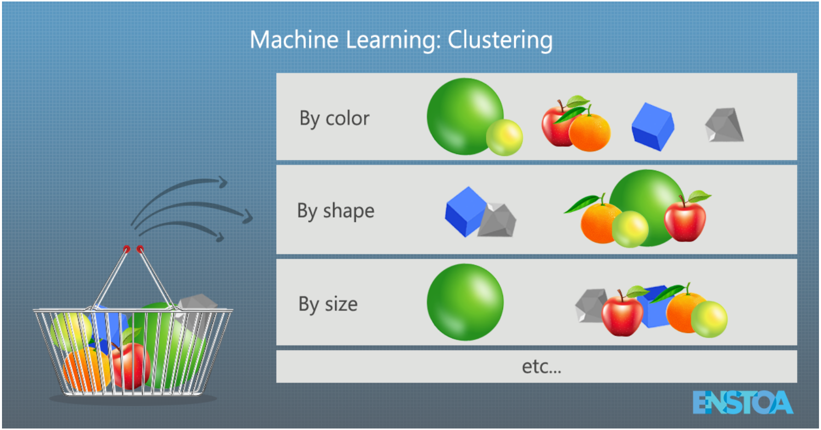
# Clustering

# What is clustering?

Clustering is grouping data points into groups where data points in one group are `similar` to each other.

# What is clustering?



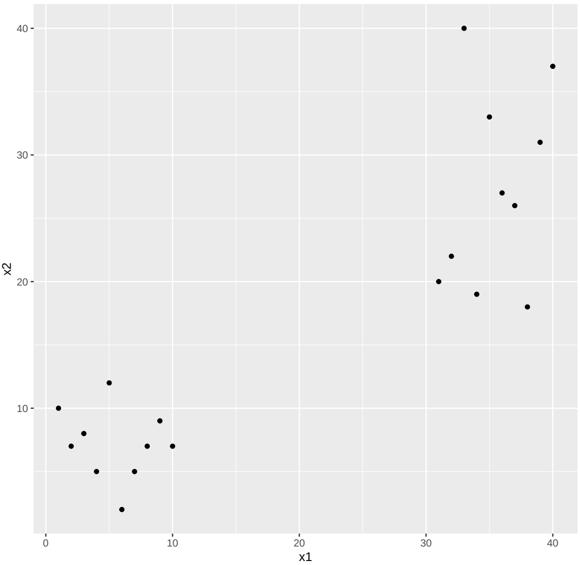
# Methods of Clustering

We will cover two clustering methods:

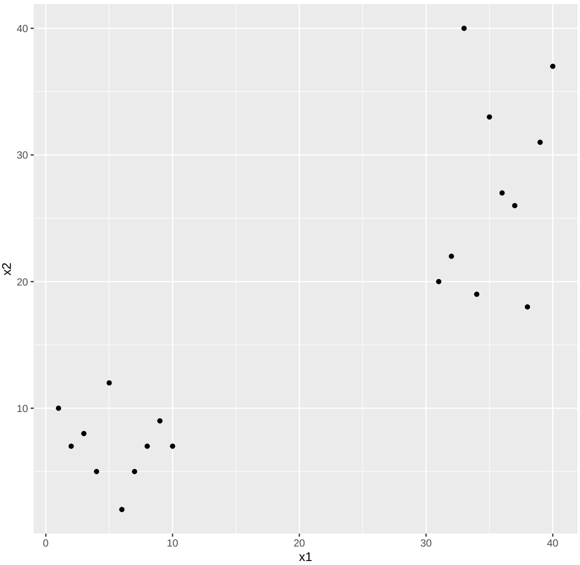
- K-means clustering and
- Hierarchical clustering

