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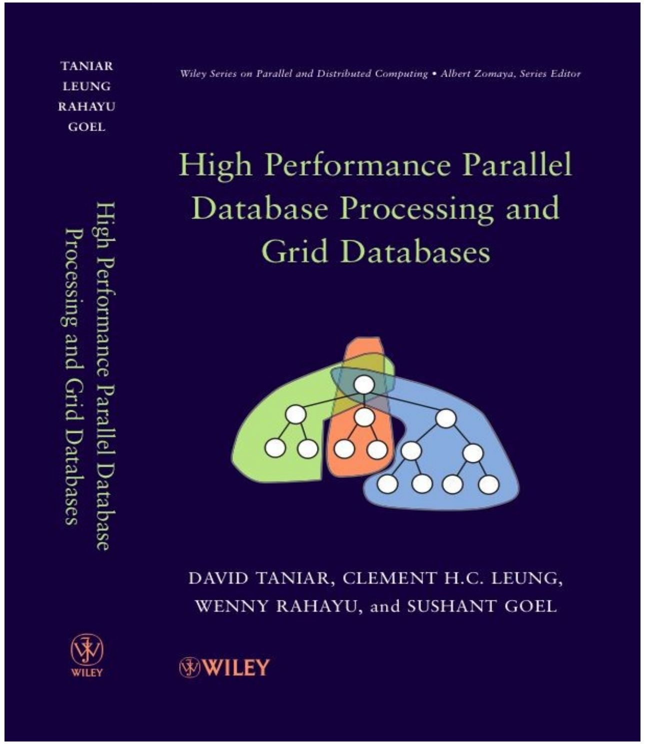
INFORMATION
TECHNOLOGY

Machine Learning: Clustering

Prajwol Sangat
Updated by Chee-Ming Ting (15 April 2022)

GROUP OF EIGHT AUSTRALIA

This week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Wiley Series on Parallel and Distributed Computing • Albert Zomaya, Series Editor

High Performance Parallel Database Processing and Grid Databases

DAVID TANIAR, CLEMENT H.C. LEUNG, WENNY RAHAYU, and SUSHANT GOEL

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Chapter 17 Parallel Clustering and Classification

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Machine Learning Fundamentals - Revision

- Supervised learning vs. unsupervised learning
- Supervised learning: discover patterns in the data that relate to data attributes with a target (class) attribute.
  - These patterns are then utilized to predict the values of the target attribute in future data instances.
- Unsupervised learning: The data have no target attribute.
  - Exploring the data to find some intrinsic structures in them.

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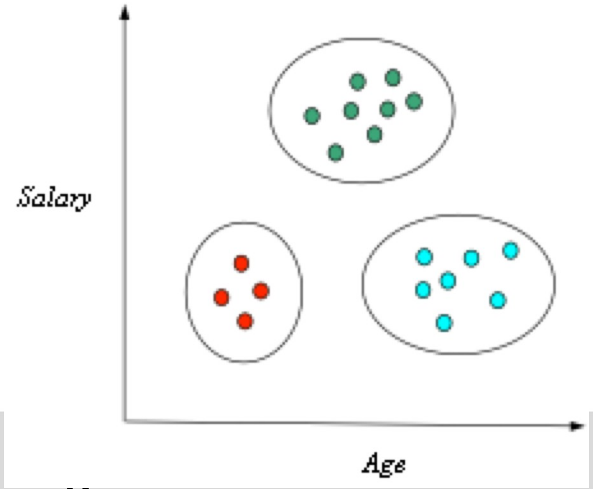
Clustering: an illustration

- Finds groups (or clusters) of data
- A cluster comprises a number of "similar" objects
- A member is closer to another member within the same group than to a member of a different group (data points are similar within a cluster, less similar between clusters)
- Groups have no category or label
- Unsupervised learning

Definition:
Membership of a data point
- Indicates which cluster a point belong to



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What is clustering for?

- Let’s see some real-life examples
- Example 1: Cluster students based on their examination marks, gender, heights, nationality, etc.
- Example 2: In marketing, segment customers according to their similarities
  - To do targeted marketing.

What is clustering for?

