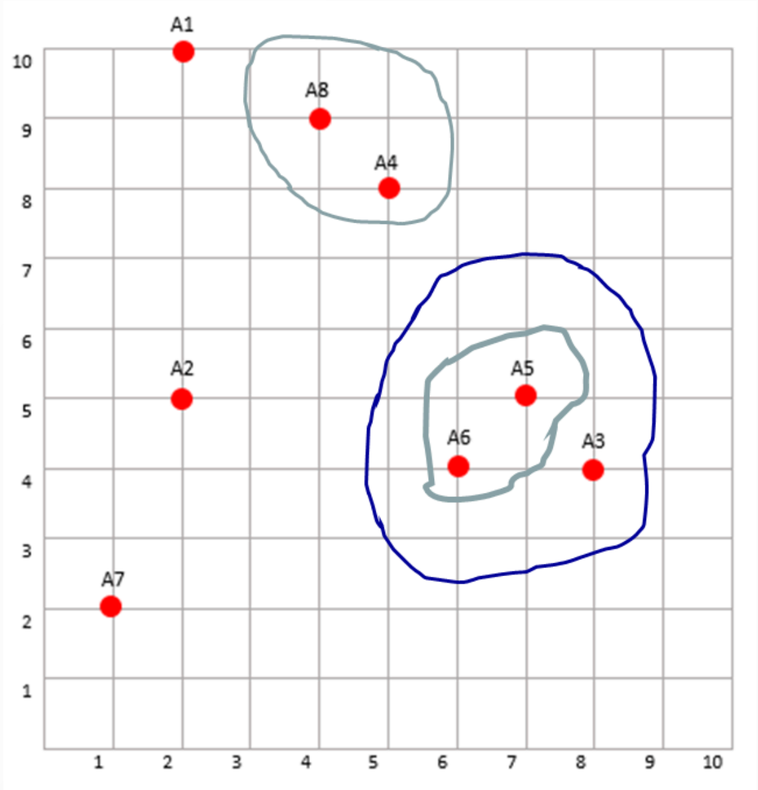

| | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 3.6 | 7.1 | 7.2 | 8.1 | 2.2 |
| A2 | | 0 | 6.1 | 4.2 | 5 | 4.1 | 3.1 | 4.5 |
| A3 | | | 0 | 5 | 1.4 | 1.4 | 7.2 | 6.4 |
| A4 | | | | 0 | 3.6 | 4.1 | 7.2 | 1.4 |
| A5 | | | | | 0 | 1.4 | 6.7 | 5 |
| A6 | | | | | | 0 | 5.4 | 5.4 |
| A7 | | | | | | | 0 | 7.6 |
| A8 | | | | | | | | 0 |

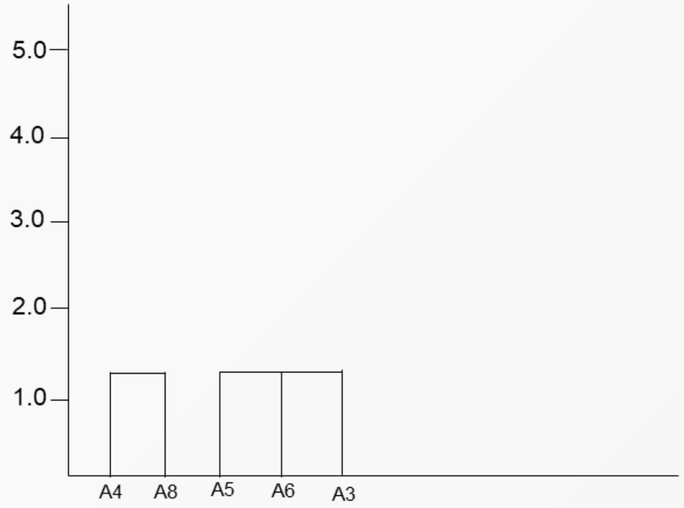


# Steps to Perform Clustering

## 2nd clustering cycle

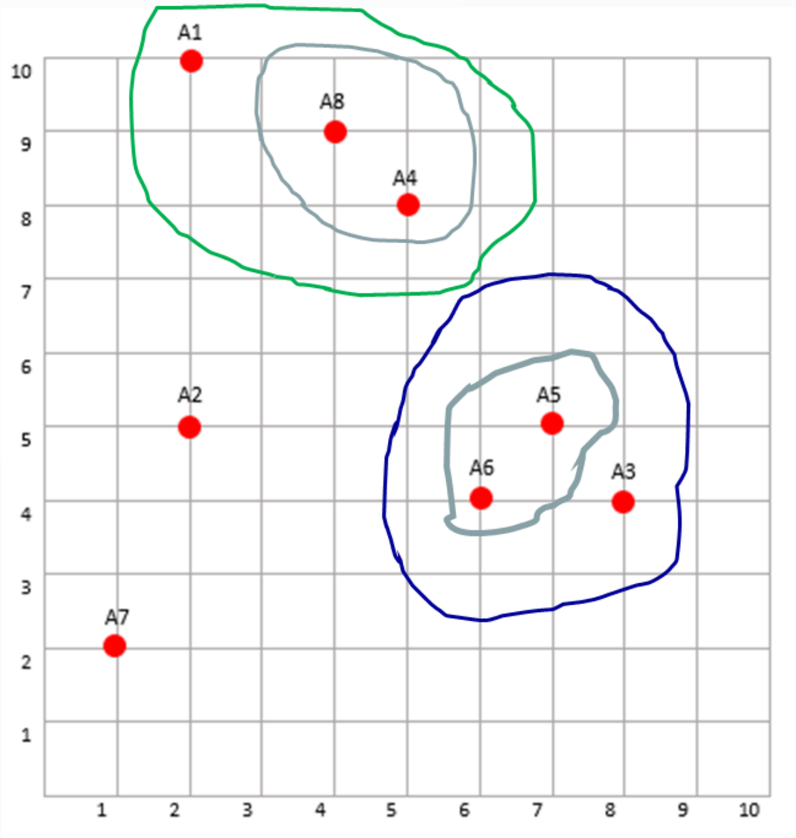
| | A1 | A2 | A3 | A4, A8 | A5, A6 | A7 |
|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 2.2 | 7.1 | 8.1 |
| A2 | | 0 | 5 | 4.2 | 4.1 | 3.1 |
| A3 | | | 0 | 5 | 1.4 | 7.2 |
| A4, A8 | | | | 0 | 3.6 | 7.2 |
| A5, A6 | | | | | 0 | 5.4 |
| A7 | | | | | | 0 |