# Algorithm Example

# Data



# Step 1: Randomly Assign Points to Clusters



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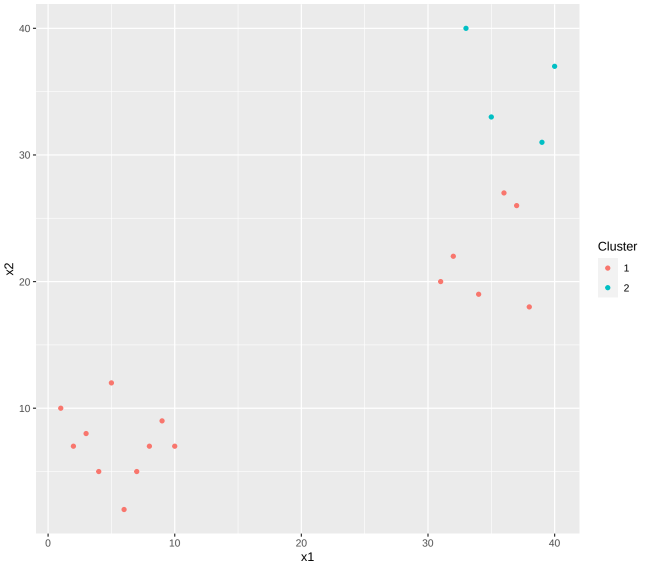
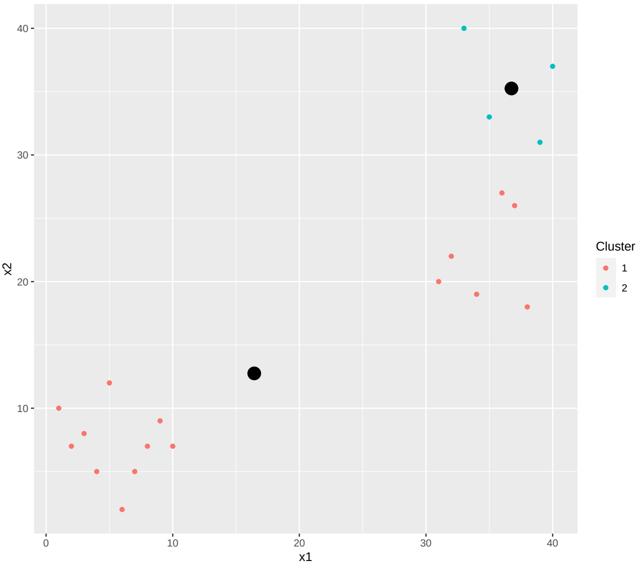
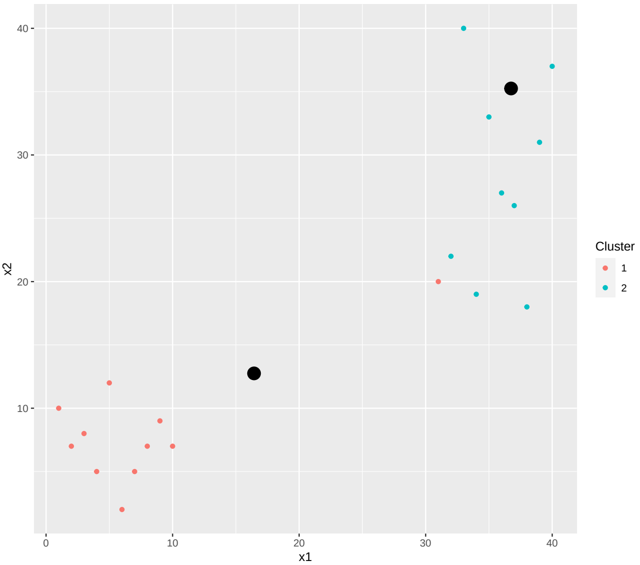


