Unsupervised learning
Part I: Clustering

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Outline

- Introduction of Unsupervised Learning
- Introduction of Clustering
  - What is clustering
  - Applications
- K-means Algorithm
  - What is k-means
  - How does k-means work
  - Loss function
  - Strengths and weakness

Introduction of unsupervised learning

Supervised learning vs.Unsupervised learning

Supervised learning: discover patterns in the data that relate data attributes with a target (class) attribute.

- ➢ These patterns are then utilized to predict the values of the target attribute in future data instances.

Examples: Regression, Classification

Unsupervised learning: The data have no target attribute.

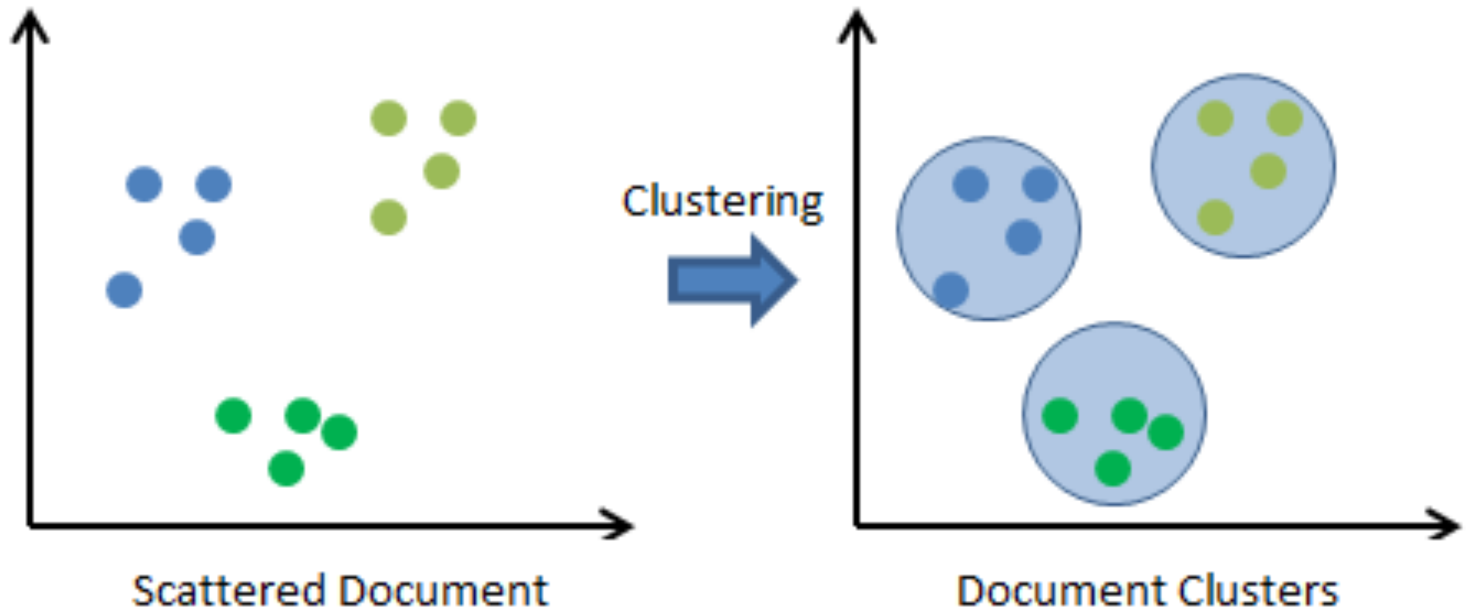
- ➢ We want to explore the data to find some intrinsic structures in them.

Examples: Clustering, Dimensionality reduction

Clustering

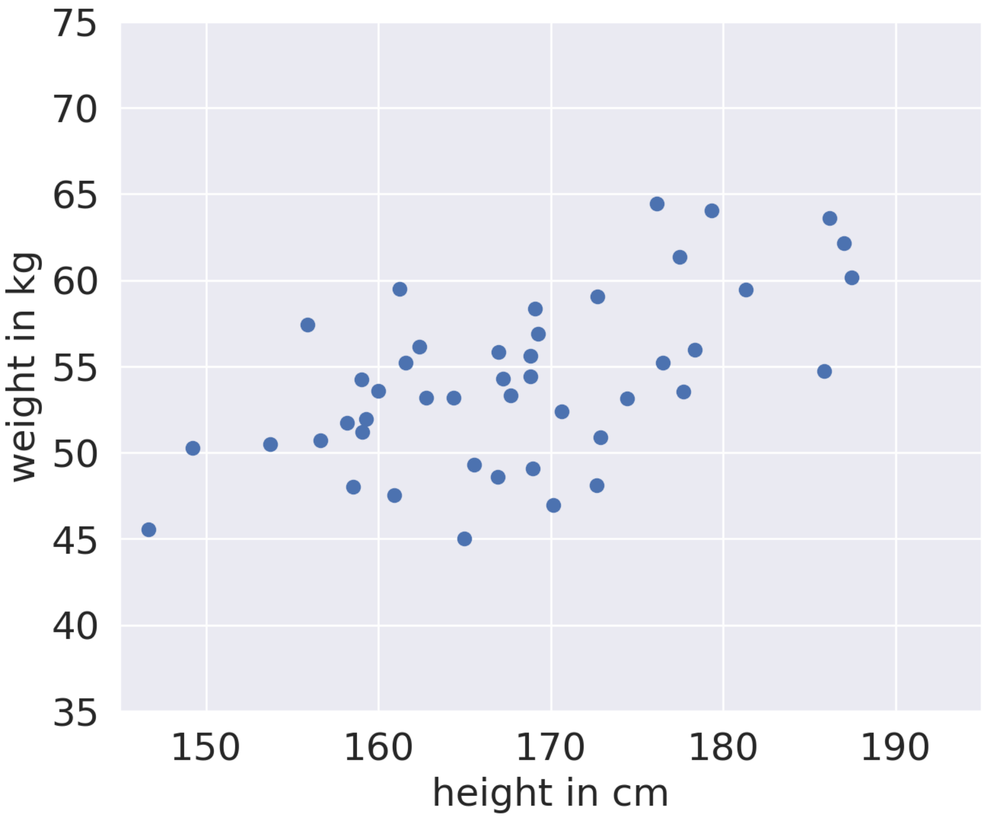
What is clustering?