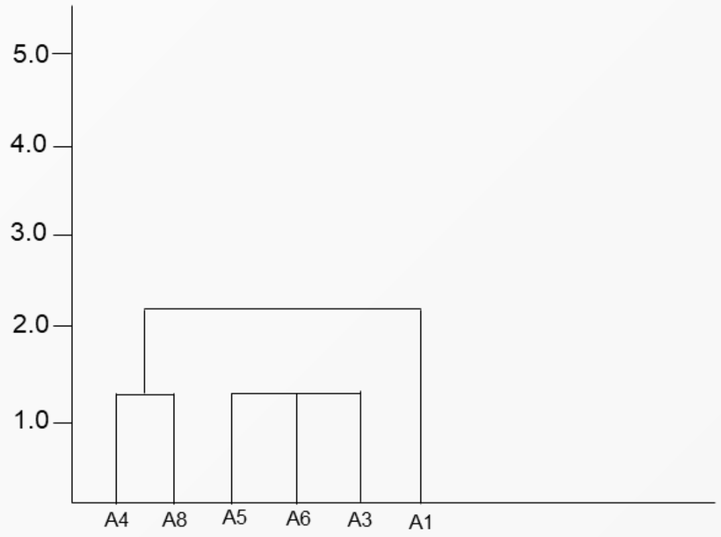



# Steps to Perform Clustering

## 3rd clustering cycle



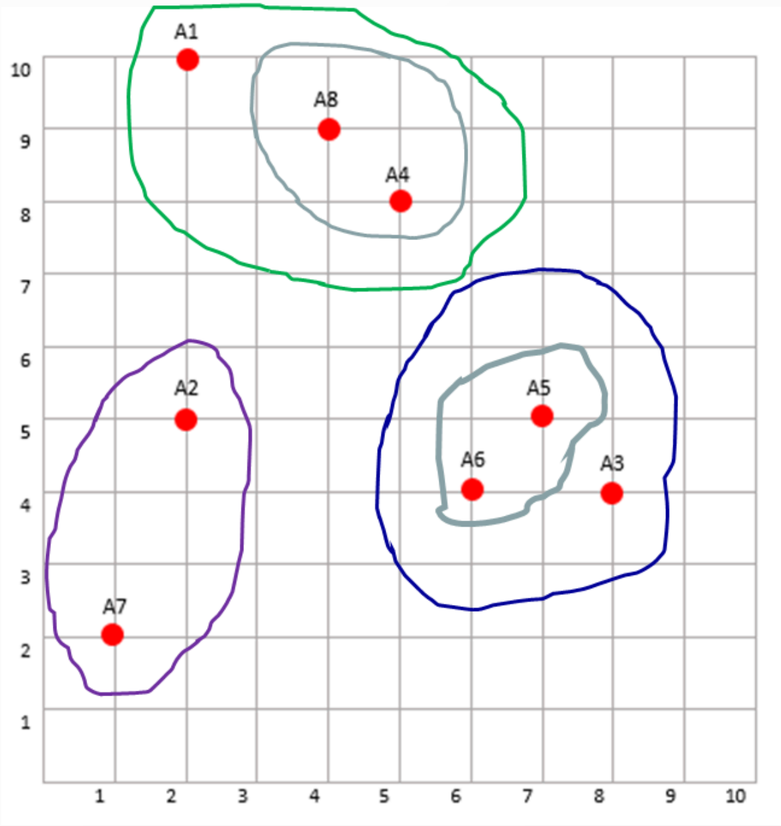

| | A1 | A2 | A4, A8 | A3, A5, A6 | A7 |
|---|---|---|---|---|---|
| A1 | 0 | 5 | 2.2 | 6 | 8.1 |
| A2 | | 0 | 4.2 | 4.1 | 3.1 |
| A4, A8 | | | 0 | 3.6 | 7.2 |
| A3, A5, A6 | | | | 0 | 5.4 |
| A7 | | | | | 0 |

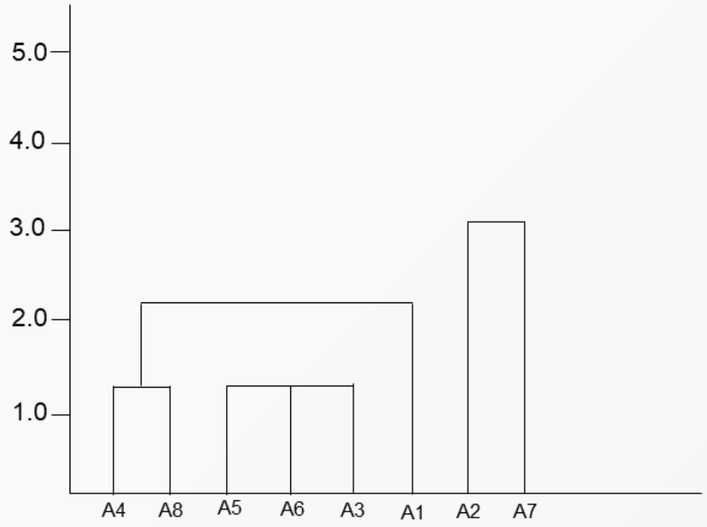


# Steps to Perform Clustering

## 4th clustering cycle

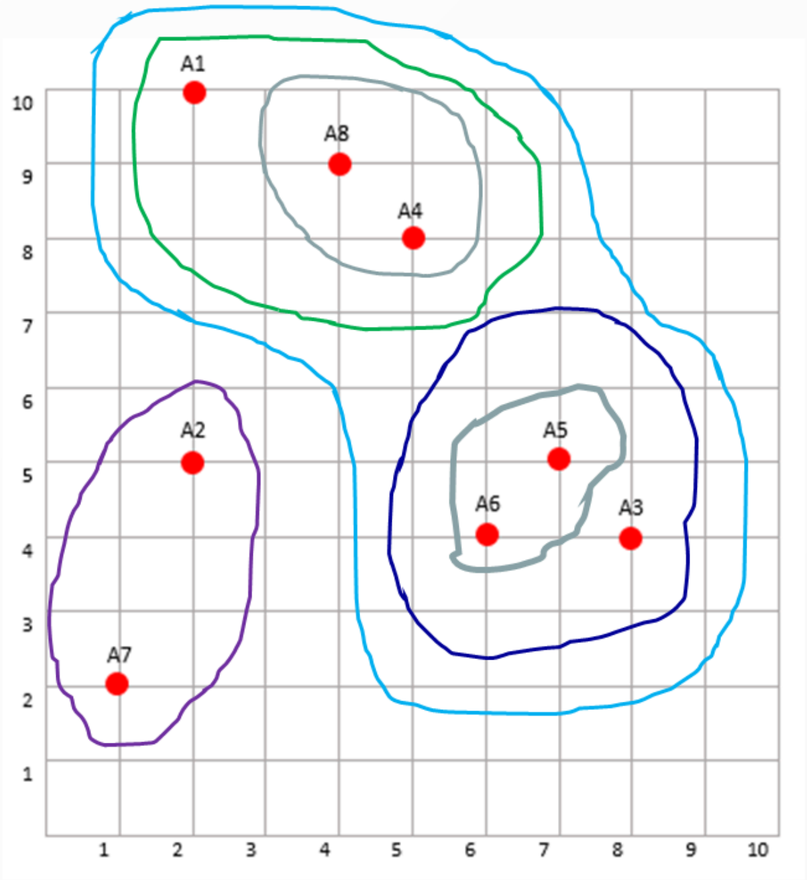
| | A2 | A1, A4, A8 | A3, A5, A6 | A7 |
|---|---|---|---|---|
| A2 | 0 | 4.2 | 4.1 | 3.1 |
| A1, A4, A8 | | 0 | 3.6 | 7.2 |
| A3, A5, A6 | | | 0 | 5.4 |
| A7 | | | | 0 |