- Clustering is one of the most utilized machine learning techniques.
  - Used in almost every field, e.g., medicine, psychology, botany, sociology, biology, archeology, marketing, insurance, libraries, etc.
  - Most popular applications of clustering are:
    - recommendation engines,
    - market segmentation,
    - social network analysis,
    - image segmentation,
    - anomaly detection

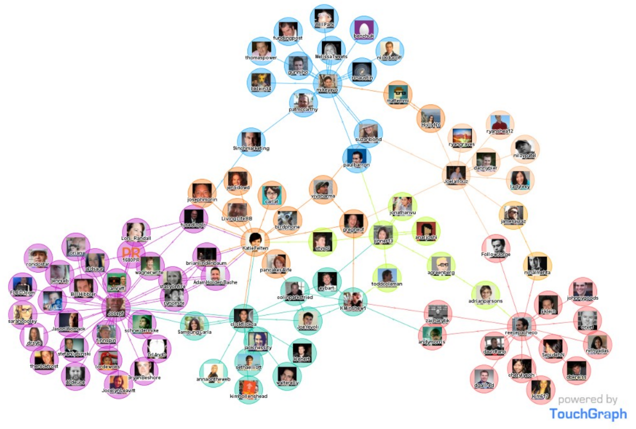


Image from: http://www.touchgraph.com/news

Some Applications in Digital Health

Partitioning of Heart sound signals

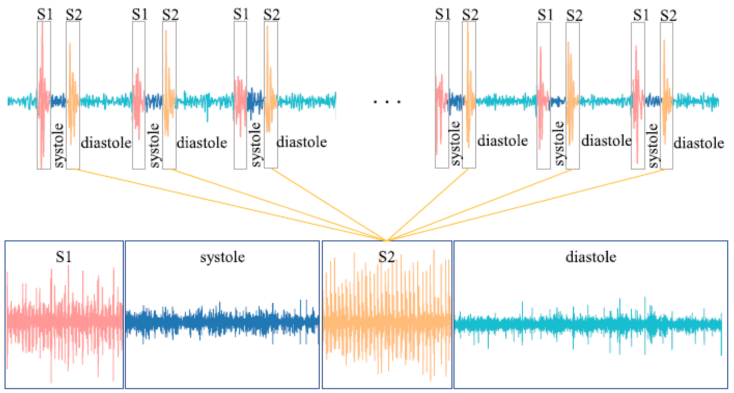
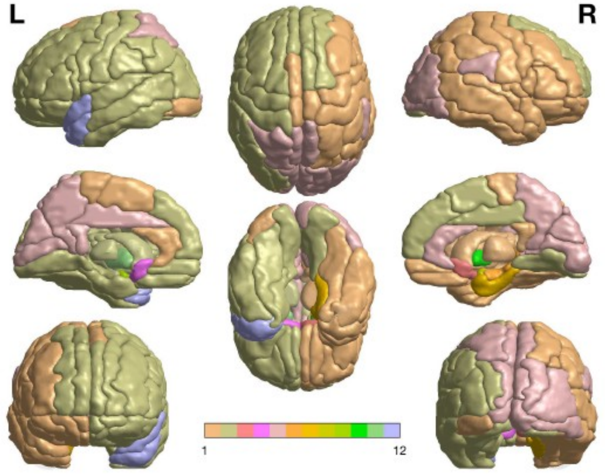


Fig. 2. Dynamic clustering of heart sound into four fundamental components.

Noman, Fuad, Sh-Hussain Salleh, Chee-Ming Ting. "A markov-switching model approach to heart sound segmentation and classification." *IEEE Journal of Biomedical and Health Informatics* 24, no. 3 (2019).

Partitioning of brain regions into clusters (communities)

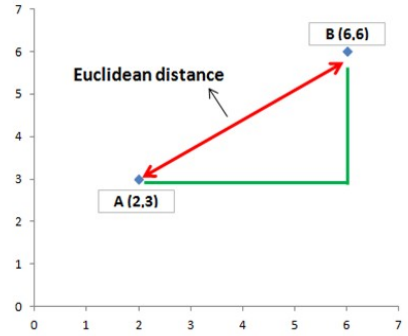


Ting, Chee-Ming, et al. "Detecting Dynamic Community Structure in Functional Brain Networks Across Individuals: A Multilayer Approach." *IEEE Trans Medical Imaging* (2020).

What is clustering for?