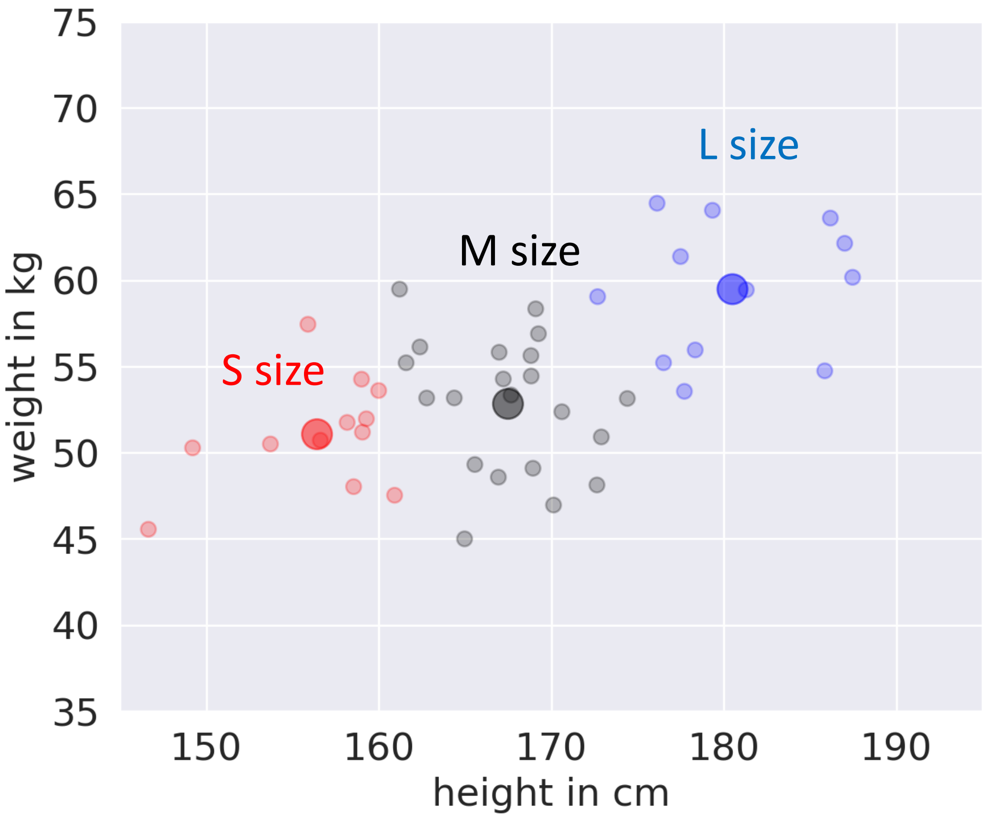
Clustering is to group a set of objects such that similar objects are in the same group and dissimilar objects are separated into different groups