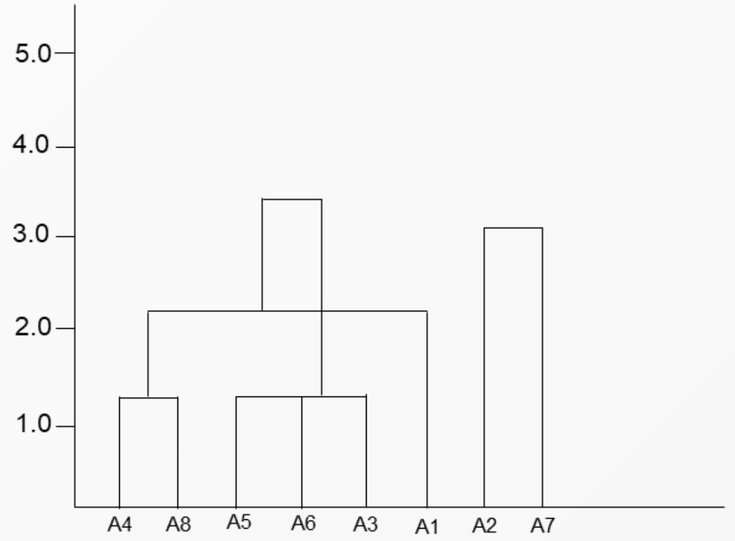



# Steps to Perform Clustering

## 5th clustering cycle

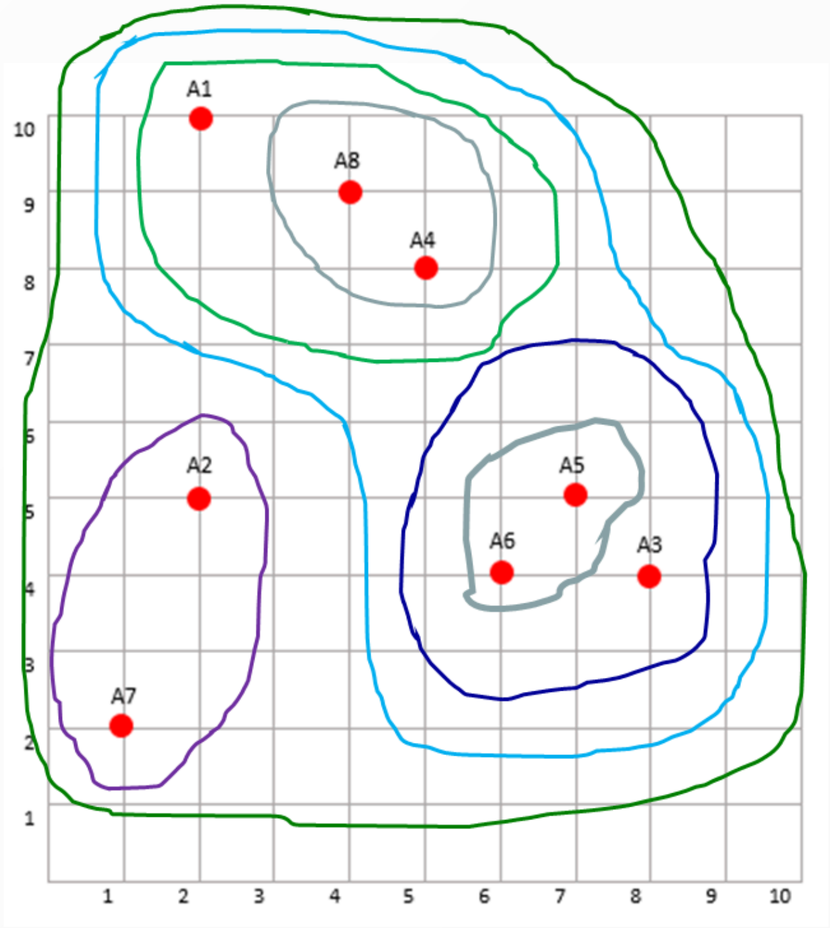



| | A2, A7 | A1, A4, A8 | A3, A5, A6 |
|---|---|---|---|
| A2, A7 | 0 | 4.2 | 4.1 |
| A1, A4, A8 | | 0 | 3.6 |
| A3, A5, A6 | | | 0 |

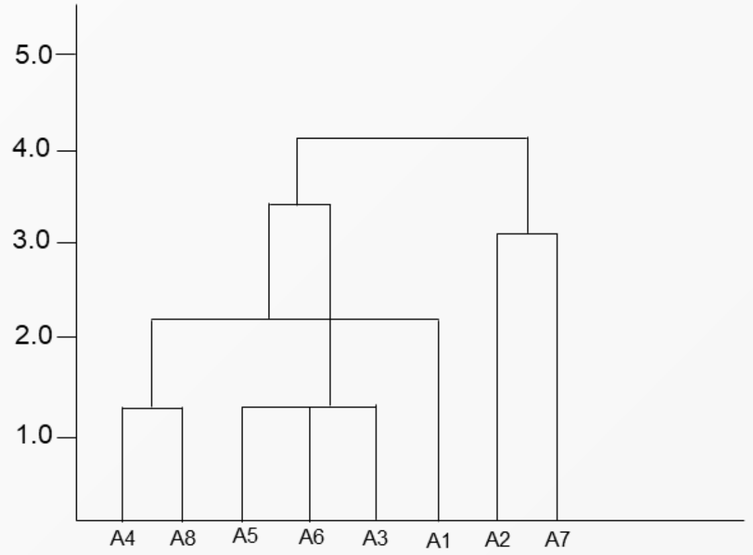


# Steps to Perform Clustering

## 6th clustering cycle

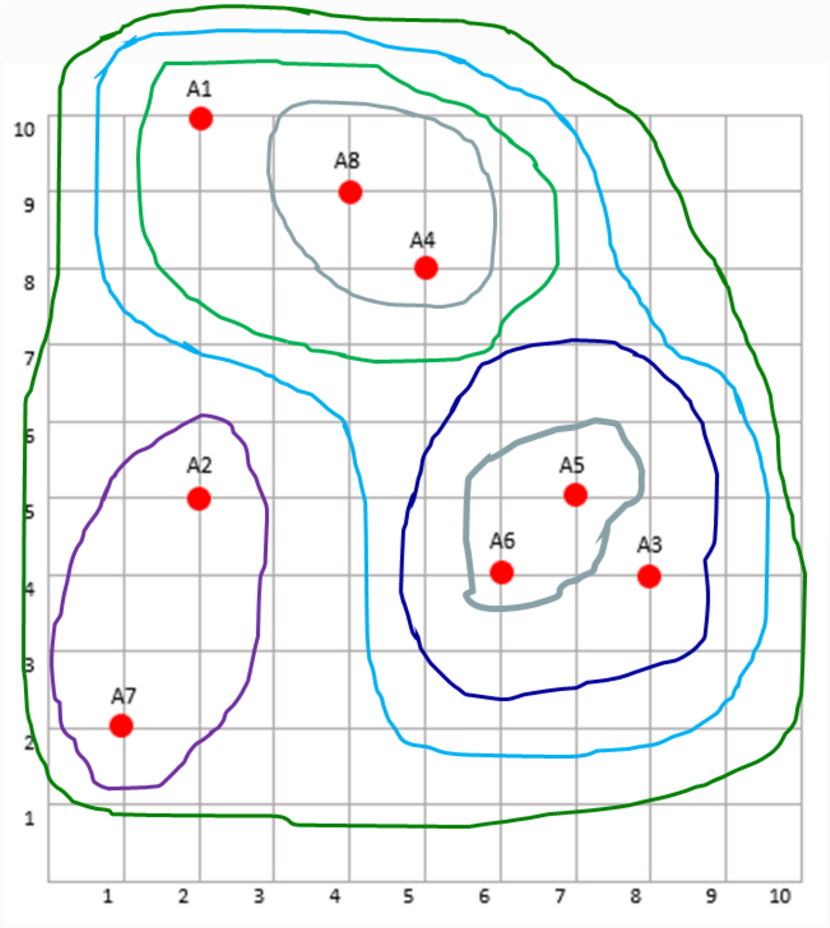



| | A2, A7 | A1, A4, A8, A3, A5, A6 |
|---|---|---|
| A2, A7 | 0 | 4.1 |
| A1, A4, A8, A3, A5, A6 | | 0 |

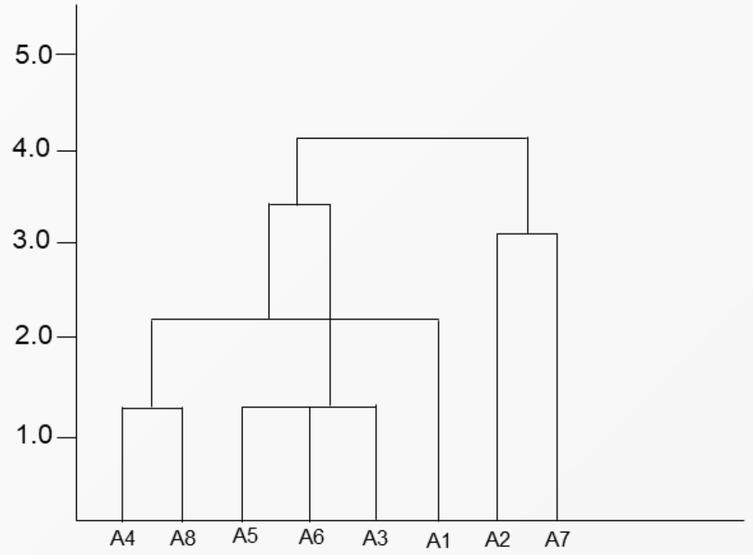


# Steps to Perform Clustering

## 6th clustering cycle




| | A2, A7 | A1, A4, A8, A3, A5, A6 |
|---|---|---|
| A2, A7 | 0 | 4.1 |
| A1, A4, A8, A3, A5, A6 | | 0 |



# Steps to Perform Clustering

## 2. Partitioning methods

- The most common one is k-means
- However, for partitioning methods, we need to determine our initial cluster.
- We will get back to k-means later