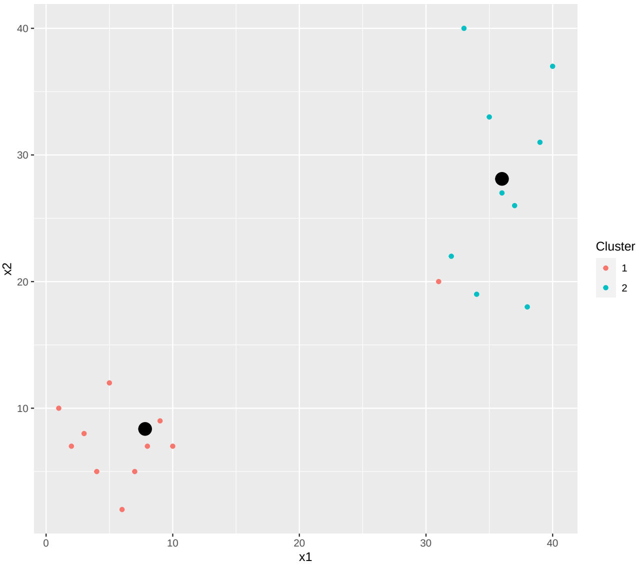
# Locate centroids



# Reassign Points to clusters



# Relocate centroids



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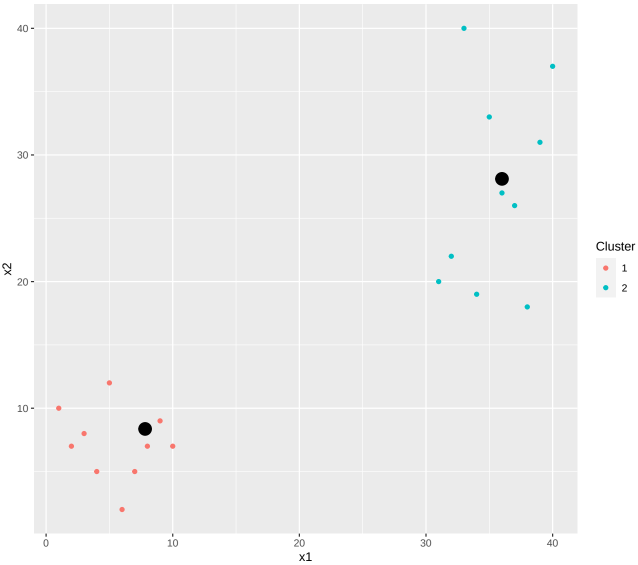

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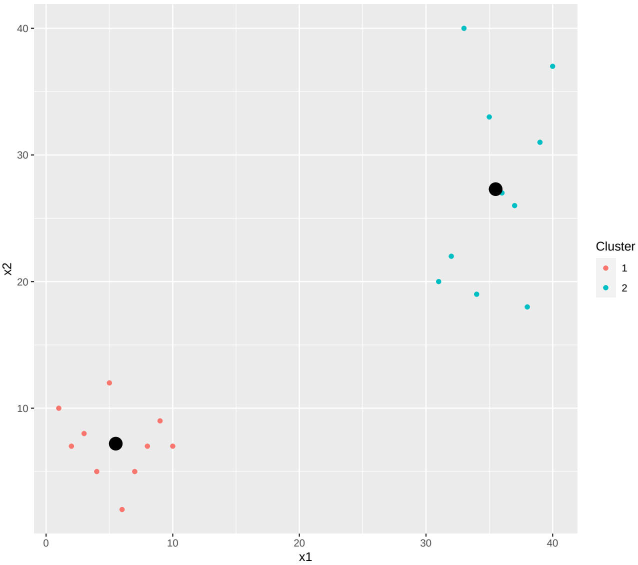

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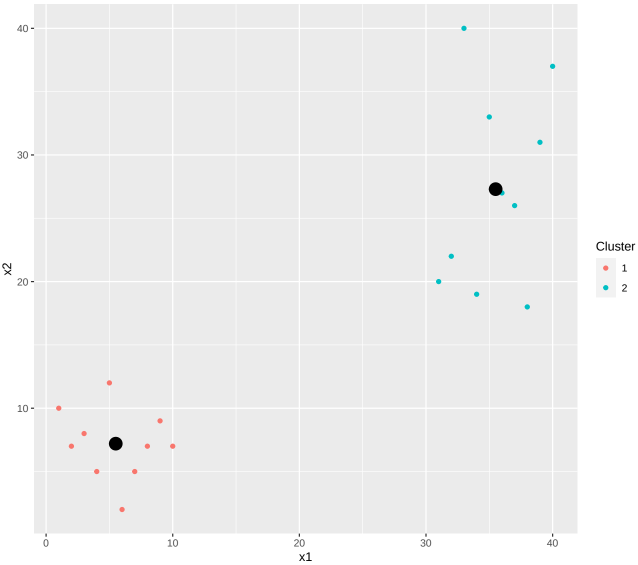