- **Similarities Measures**
  - Key factor in clustering is the similarity measure
  - Measure the degree of similarity between two objects
  - Distance measure: the shorter the distance, the more similar are the two objects (zero distance means identical objects)
  - Euclidean Dis

$$dist(x_i, x_j) = \sqrt{\sum_{k=1}^{h}\left(x_{ik} - x_{jk}\right)^2}$$



$$\textit{Euclidean distance } (a,b) = \sqrt{(a_1 - b_1)^2 + (a_2 - b_2)^2}$$

d(x1,x2)

$$= \sqrt{(x_{11} - x_{12})^2 + (x_{21} - x_{22})^2}$$

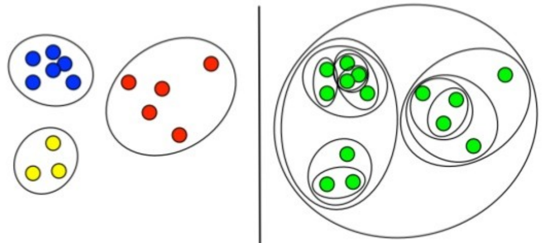
$$= \sqrt{(2-6)^2 + (3-6)^2}$$

h = number of features (or attributes)

Clustering Techniques

- **Goal of clustering:**
  - maximize intra-cluster similarity & minimize inter-cluster similarity
- **Hierarchical** clustering (nested clustering)
  - Seeks to build a hierarchy of clusters (clusters within clusters)
  - Strategies:
    - *Agglomerative*: Bottom up approach
    - *Divisive*: Top down approach.
- **Partitional** clustering (non-overlapping clustering)
  - Partitions the data objects based on a clustering criterion.
  - Places the data objects into clusters to maximise intra-cluster similarity.
  - So that data in a cluster are more similar to each other than to data in different clusters.

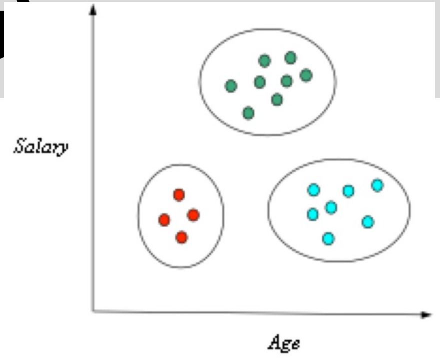
Partitional vs Hierarchical



Each sample(point) is assigned to a unique cluster

Creates a nested and hierarchical set of partitions/clusters

K-Means clustering (Partitional clustering



- K-means is a partitional clustering algorithm
- Let a set of data points (or instances) *D* be

  $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$,

  where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ir})$ is a vector in a real-valued space $X \subseteq R^r$, and *r* is the number of attributes (dimensions) in the data.
- The *k*-means algorithm partitions the given data into *k* clusters.
  - Each cluster has a cluster **center**, called **centroid**.
  - Centroid can be mean/average of member data points in each cluster
  - *k* is specified by the user

sub	salary	age
x1		
x2		
x3		
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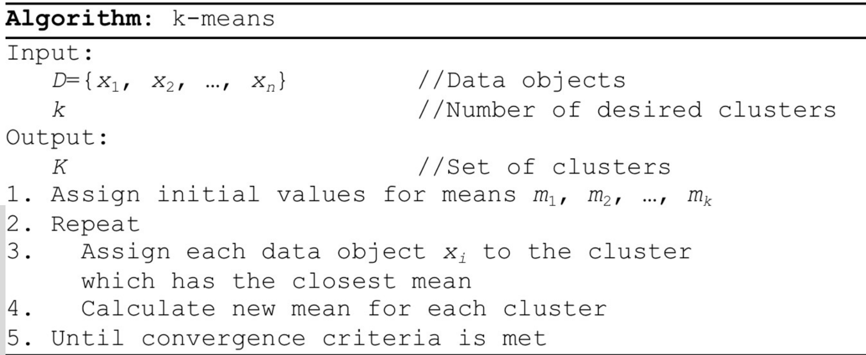
K-Means clustering

- **Algorithm** k-Means:
  - (**Initialization**) Specifies *k* number of clusters, and guesses the *k* seed cluster centroid
  - (**Assignment Step**) Assign each data point to the cluster with the closest centroid
    - Current clusters may receive or loose their members
  - (**Update Step**) Each cluster must re-calculate the mean (centroid) based on the newly assigned members
  - The process is repeated until the clusters are stable (no change of members)