# Steps to Perform Clustering

**Step 3:**
**Decide on the number of clusters**

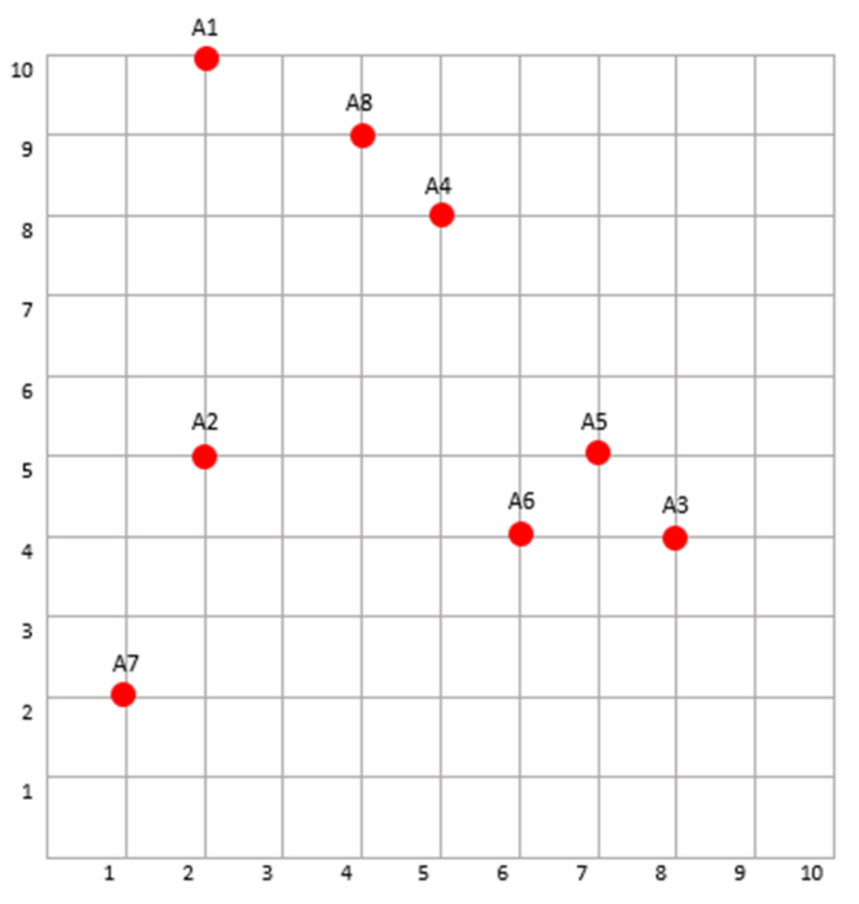
- The main objective is:
- To achieve **maximum inter-variance** and **minimum intra-variance**
- One of the method to determine number of clusters is by using **elbow plot**

# Steps to Perform Clustering

- Steps to perform k-means cluster analysis:
  - Choose the number of cluster, k
  - Generate k random points as cluster centroids
  - Assign each point to the nearest cluster centroid
  - Recompute the new cluster centroid
  - Repeat the two previous steps until the convergence criterion is met

# Steps to Perform Clustering

- Let's say we use the same data set:




| | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 |
|---|---|---|---|---|---|---|---|---|
| A1 | 0 | 5 | 6 | 3.6 | 7.1 | 7.2 | 8.1 | 2.2 |
| A2 | | 0 | 6.1 | 4.2 | 5 | 4.1 | 3.1 | 4.5 |
| A3 | | | 0 | 5 | 1.4 | 1.4 | 7.2 | 6.4 |
| A4 | | | | 0 | 3.6 | 4.1 | 7.2 | 1.4 |
| A5 | | | | | 0 | 1.4 | 6.7 | 5 |
| A6 | | | | | | 0 | 5.4 | 5.4 |
| A7 | | | | | | | 0 | 7.6 |
| A8 | | | | | | | | 0 |

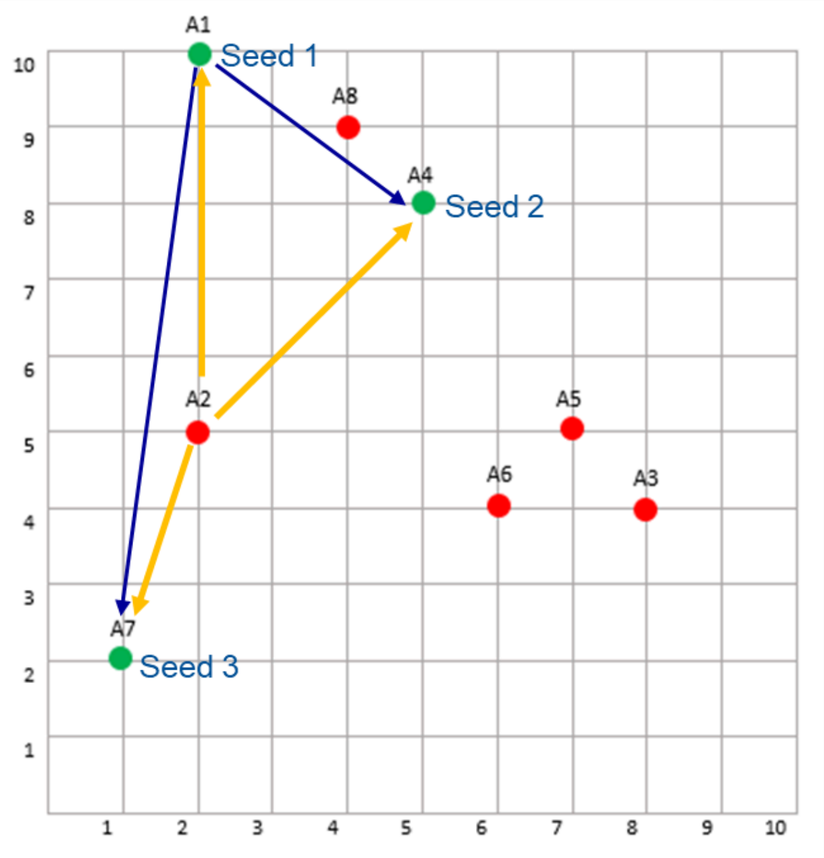
# Steps to Perform Clustering

- Steps to perform k-means cluster analysis:

1. Choose the number of cluster, k
    - Let’s say we start with k=3
2. Generate k random points as cluster centroids
    - And we choose the following points as the cluster centroids
    - A1, A4, A7

# Steps to Perform Clustering

- Then, we need to calculate the distance for each point to each centroid (seed)




| Distance from A1 to: | |
|---|---|
| Seed 1 | 0 |
| Seed 2 | 3.6 |
| Seed 3 | 8.1 |

| Distance from A2 to: | |
|---|---|
| Seed 1 | 5 |
| Seed 2 | 4.2 |
| Seed 3 | 3.1 |

| Distance from A3 to: | |
|---|---|
| Seed 1 | 6 |
| Seed 2 | 5 |
| Seed 3 | 7.2 |