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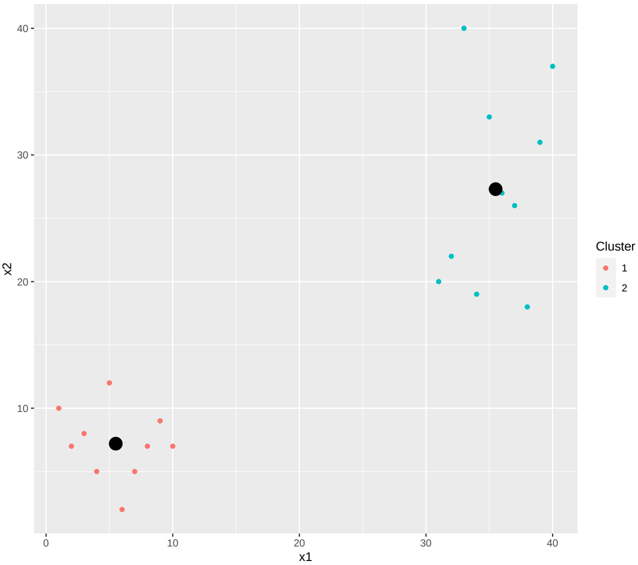
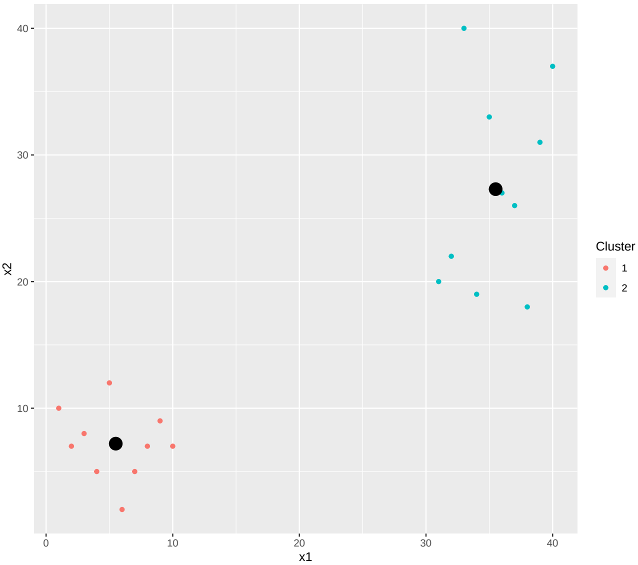
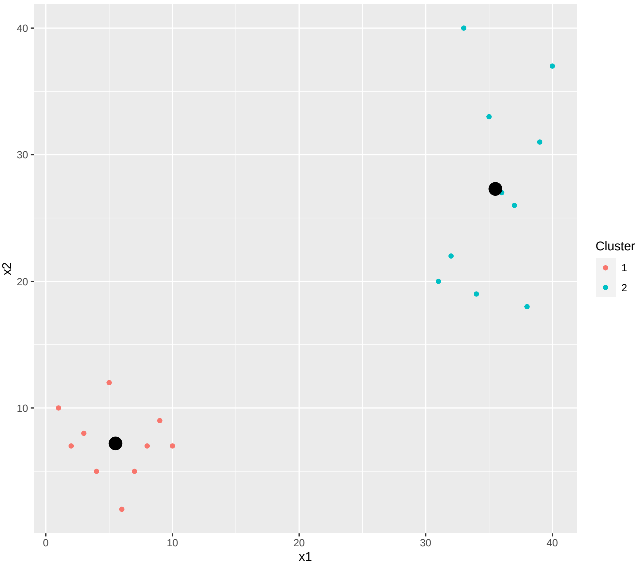


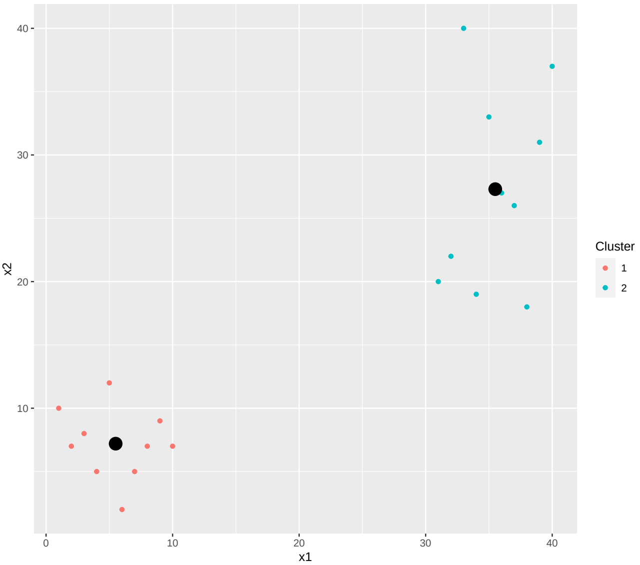
# Step 2: Reassign Points to clusters



# Step 2: Relocate centroids



# Step 2: Reassign Points to clusters



# Centroids

| Cluster | x1 | x2 |
|---|---|---|
| 1 | 5.5 | 7.2 |
| 2 | 35.5 | 27.3 |

# K-means Algorithm

- 1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
- 2. Iterate until the cluster assignments stop changing:
  - (a) For each of the K clusters, compute the cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
  - (b) Assign each observation to the cluster whose centroid is closest (where closest is defined using Euclidean distance).