Applications

-Customer categorisation





Applications

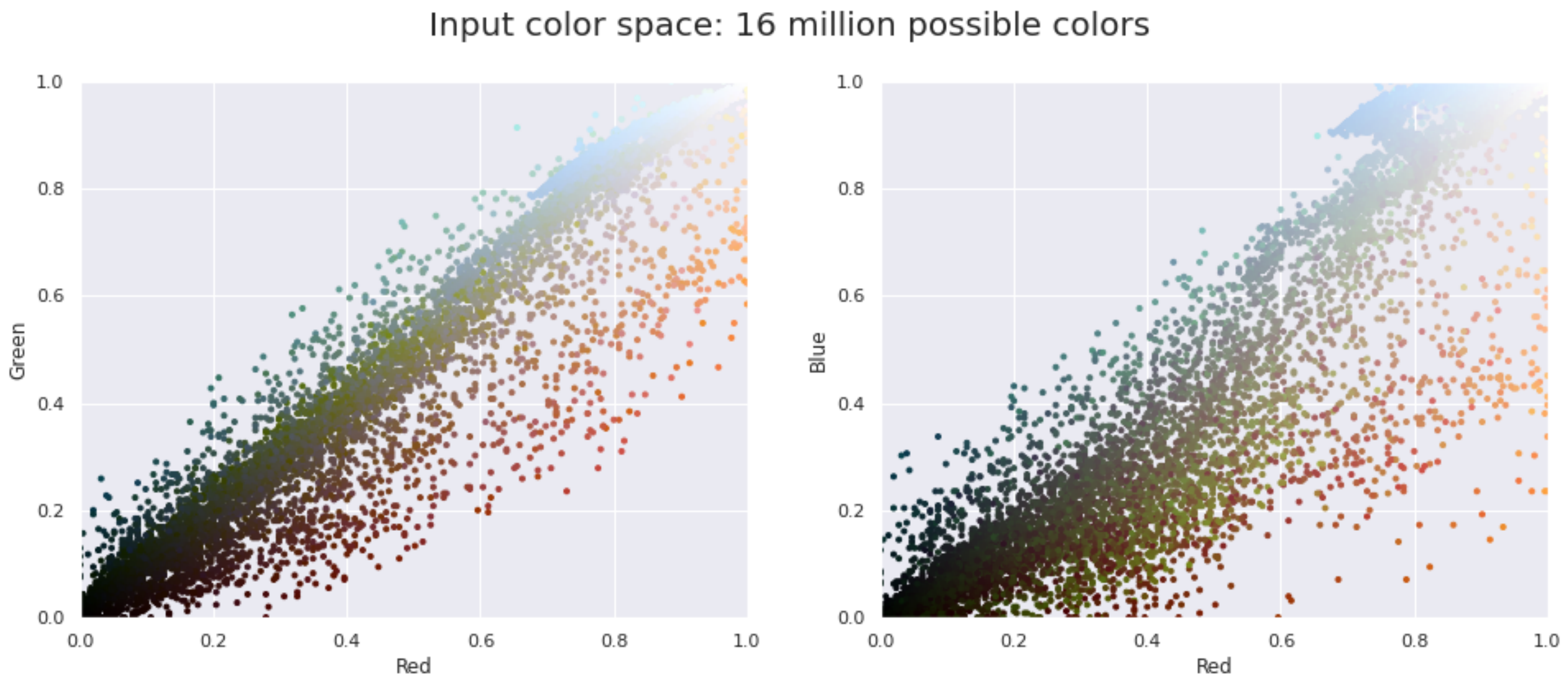
-Image compression

Number of possible colours: $256^3 = 16777216$

From scikit-learn (https://scikit-learn.org/stable/index.html) sample images

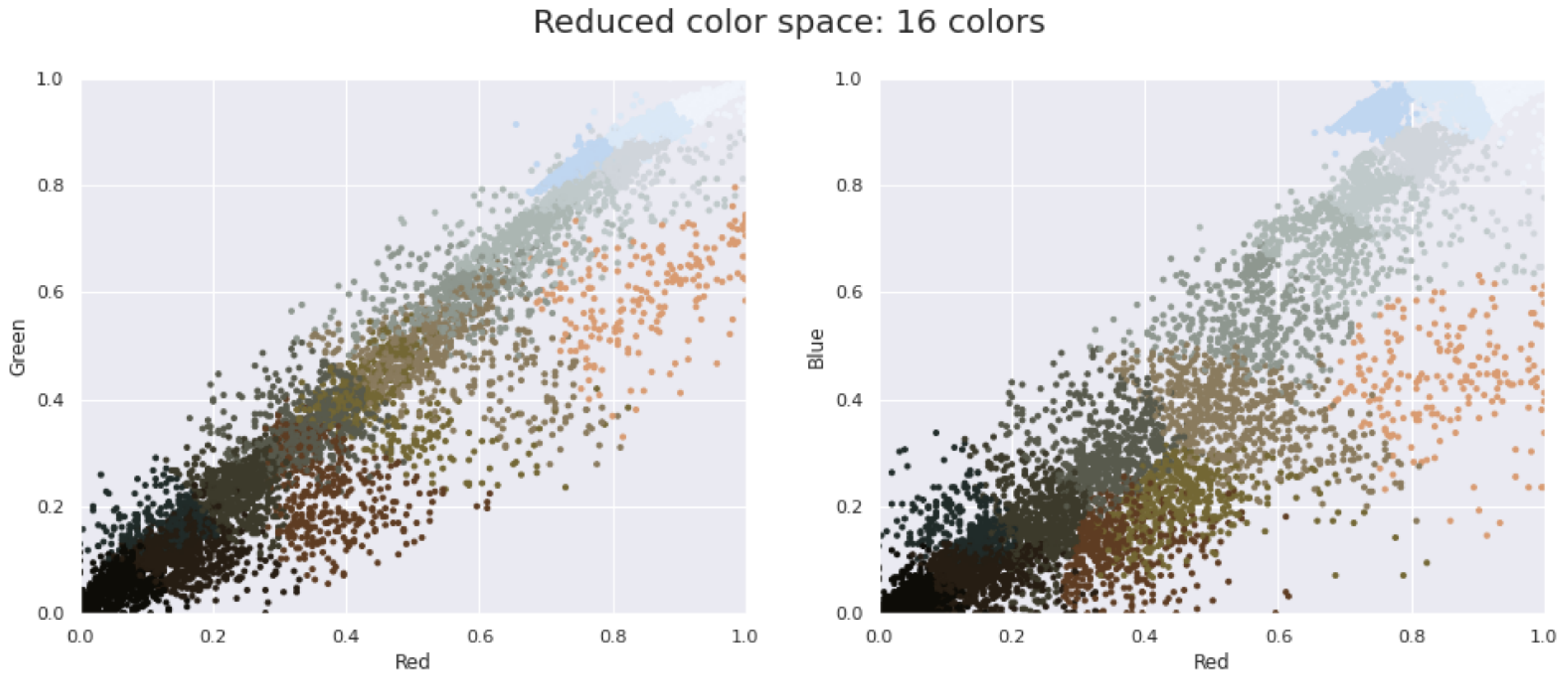
Applications

-Image compression



Applications

-Image compression

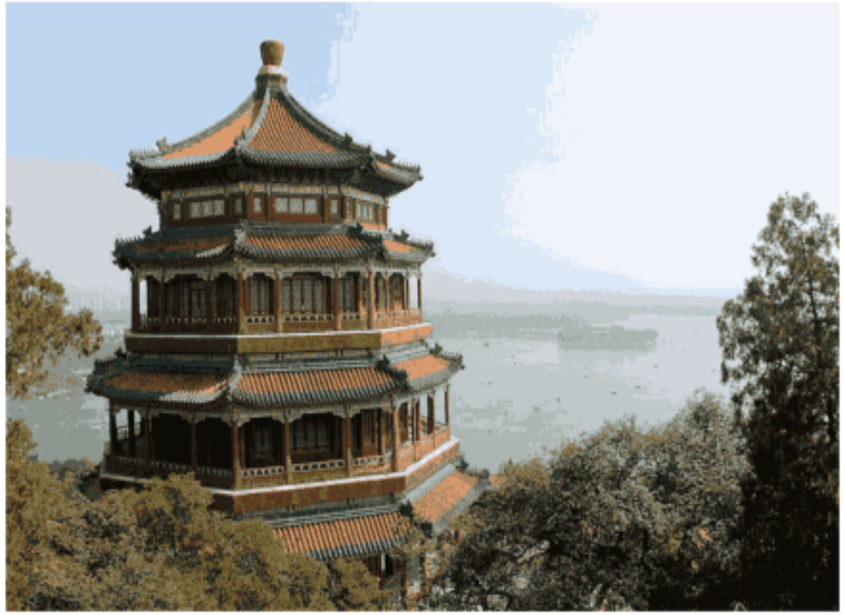


Applications

-Image compression

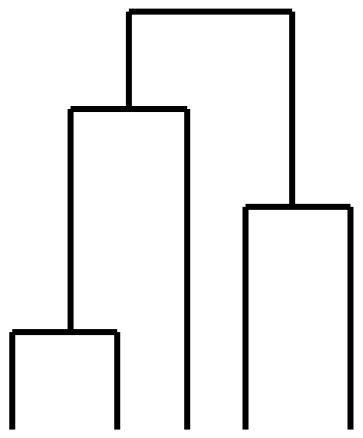
Original Image

16-color Image

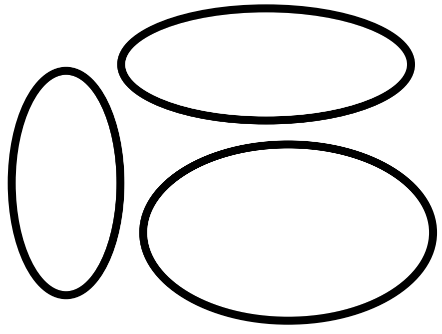


Types of clustering

1. **Hierarchical algorithms**: find successive clusters using previously established clusters.
   - Agglomerative("bottom-up"): begin with each element as a separate cluster and merge them into successively larger clusters.
   - Divisive("top-down"): begin with the whole set and proceed to divide it into successively smaller clusters.