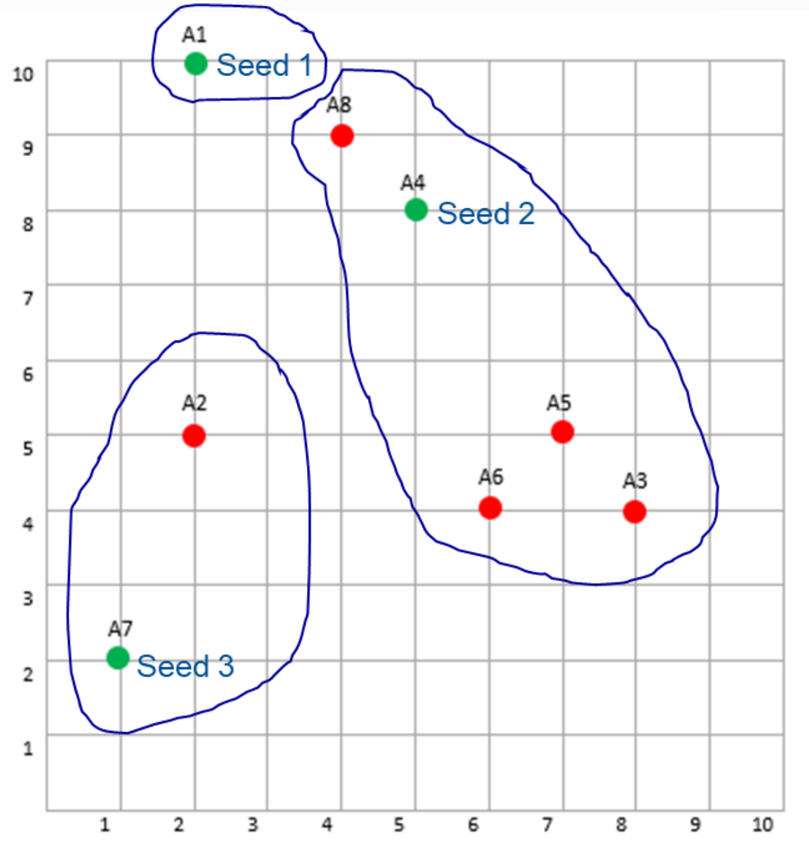
| Distance from A4 to: | |
|---|---|
| Seed 1 | 3.6 |
| Seed 2 | 0 |
| Seed 3 | 7.2 |

| Distance from A5 to: | |
|---|---|
| Seed 1 | 7.1 |
| Seed 2 | 3.6 |
| Seed 3 | 6.7 |

| Distance from A6 to: | |
|---|---|
| Seed 1 | 7.2 |
| Seed 2 | 4.1 |
| Seed 3 | 5.4 |

# Steps to Perform Clustering

- Assign each point to the nearest cluster centroid




| Distance from A1 to: | |
|---|---|
| Seed 1 | 0 |
| Seed 2 | 3.6 |
| Seed 3 | 8.1 |

| Distance from A2 to: | |
|---|---|
| Seed 1 | 5 |
| Seed 2 | 4.2 |
| Seed 3 | 3.1 |

| Distance from A3 to: | |
|---|---|
| Seed 1 | 6 |
| Seed 2 | 5 |
| Seed 3 | 7.2 |

| Distance from A4 to: | |
|---|---|
| Seed 1 | 3.6 |
| Seed 2 | 0 |
| Seed 3 | 7.2 |

| Distance from A5 to: | |
|---|---|
| Seed 1 | 7.1 |
| Seed 2 | 3.6 |
| Seed 3 | 6.7 |

| Distance from A6 to: | |
|---|---|
| Seed 1 | 7.2 |
| Seed 2 | 4.1 |
| Seed 3 | 5.4 |

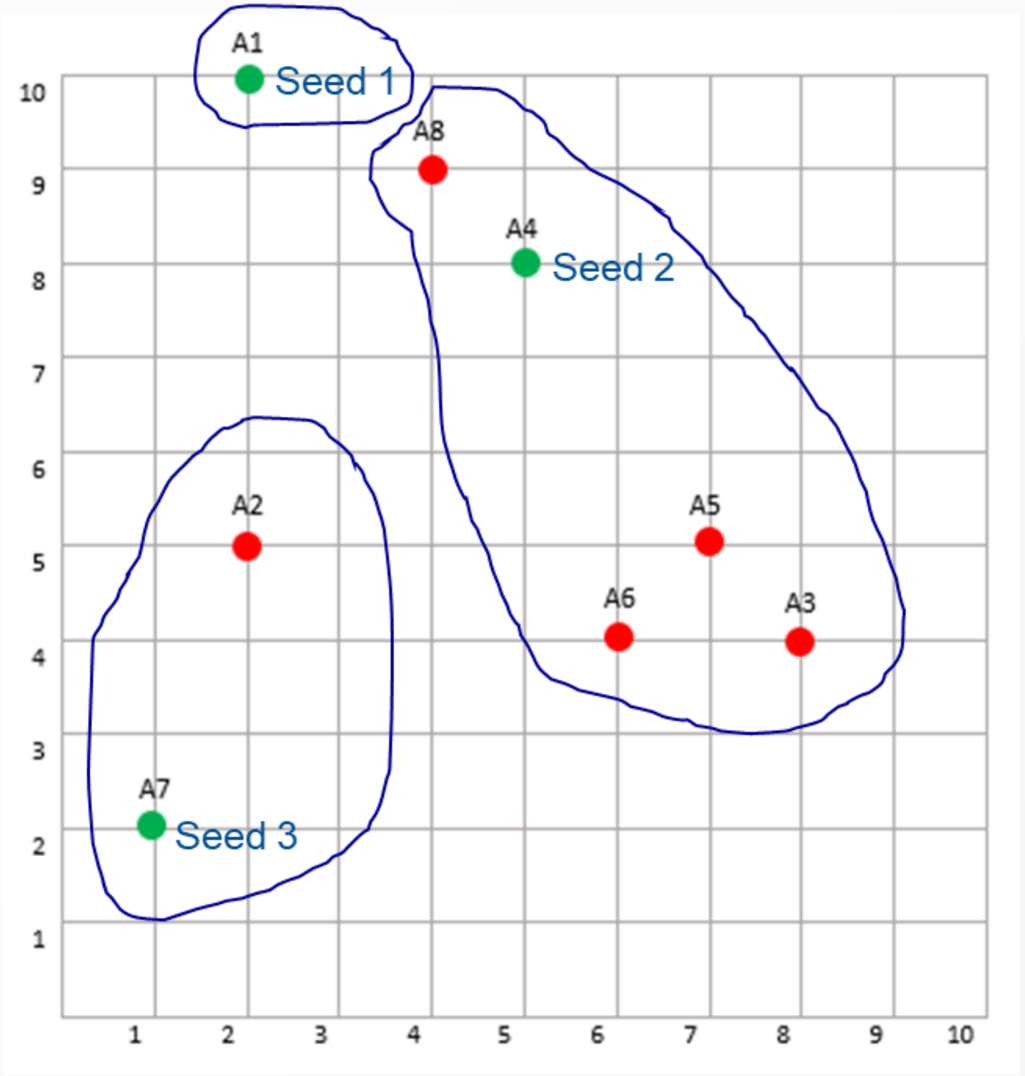
| Distance from A7 to: | |
|---|---|
| Seed 1 | 8.1 |
| Seed 2 | 7.2 |
| Seed 3 | 0 |

| Distance from A8 to: | |
|---|---|
| Seed 1 | 2.2 |
| Seed 2 | 1.4 |
| Seed 3 | 7.6 |