# Dataset

| Point | x | y |
|---|---|---|
| A | 1 | 3 |
| B | 2 | 2 |
| C | 3 | 5 |
| D | 4 | 5 |
| E | 5 | 6 |

# Randomly Assign Cluster to Points

| Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 2 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 1 | D | 4 | 5 |
| 2 | E | 5 | 6 |

# Total Variance within

- Cluster 1 $= \{$A, C, D$\}$
- Cluster 2 $= \{$B, E$\}$
- Let M and N are the centroids of cluster 1 and 2 respectively

- Total Variance within

$$
\begin{aligned}
&= 2 \cdot (MA^2 + MC^2 + MD^2 + NB^2 + ND^2) \\
&= \frac{1}{3}(AB^2 + AC^2 + AD^2) + \frac{1}{2} \cdot BE^2
\end{aligned}
$$

| Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 2 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 1 | D | 4 | 5 |
| 2 | E | 5 | 6 |

- Total Variance within

| Cluster | Point | x | y |
|---|---|---|---|
| 1 | A | 1 | 3 |
| 2 | B | 2 | 2 |
| 1 | C | 3 | 5 |
| 1 | D | 4 | 5 |
| 2 | E | 5 | 6 |

- Total Variance within 19.83

| Cluster | Point | x | y | C_1x | C_1y | C_2x | C_2y |
|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.67 | 4.33 | 3.5 | 4 |
| 2 | B | 2 | 2 | 2.67 | 4.33 | 3.5 | 4 |
| 1 | C | 3 | 5 | 2.67 | 4.33 | 3.5 | 4 |
| 1 | D | 4 | 5 | 2.67 | 4.33 | 3.5 | 4 |
| 2 | E | 5 | 6 | 2.67 | 4.33 | 3.5 | 4 |

| Cluster | Point | x | y | C_1x | C_1y | C_2x | C_2y | dc1 | dc2 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.67 | 4.33 | 3.5 | 4 | 2.13 | 2.69 |
| 2 | B | 2 | 2 | 2.67 | 4.33 | 3.5 | 4 | 2.42 | 2.50 |
| 1 | C | 3 | 5 | 2.67 | 4.33 | 3.5 | 4 | 0.75 | 1.12 |
| 1 | D | 4 | 5 | 2.67 | 4.33 | 3.5 | 4 | 1.49 | 1.12 |
| 2 | E | 5 | 6 | 2.67 | 4.33 | 3.5 | 4 | 2.87 | 2.50 |

| Cluster | Point | x | y | dc1 | dc2 | min_distance |
|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.13 | 2.69 | 2.13 |
| 2 | B | 2 | 2 | 2.42 | 2.50 | 2.42 |
| 1 | C | 3 | 5 | 0.75 | 1.12 | 0.75 |
| 1 | D | 4 | 5 | 1.49 | 1.12 | 1.12 |
| 2 | E | 5 | 6 | 2.87 | 2.50 | 2.50 |

| Cluster | Point | x | y | dc1 | dc2 | min_distance | New_Cluster |
|---|---|---|---|---|---|---|---|
| 1 | A | 1 | 3 | 2.13 | 2.69 | 2.13 | 1 |
| 2 | B | 2 | 2 | 2.42 | 2.50 | 2.42 | 1 |
| 1 | C | 3 | 5 | 0.75 | 1.12 | 0.75 | 1 |
| 1 | D | 4 | 5 | 1.49 | 1.12 | 1.12 | 2 |
| 2 | E | 5 | 6 | 2.87 | 2.50 | 2.50 | 2 |

# Total Variance within

- Cluster 1 = {A, B, C}
- Cluster 2 = {D, E}
- Let H and K are the centroids of cluster 1 and 2, respectively.

- Total Variance within

$$
\begin{aligned}
&= 2 \cdot (HA^2 + HB^2 + HC^2 + KD^2 + KE^2) \\
&= \frac{1}{3}(AB^2 + AC^2 + BC^2) + \frac{1}{2} \cdot DE^2
\end{aligned}
$$

- Total Variance within 7.67
- The process of k-means will minimize the total variance within

# Example

You apply 2-means clustering to a set of five observations with two features. You are given the following initial cluster assignments:

| Observation | $X_1$ | $X_2$ | Initial cluster |
|---|---|---|---|
| A | 1 | 1 | 1 |
| B | 0 | 0 | 1 |
| C | 0 | 1 | 1 |
| D | 2 | 1 | 2 |
| E | 1 | 0 | 2 |

Calculate the total within-cluster variation of the initial cluster assignments, based on Euclidean distance measure.