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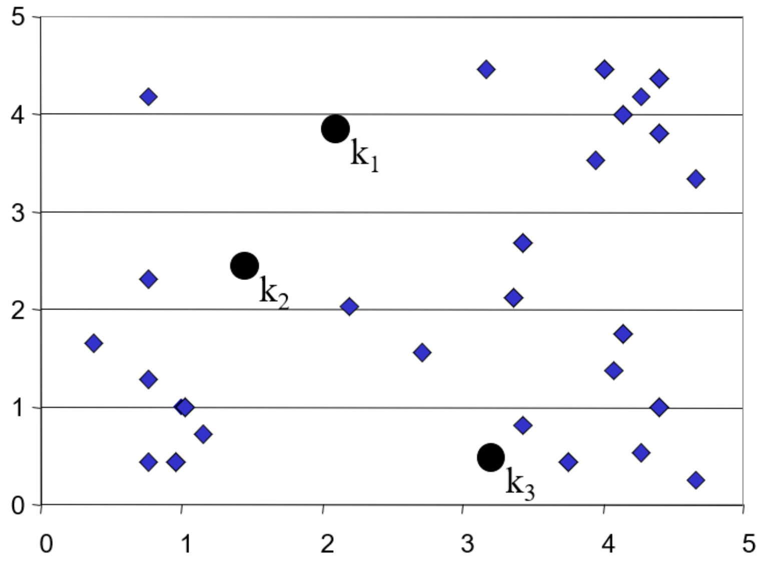
Algorithm: k-means
Input:
    $D=\{x_1, x_2, \dots, x_n\}$          //Data objects
    $k$                           //Number of desired clusters
Output:
    $K$                           //Set of clusters
1. Assign initial values for means $m_1, m_2, \dots, m_k$
2. Repeat
3.     Assign each data object $x_i$ to the cluster
       which has the closest mean
4.     Calculate new mean for each cluster
5. Until convergence criteria is met
```

K-Means Clustering: Step 1

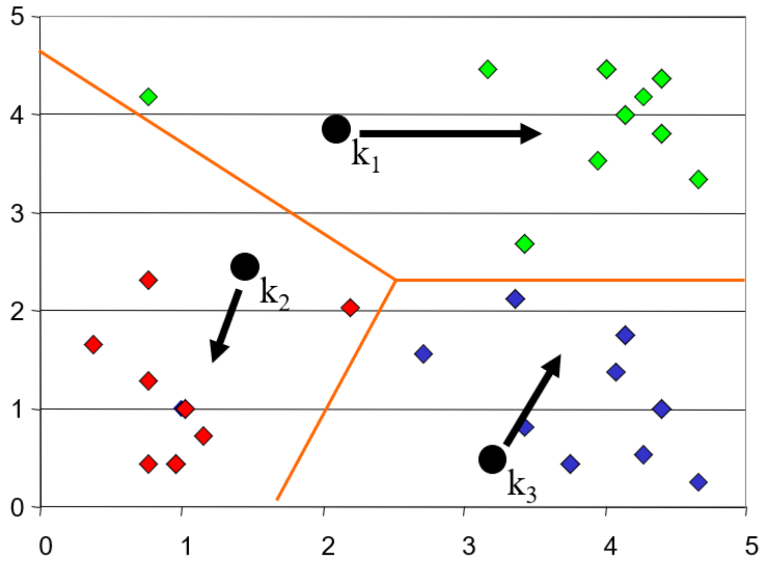
- Algorithm: k-means, Distance Metric: Euclidean Distance



- (**Initialization**)
  Specifies *k* number of clusters, and guesses the *k* seed cluster centroid

K-Means Clustering: Step 2

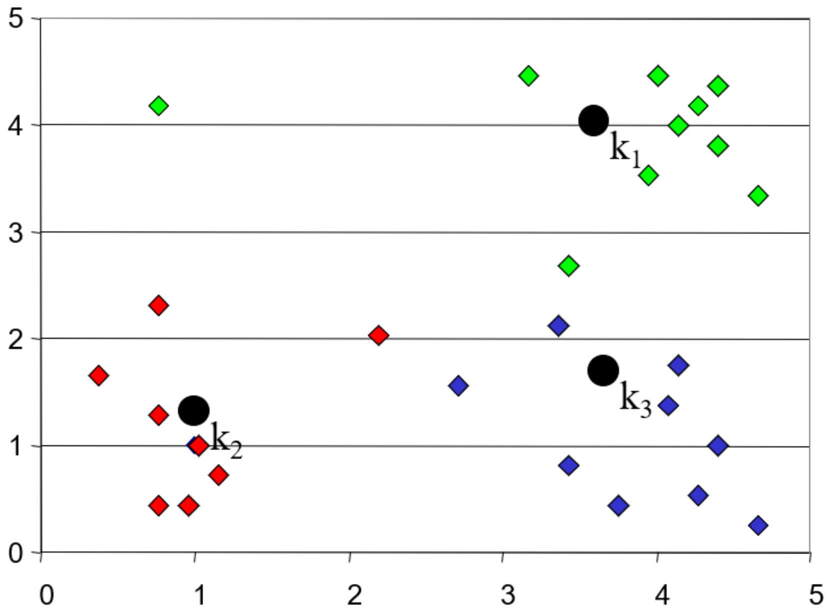
- Algorithm: k-means, Distance Metric: Euclidean Distance