# Steps to Perform Clustering

- Recompute the new cluster centroid

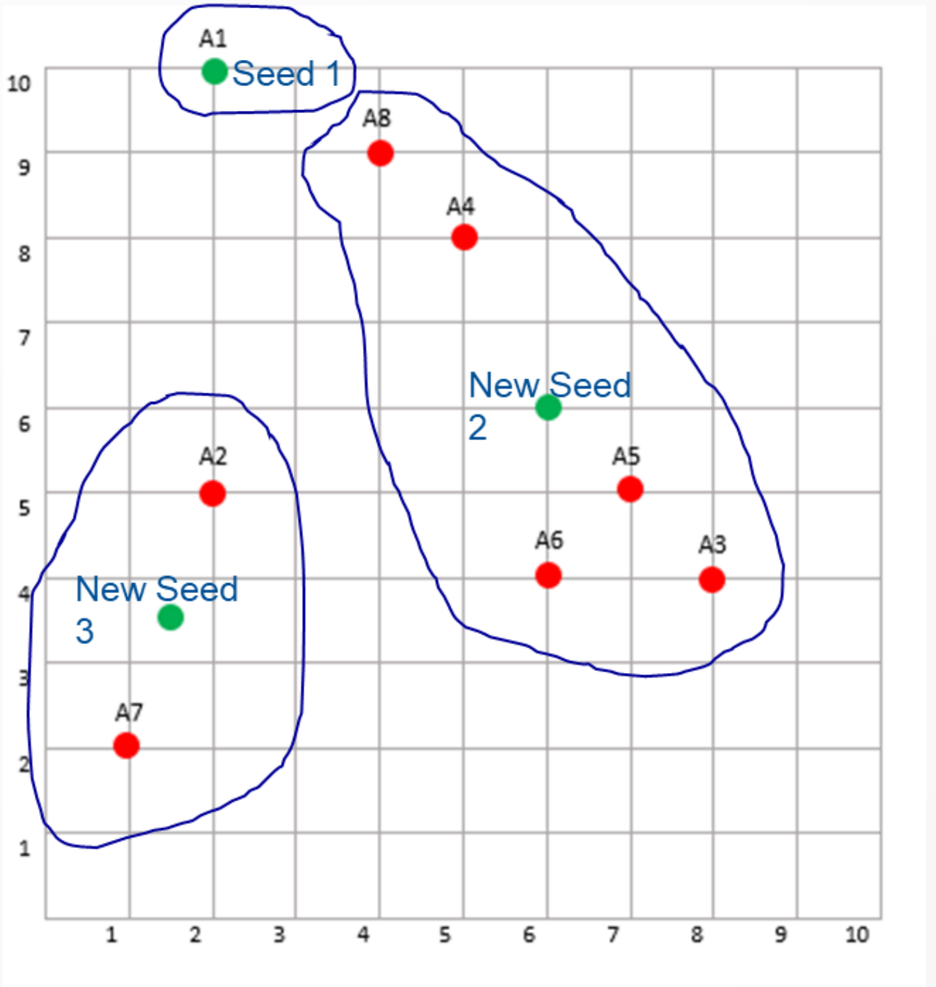
**Seed 1 = (2,10)**
**Seed 2** = (8+5+7+6+4)/5,
=(4+8+5+4+9)/5
= **(6, 6)**
**Seed 3** = (2+1)/2, (5+2)/2
= (1.5, 3.5)



# Steps to Perform Clustering

- Recompute the new cluster centroid

**Seed 1 = (2,10)**
**Seed 2** = (8+5+7+6+4)/5,
=(4+8+5+4+9)/5
= **(6, 6)**
**Seed 3** = (2+1)/2, (5+2)/2
= (1.5, 3.5)



# Steps to Perform Clustering

- Repeat the two previous steps until the convergence criterion is met
- Convergence criterion – when the assignment of points in clusters do not change over multiple iterations

# Steps to Perform Clustering

**Step 4:**
**Validate and Interpret cluster solution**

- Stability and Validity
- Stability is evaluated using different clustering procedures on the same data and testing whether these yield the same results.
- Eg: for hierarchical clustering, use different distance measures
- Validity can be evaluated using criterion validity

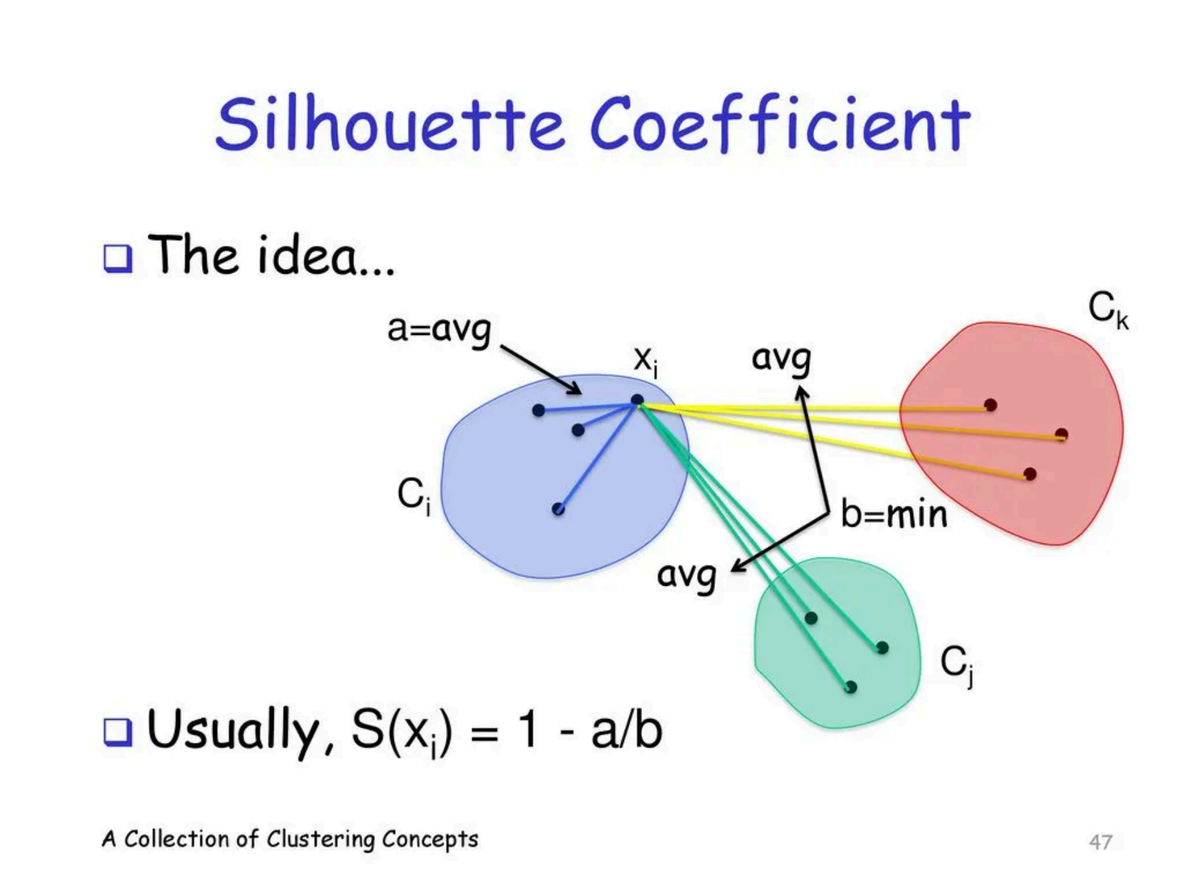
# Steps to Perform Clustering

**Step 4:**
**Validate and Interpret cluster solution**

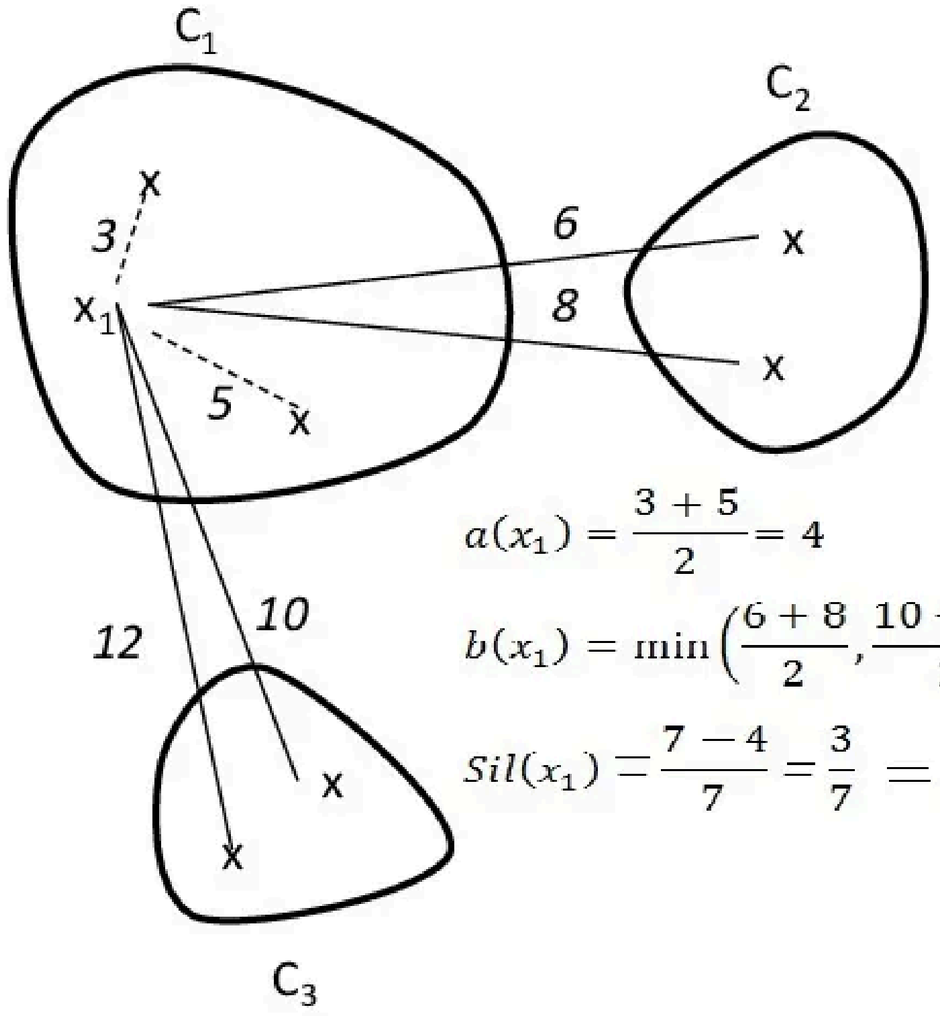
- Profiling of cluster
- Interpreting the clusters by examining the cluster centroids
- It helps to shed light on whether the segments are conceptually distinguishable
- This information will also help to find the meaningful label or name for the cluster to adequately reflects the objects in the cluster

