Clustering

What is clustering?

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

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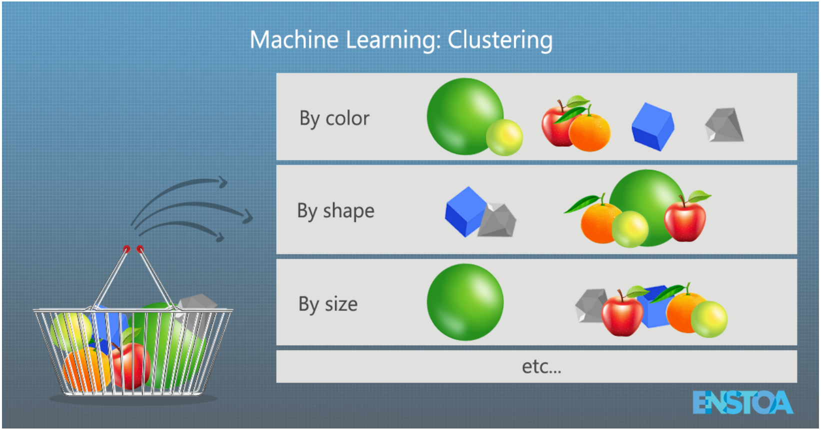


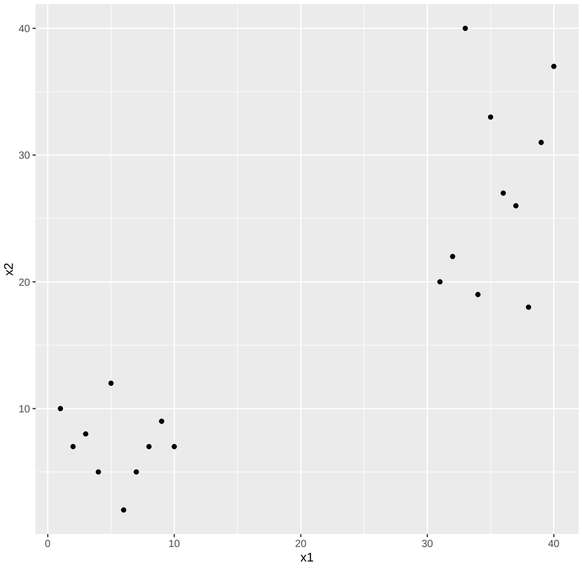
Methods of Clustering

We will cover two clustering methods:

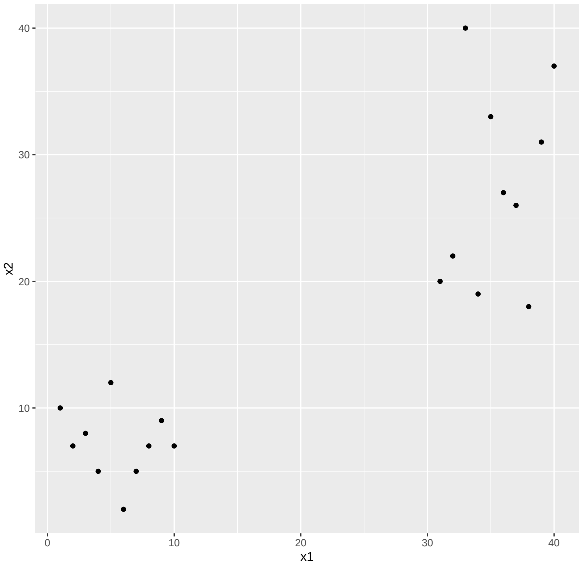
- K-means clustering and
- Hierarchical clustering