2. **Partitional clustering:** determine all clusters at once.
   - ***K*-means**
   - Fuzzy *c*-means clustering



K-means

What is k-means?

The k-means algorithm is an algorithm to cluster m objects based on attributes into k clusters, where k < m.

- Each cluster has a cluster center, called centroid.
- The centroid of the cluster is the mean of the value of the data points that belong to the cluster
- *k* is specified by the user

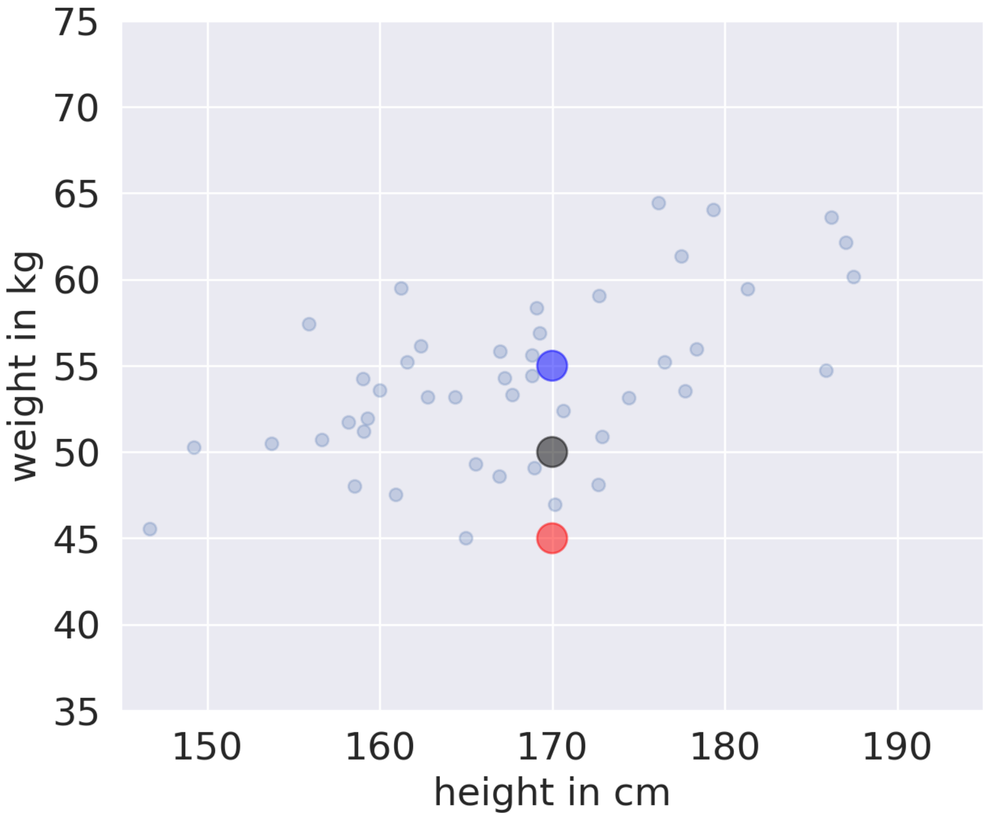
How does K-means work?

- Step 1: Begin with a decision of the value of k
- Step 2: randomly select initial cluster centroids

Repeat

- Step 3: calculate distance from each object to each cluster centroid.
- Step 4: Assign each object to the closest cluster
- Step 5: Compute the new centroid for each cluster