# Silhouette Score

- The silhouette value is a measure of how similar an object is to its own cluster (cohesion) compared to other clusters (separation).
- The Silhouette coefficient is a value between -1 and 1, where higher values indicate a better clustering.



# Silhouette Score



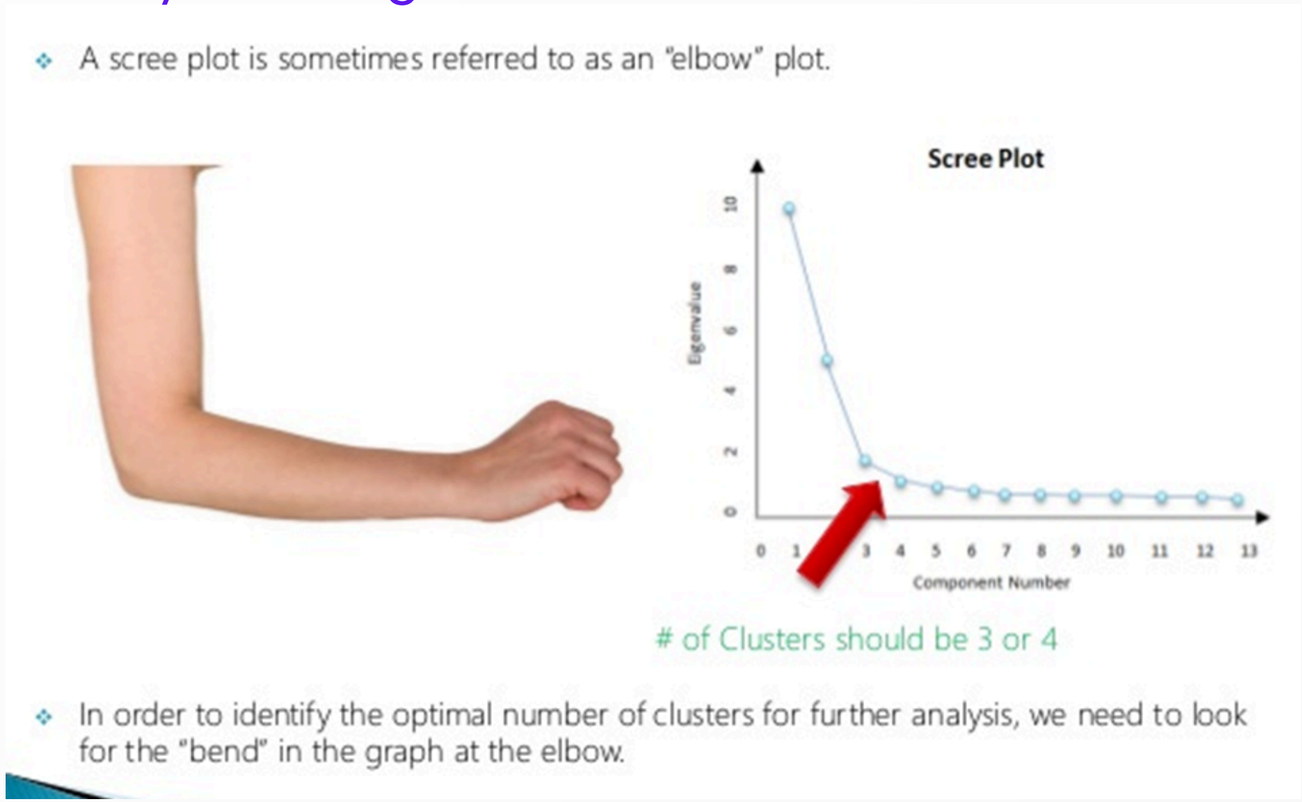

$$a(x_1) = \frac{3+5}{2} = 4$$

$$b(x_1) = \min\left(\frac{6+8}{2}, \frac{10+12}{2}\right) = 7$$

$$Sil(x_1) = \frac{7-4}{7} = \frac{3}{7} = 0.42$$

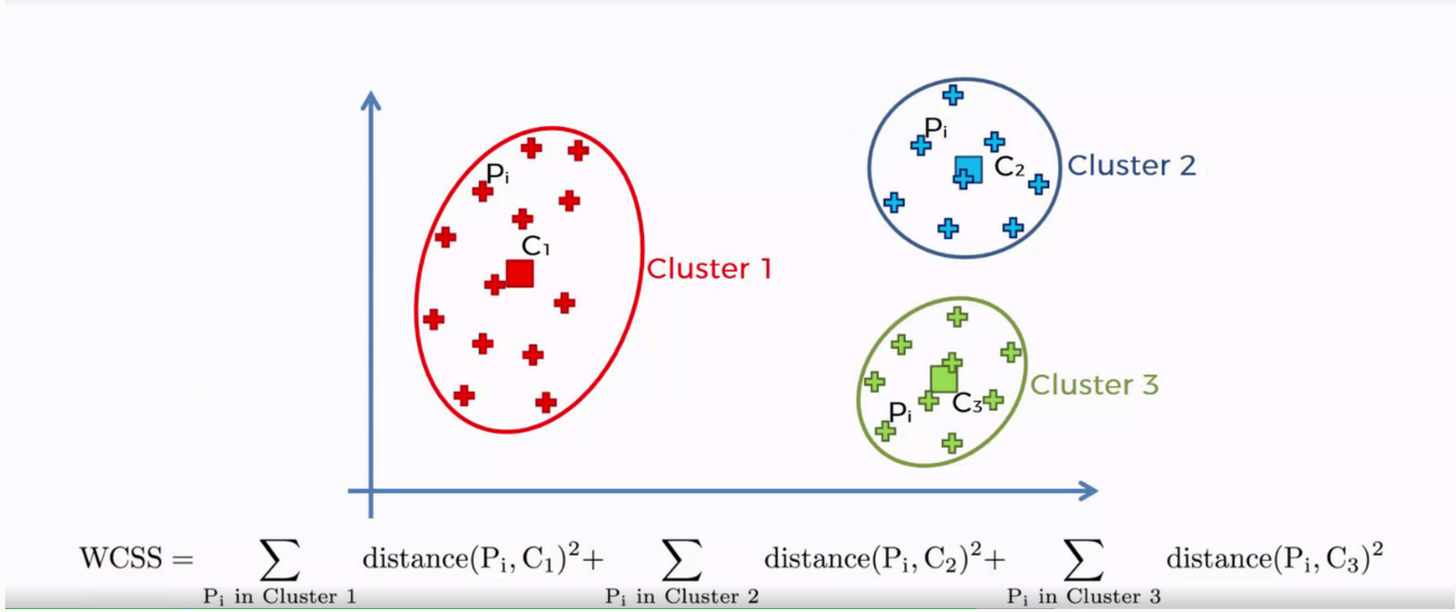
# Elbow Method

- When using K-Means algorithm, you need to always specify the number of clusters that you need the data set clustered into.
- The most easiest way of doing this is the use of Elbow method.