K-means clustering

Example - Data



Step 1: Randomly Assign Points to Clusters



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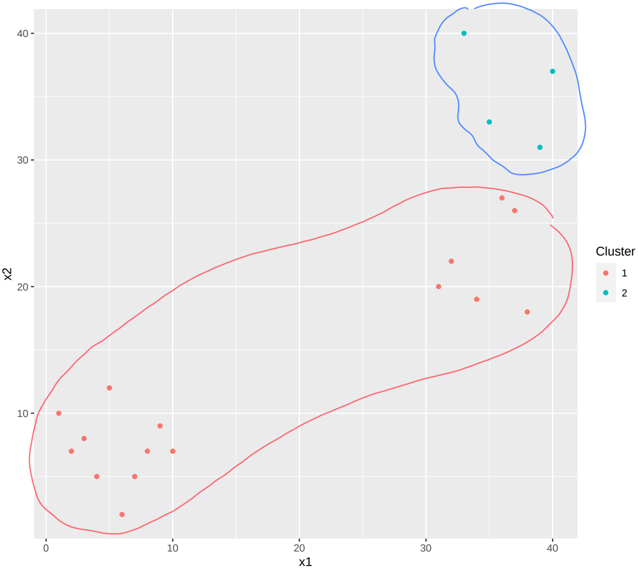
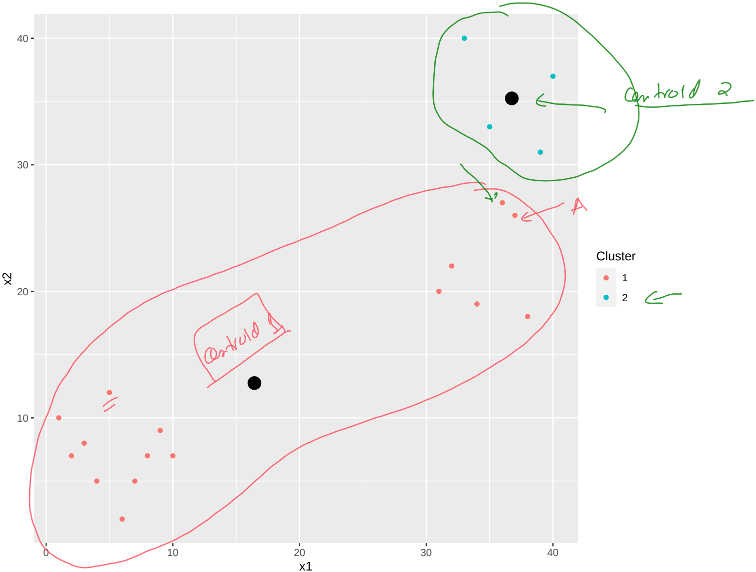
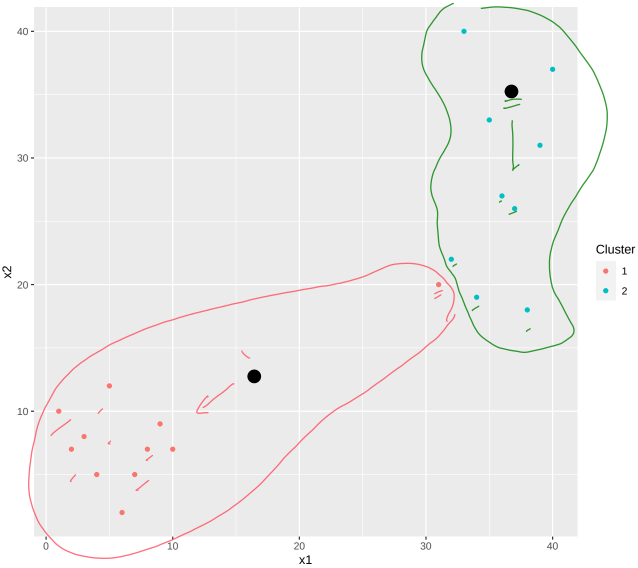