until *no change in clusters*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weight in kg
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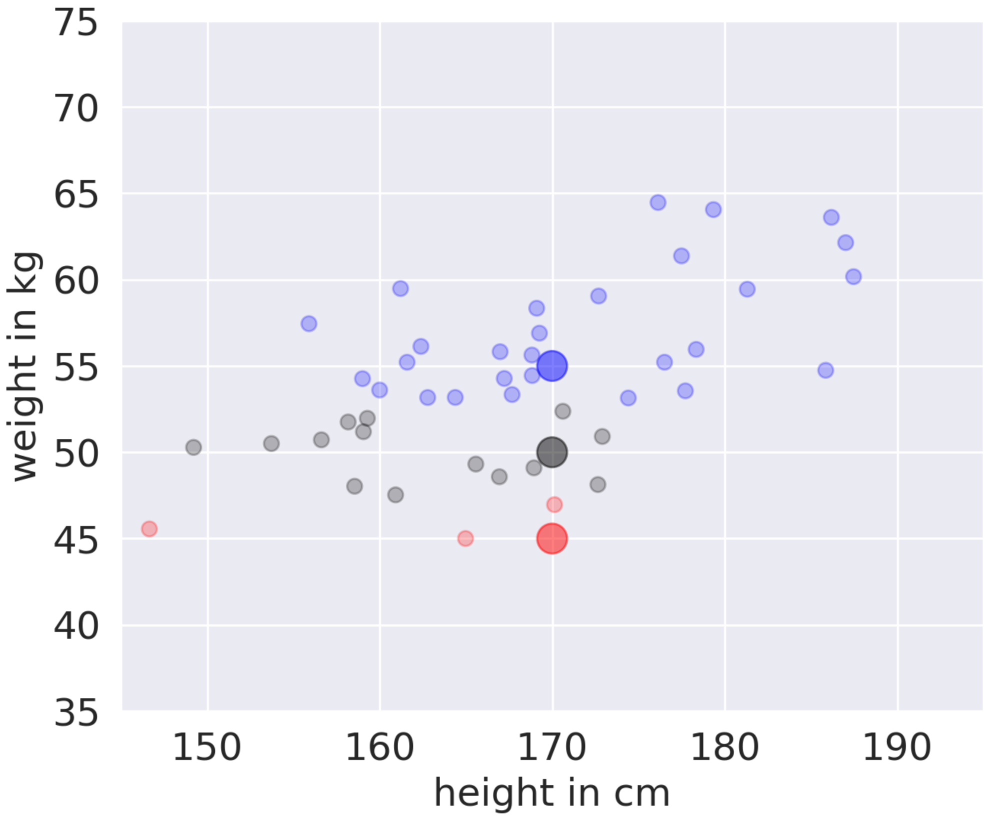
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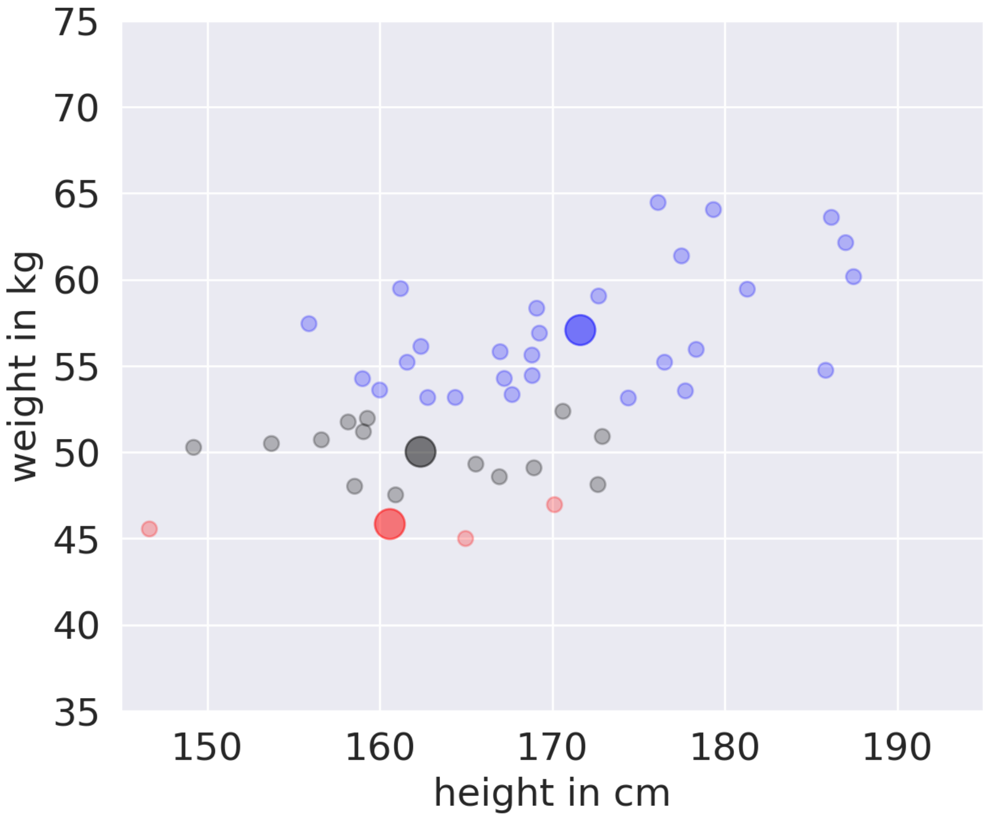
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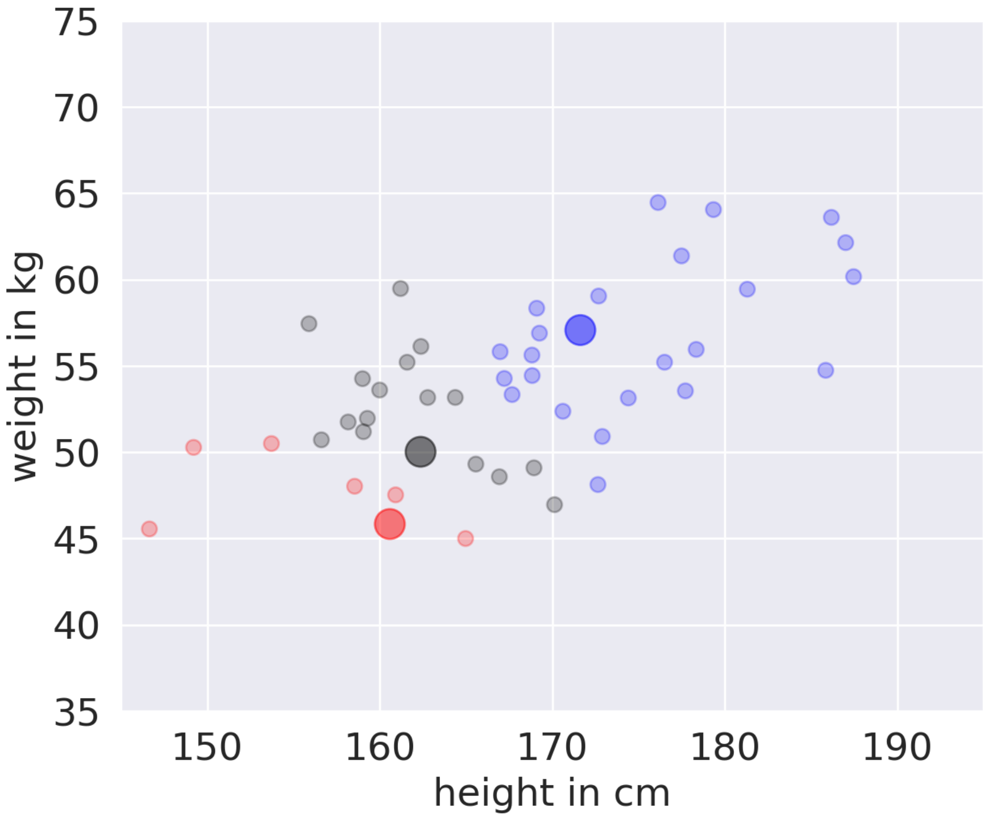
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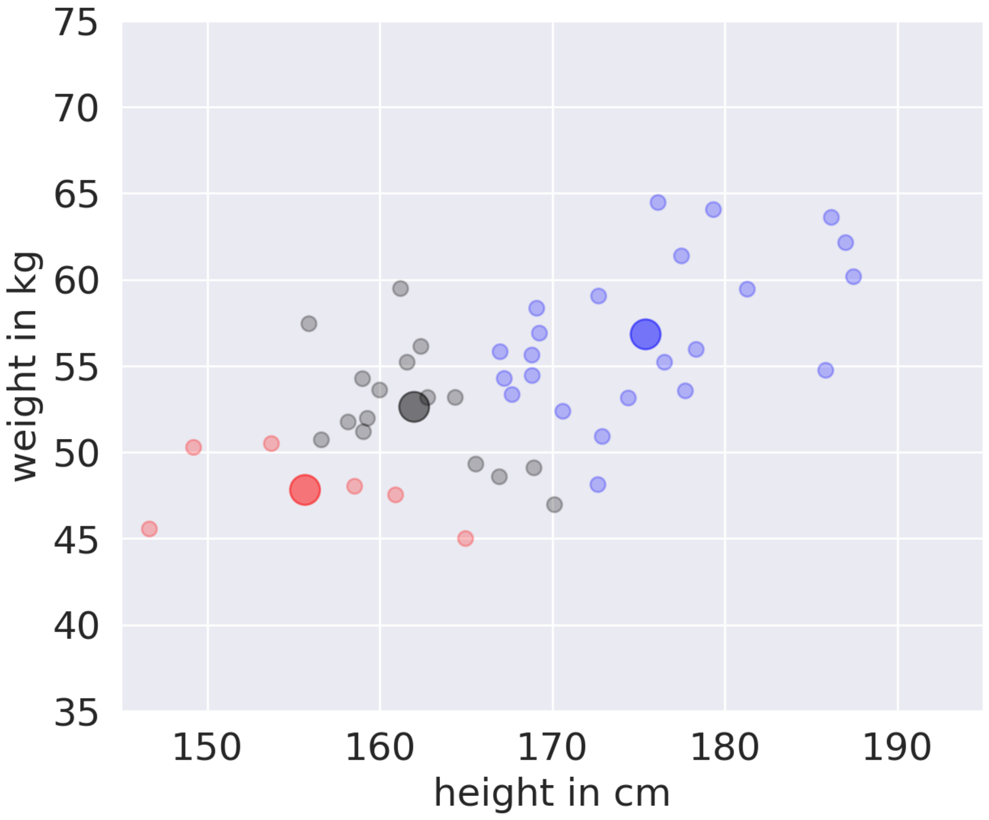