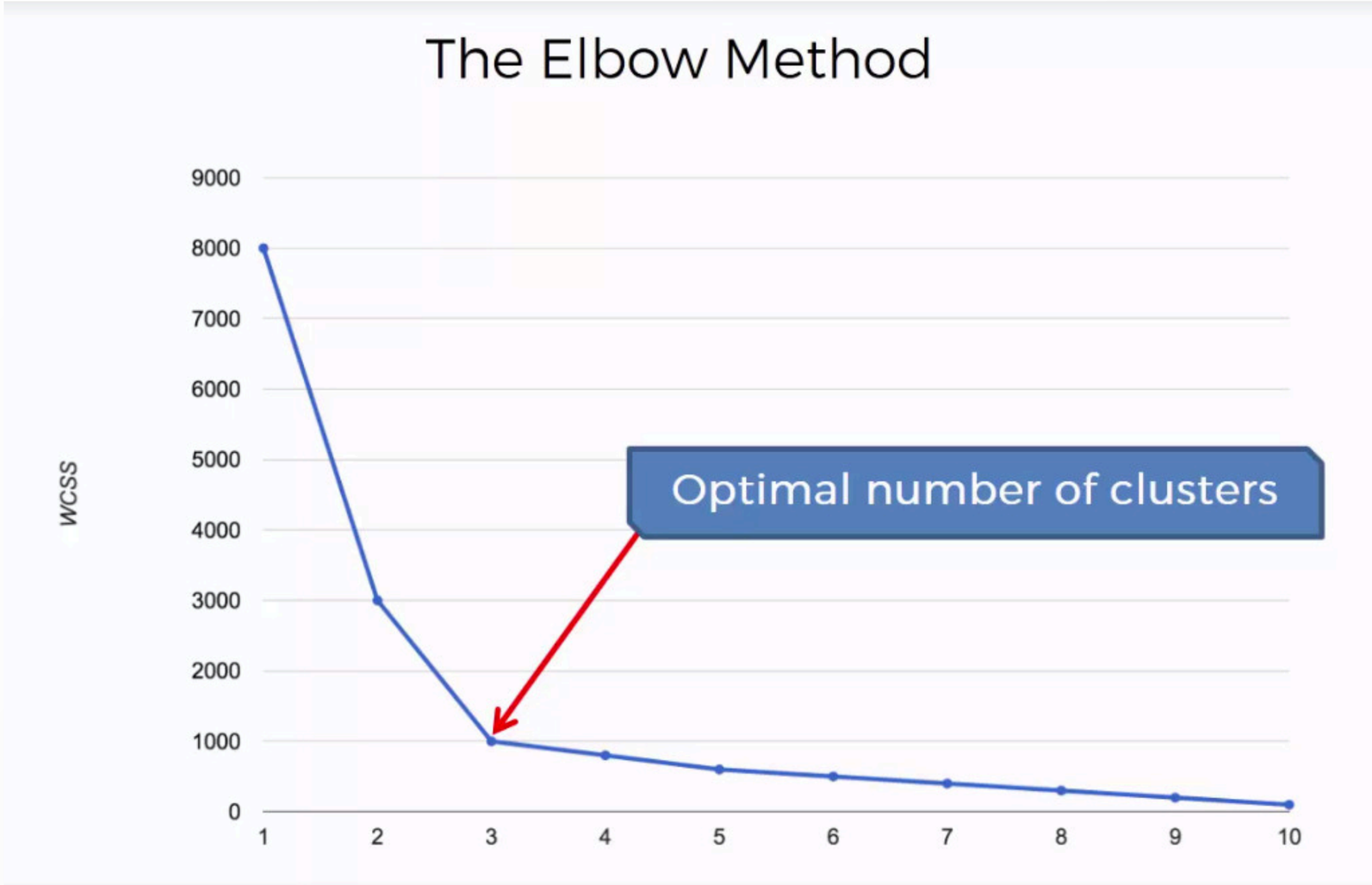


# Elbow Method

- When using K-Means algorithm, you need to always specify the number of clusters that you need the data set clustered into.
- The most easiest way of doing this is the use of Elbow method.
- Most of the time, Elbow method is used with either squared error(sse) or within cluster sum of errors(wcss)



# Elbow Method



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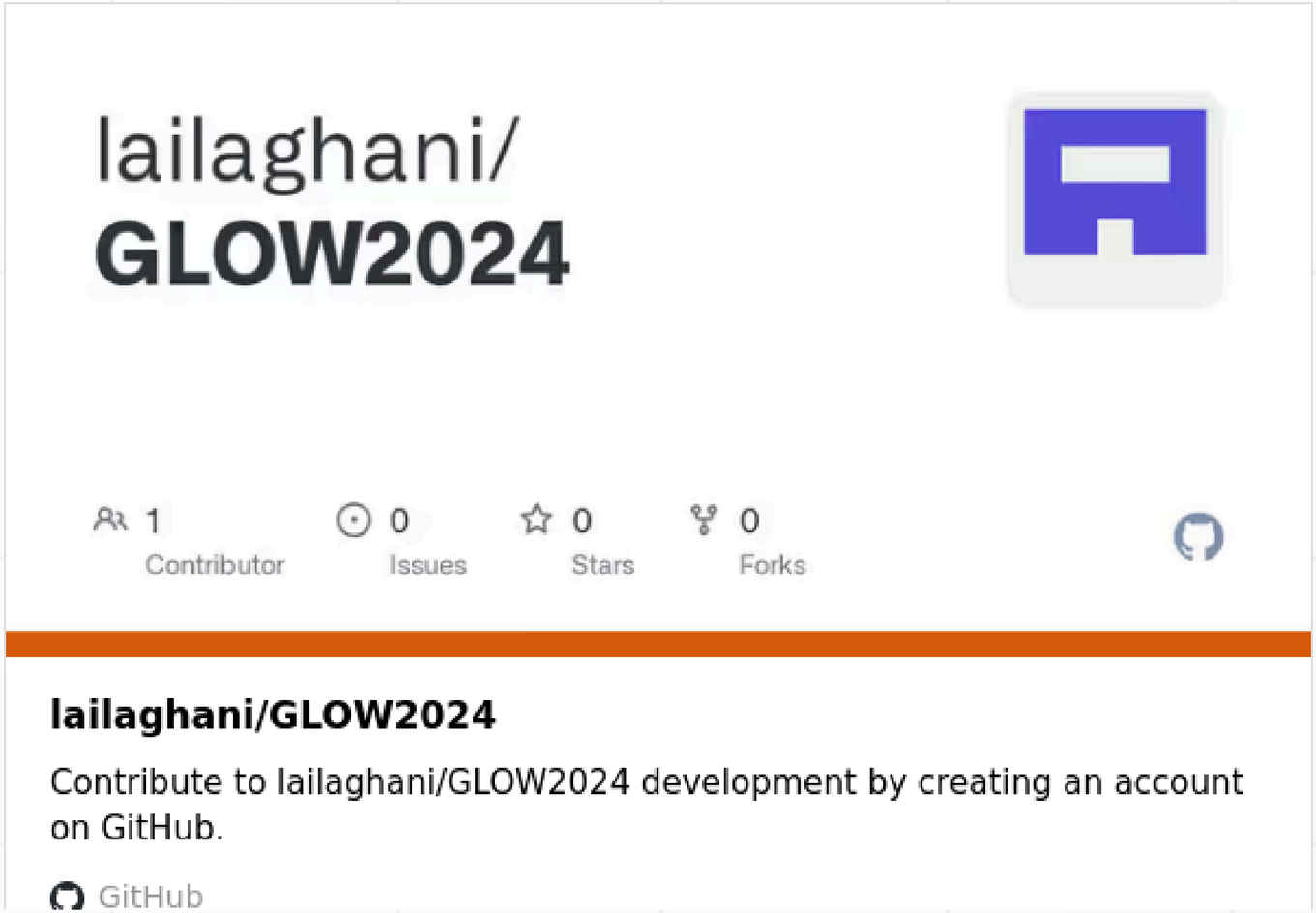
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