Locate centroids



Reassign Points to clusters



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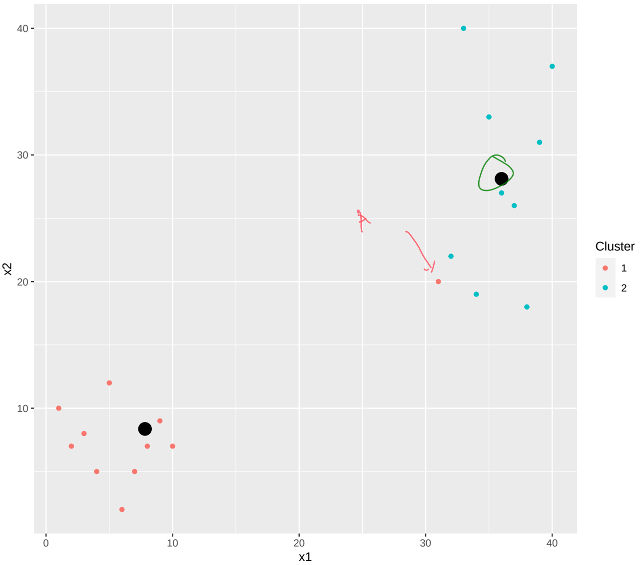

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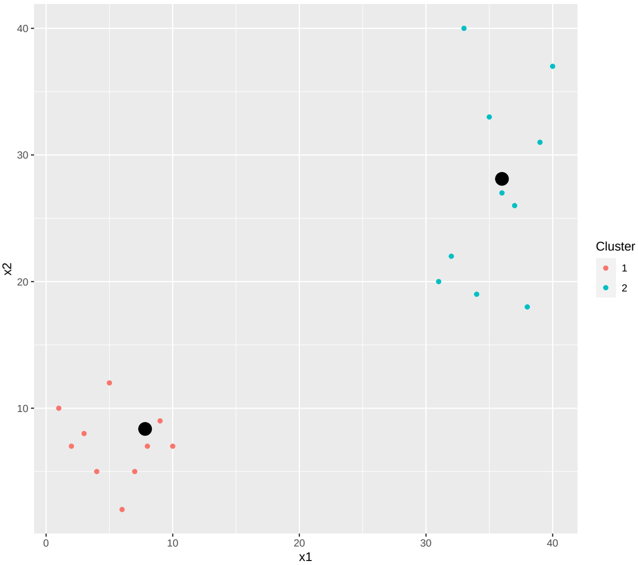

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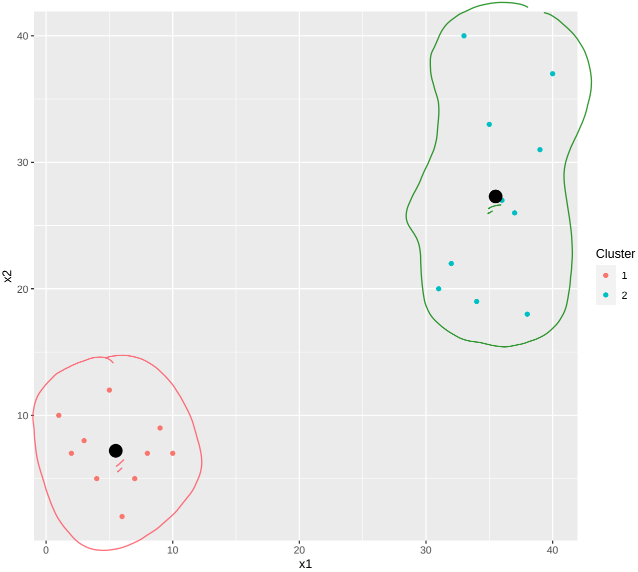