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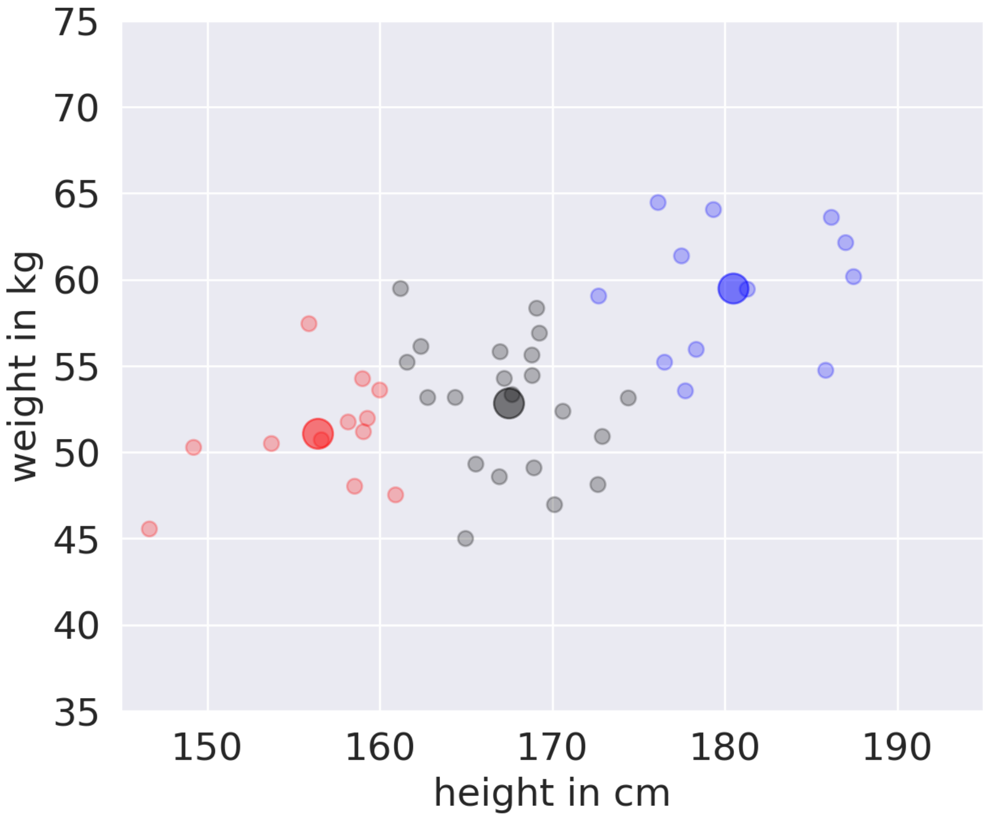

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weight in kg
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height in cm

A simple example of implementation of k-means (using k=2)

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

Step 1:

Initialization: Randomly we choose following two centroids (k=2) for two clusters.

In this case the 2 centroid are: m1=(1.0,1.0) and m2=(5.0,7.0).

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

	Individual	Mean Vector
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

Step 2:

- Thus, we obtain two clusters containing:

  {1,2,3} and {4,5,6,7}.

- Their new centroids are:

$$m_1 = \left(\frac{1}{3}(1.0+1.5+3.0), \frac{1}{3}(1.0+2.0+4.0)\right) = (1.83, 2.33)$$

$$m_2 = \left(\frac{1}{4}(5.0+3.5+4.5+3.5), \frac{1}{4}(7.0+5.0+5.0+4.5)\right)$$
$$= (4.12, 5.38)$$

Individual	Centroid 1	Centroid 2
1	0	7.21
2 (1.5, 2.0)	1.12	6.10
3	3.61	3.61
4	7.21	0
5	4.72	2.5
6	5.31	2.06
7	4.30	2.92

$$d(m_1, 2) = \sqrt{|1.0-1.5|^2 + |1.0-2.0|^2} = 1.12$$
$$d(m_2, 2) = \sqrt{|5.0-1.5|^2 + |7.0-2.0|^2} = 6.10$$

Step 3:

- Now using these centroids we compute the Euclidean distance of each object, as shown in table.