(**Assignment Step**)
Iteratively looks at each data point and assigns it to the closest centroid

K-Means Clustering: Step 3

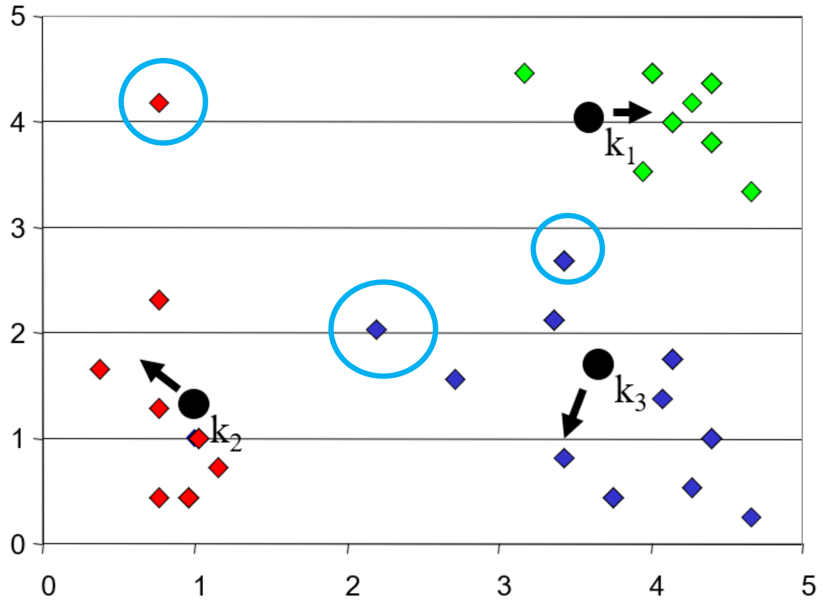
- Algorithm: k-means, Distance Metric: Euclidean Distance



(**Update Step**) Re-calculate the mean (centroid) for each cluster based on the membership of the cluster

K-Means Clustering: Step 4

- Algorithm: k-means, Distance Metric: Euclidean Distance

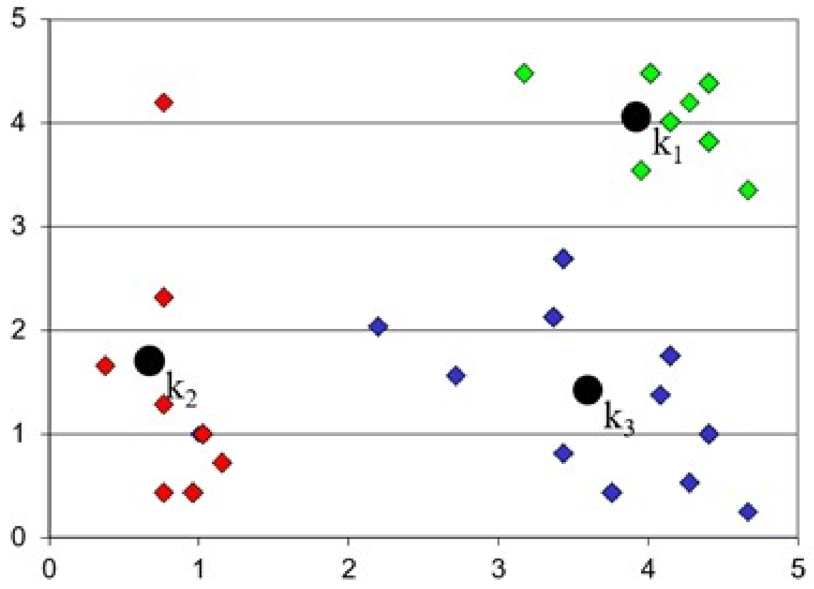


Iteratively looks at each data point and assigns it to the closest centroid,

Current clusters may receive or loose their members

K-Means Clustering: Step 5

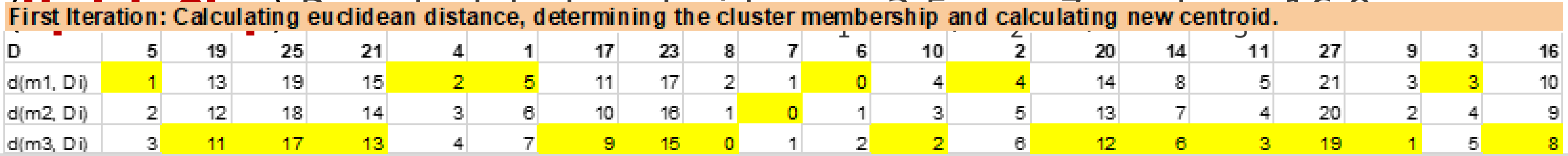
- Algorithm: k-means, Distance Metric: Euclidean Distance



Re-calculate the mean (centroid) for each cluster based on the membership of the cluster

k-Means: Step-By-Step Example

- Data D = {5, 19, 25, 21, 4, 1, 17, 23, 8, 7, 6, 10, 2, 20, 14, 11, 27, 9, 3, 16}