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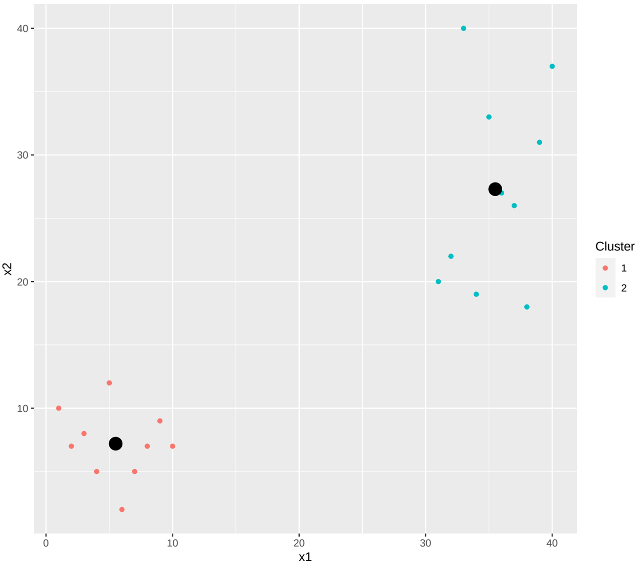

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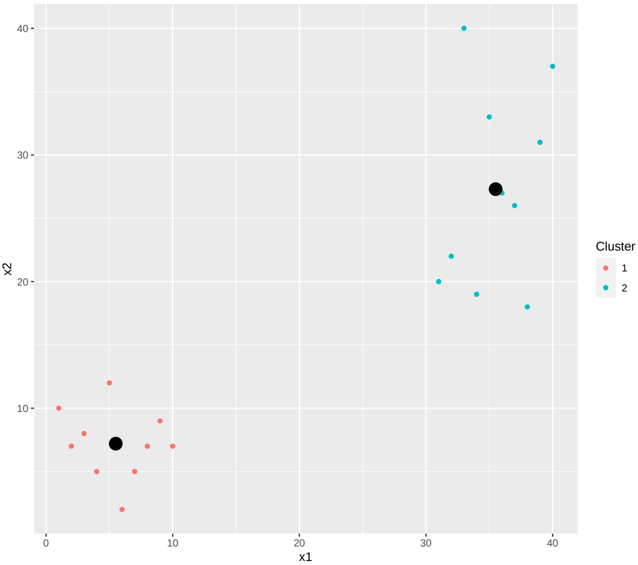
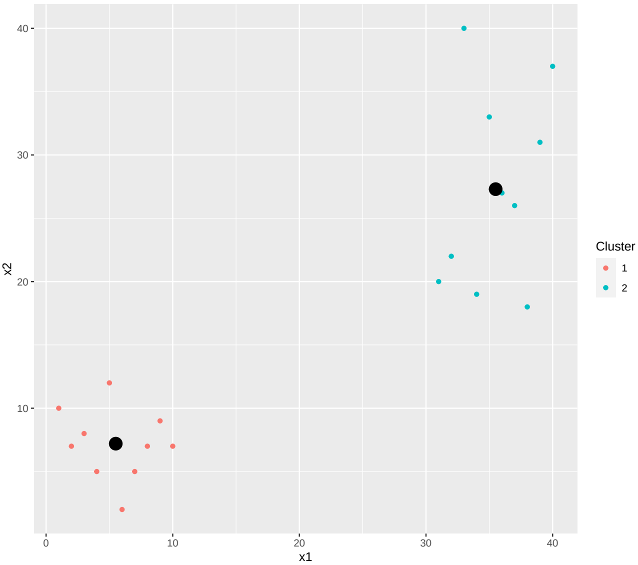


Step 2: Reassign Points to clusters



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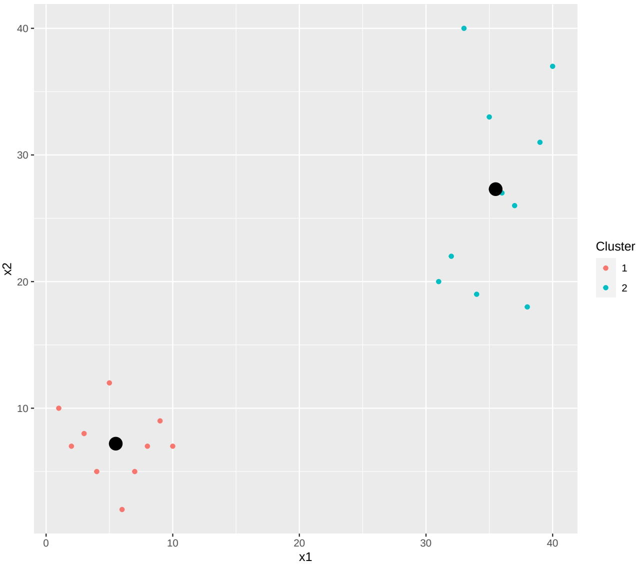