- Therefore, the new clusters are:

  {1,2} and {**3**,4,5,6,7}

- Next centroids are: m1=(1.25,1.5) and m2 = (3.9,5.1)

Individual	Centroid 1	Centroid 2
1	1.57	5.38
2	0.47	4.28
3	2.04	1.78
4	5.64	1.84
5	3.15	0.73
6	3.78	0.54
7	2.74	1.08

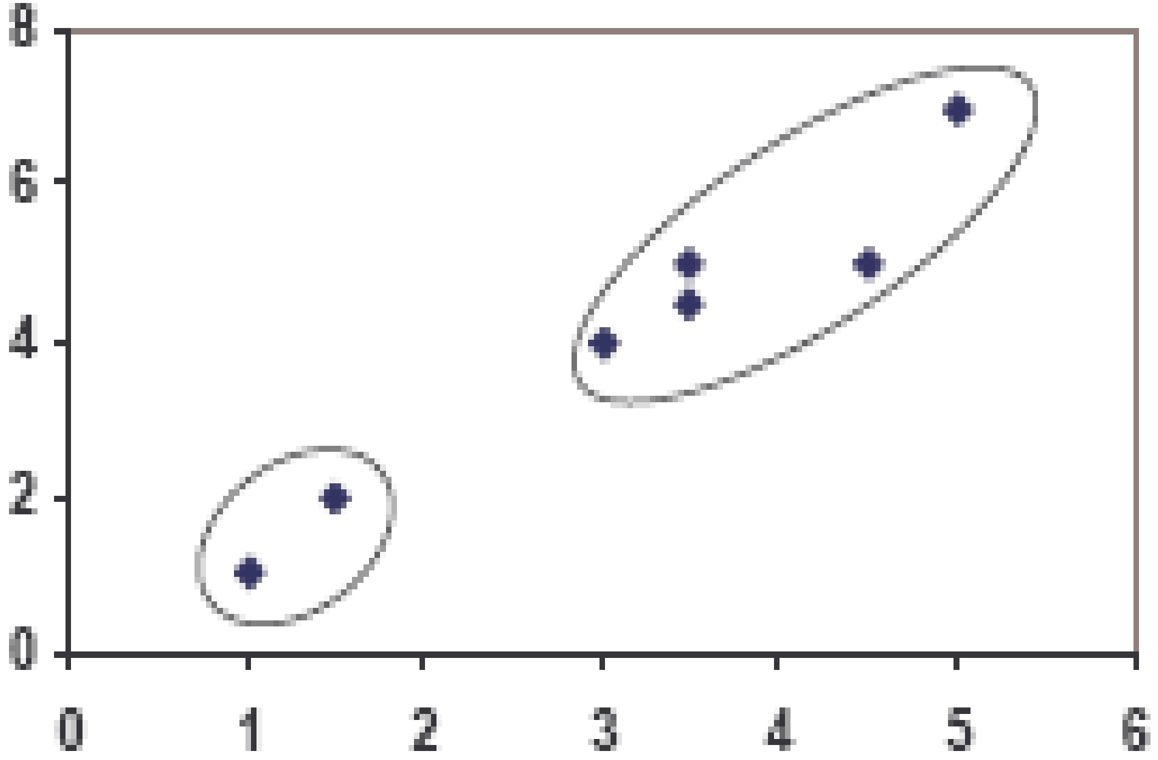
- **Step 4** :

  The clusters obtained are:

  {1,2} and {3,4,5,6,7}

- Therefore, there is no change in the cluster.
- Thus, the algorithm comes to a halt here and final result consist of 2 clusters {1,2} and {3,4,5,6,7}.

Individual	Centroid 1	Centroid 2
1	0.56	5.02
2	0. 56	3.92
3	3.05	1.42
4	6.66	2.20
5	4.16	0.41
6	4.78	0.61
7	3.75	0.72



8
6
4
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0
0
1
2
3
4
5
6

Loss function

Data (m examples): $\boldsymbol{x}^{(0)}, \boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m-1)} \in \mathbb{R}^n$

The centroid of ℓ-th cluster: $\boldsymbol{\mu}^{[\ell]} \in \mathbb{R}^n$ ($\ell = 0,1,\dots,k-1$)

Cluster indicator: $\boldsymbol{z}^{(i)} \in \mathbb{R}^k$ (an one hot vector, $i = 0,1,\dots,m-1$).

$$z_\ell^{(i)} = \begin{cases} 1 & \text{if the } i\text{–th example belongs to the } \ell\text{–th cluster,} \\ 0 & \text{otherwise.} \end{cases}$$

Loss function $J\left(\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}, \boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}\right)$

$$:= \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_\ell^{(i)} \left\|\boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]}\right\|^2$$

Non-zero only for the cluster $\boldsymbol{x}^{(i)}$ belongs to

Loss function

Data (m examples): $\boldsymbol{x}^{(0)}, \boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m-1)} \in \mathbb{R}^n$

The centroid of ℓ-th cluster: $\boldsymbol{\mu}^{[\ell]} \in \mathbb{R}^n$ $(\ell = 0,1,\dots,k-1)$

Cluster label: $\boldsymbol{z}^{(i)} \in \mathbb{R}^k$ (an one hot vector, $i = 0,1,\dots,m-1$).

$$z_\ell^{(i)} = \begin{cases} 1 & \text{if the } i\text{–th example belongs to the } \ell\text{–th cluster,} \\ 0 & \text{otherwise.} \end{cases}$$

Loss function $J\left(\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}, \boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}\right)$

$$:= \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_\ell^{(i)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]} \right\|^2$$

The square distance between $\boldsymbol{x}^{(i)}$
and the centroid of the cluster $\boldsymbol{x}^{(i)}$ belongs to

Update of cluster indicators:

Minimise $J\left(\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}, \boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}\right)$

$$\coloneqq \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_{\ell}^{(i)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]} \right\|^2$$

w.r.t. $\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}$ with $\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}$ fixed

$$z_{\ell}^{(i)} \leftarrow \begin{cases} 1 & \text{if } \ell = \operatorname*{argmin}_{\ell'} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell']} \right\|, \\ 0 & \text{otherwise.} \end{cases}$$

Update of cluster indicators:

Minimise $J\left(\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}, \boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}\right)$

$$:= \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_\ell^{(i)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]} \right\|^2$$

w.r.t. $\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}$ with $\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}$ fixed

$$z_\ell^{(i)} \leftarrow \begin{cases} 1 & \text{if } \ell = \operatorname*{argmin}_{\ell'} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell']} \right\|, \\ 0 & \text{otherwise.} \end{cases}$$

Updating the cluster indicator $\boldsymbol{z}^{(i)}$ of $\boldsymbol{x}^{(i)}$
with the cluster that has the nearest centroid to $\boldsymbol{x}^{(i)}$.