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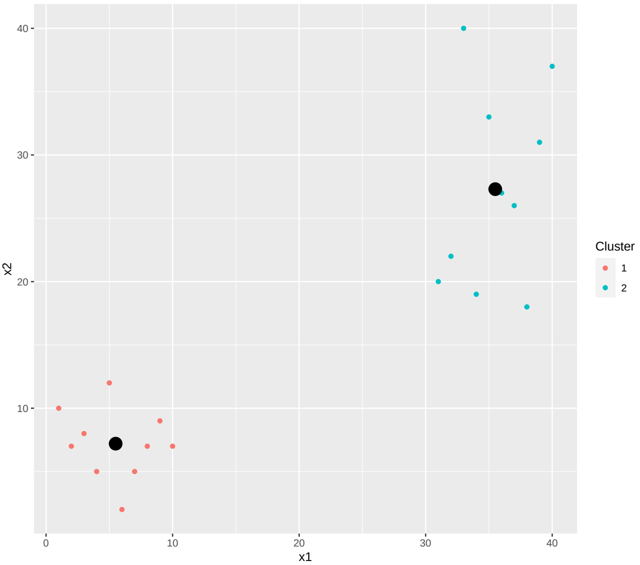

Centroids

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 k^{th} 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

cluster 1 : {A, C, D}

cluster 2 = {B, E}

$\frac{1+3+4}{3}$, $\frac{3+5+5}{3}$

Centroid 1 = $\left(\frac{8}{3}, \frac{13}{3}\right)$

Centroid 1 = (2.67, 4.33)

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

M : centroid 1

N : centroid 2

MA

NA

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

1

1

2

MA = 2.13

NA = 2.69

MA < NA

A belongs to M

or cluster M

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

cluster 1 : $\{A, B, C\}$

cluster 2 : $\{D, E\}$

Total Variance within

- With the initial Clusters:
  - 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

$$= 2 \cdot (MA^2 + MC^2 + MD^2 + NB^2 + ND^2)$$

$$= \frac{1}{3}(AB^2 + AC^2 + AD^2) + \frac{1}{2} \cdot BE^2$$

1

2

- Total Variance within 19.83

Total Variance within

- With the new Clusters:
  - 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 (Total Variance within) of the initial cluster assignments, based on Euclidean distance measure.

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

(1) cluster 1 $= \{A, B, C\} \Rightarrow V_1 = \frac{1}{3}\left(AB^2 + AC^2 + BC^2\right)$

$$= \frac{1}{3}\left[(1-0)^2 + (1-0)^2 + (1-0)^2 + (1-1)^2 + (0-0)^2 + (0-1)^2\right]$$

$$= \frac{4}{3}.$$

cluster 2 $= \{D, E\} \Rightarrow V_2 = \frac{1}{2}\left(DE^2\right) = \frac{1}{2}\left[(2-1)^2 + (1-0)^2\right]$

$$= 1$$

$$\Rightarrow V = V_1 + V_2 = \frac{4}{3} + 1 = 7/3$$

(2) using the centroid: $\begin{cases} M = \left(\frac{1}{3}, \frac{2}{3}\right) \\ N = \left(\frac{3}{2}, \frac{1}{2}\right) \end{cases} \Rightarrow V = 2\left(MA^2 + MB^2 + MC^2 + ND^2 + NE^2\right) = \boxed{7/3}$