Update of centroids:

Minimise $J\left(\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}, \boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}\right)$

$$:= \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_\ell^{(i)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]} \right\|^2$$

w.r.t. $\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \dots, \boldsymbol{\mu}^{[k-1]}$ with $\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m-1)}$ fixed

The sum of the data points that belongs to cluster ℓ

$$\boldsymbol{\mu}^{[\ell]} \leftarrow \frac{\sum_{i=0}^{m-1} z_\ell^{(i)} \boldsymbol{x}^{(i)}}{\sum_{i=0}^{m-1} z_\ell^{(i)}}$$

The number of the data points that belongs to cluster ℓ

Update of centroids:

Minimise $J\left(\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m-1)}, \boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \ldots, \boldsymbol{\mu}^{[k-1]}\right)$

$$:= \sum_{i=0}^{m-1} \sum_{\ell=0}^{k-1} z_\ell^{(i)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{[\ell]} \right\|^2$$

w.r.t. $\boldsymbol{\mu}^{[0]}, \boldsymbol{\mu}^{[1]}, \ldots, \boldsymbol{\mu}^{[k-1]}$ with $\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m-1)}$ fixed

The sum of the data points that belongs to cluster ℓ

$$\boldsymbol{\mu}^{[\ell]} \leftarrow \frac{\sum_{i=0}^{m-1} z_\ell^{(i)} \boldsymbol{x}^{(i)}}{\sum_{i=0}^{m-1} z_\ell^{(i)}}$$

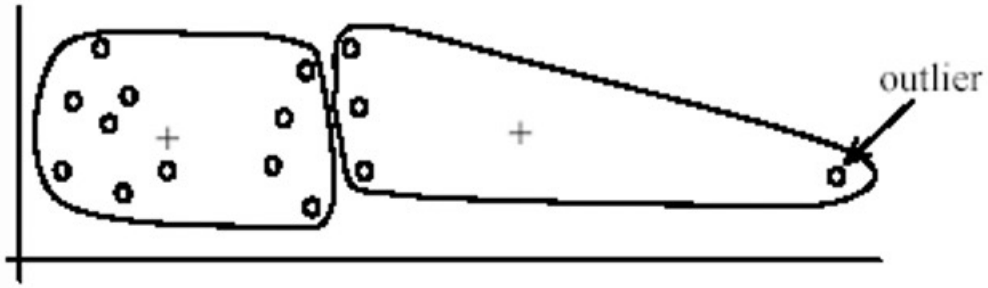
The mean of the data points that belongs to cluster ℓ

The number of the data points that belongs to cluster ℓ

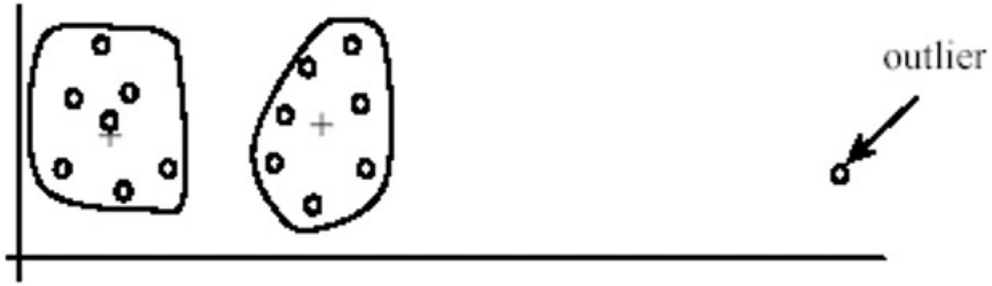
Strengths and weakness

- Strengths:
  - Simple: easy to understand and to implement
  - Efficient (linear complexity): Time complexity: $O(mkt)$, where m is the number of data points, k is the number of clusters and t is the number of iterations.
- Weakness:
  - The k needs to be specified.
  - Sensitive to outliers.
  - Not suitable for data with hyper-sphere structure.

Sensitive to outliers

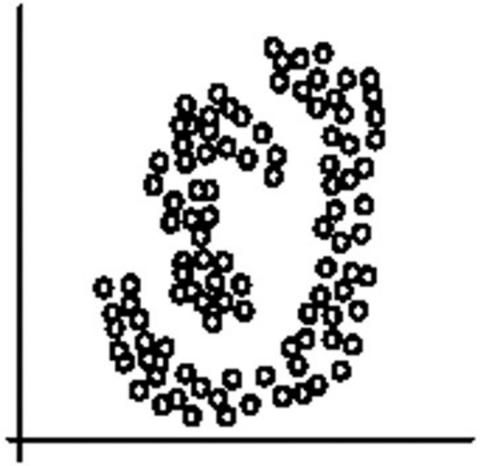


(A): Undesirable clusters

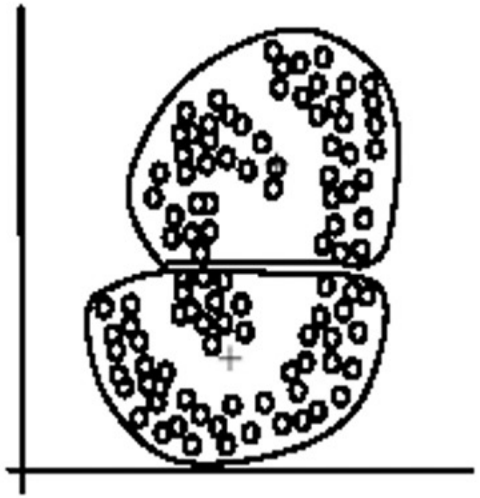


(B): Ideal clusters

Unsuitable for hyper-sphere



(A): Two natural clusters



(B): *k*-means clusters