- Number of clusters: k = 3
- Initial centroids: m_1=6, m_2=7, and m_3=8
- **First Iteration**
  - (**Assignment Step)** Clusters:
    - C_1={1, 2, 3, 4, 5, 6}
    - C_2={7}
    - C_3={8, 9, 10, 11, 14, 16, 17, 19, 20, 21, 23, 25, 27}
  -

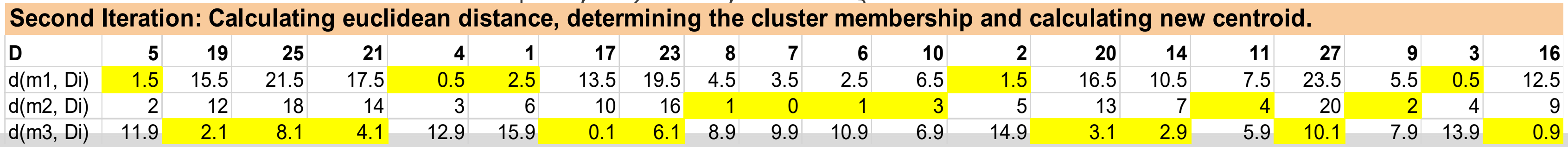


First Iteration: Calculating euclidean distance, determining the cluster membership and calculating new centroid.

D	5	19	25	21	4	1	17	23	8	7	6	10	2	20	14	11	27	9	3	16
d(m1, Di)	1	13	19	15	2	5	11	17	2	1	0	4	4	14	8	5	21	3	3	10
d(m2, Di)	2	12	18	14	3	6	10	16	1	0	1	3	5	13	7	4	20	2	4	9
d(m3, Di)	3	11	17	13	4	7	9	15	0	1	2	2	6	12	6	3	19	1	5	8

k-Means: Step-By-Step Example

- Clusters:
  - C_1={1, 2, 3, 4, 5, 6}
  - C_2={7}
  - C_3={8, 9, 10, 11, 14, 16, 17, 19, 20, 21, 23, 25, 27}
- New centroids: m_1=3.5, m_2=7, and m_3=16.9
- **Second Iteration**
  - Clusters:
    - C_1={1, 2, 3, 4, 5}
    - C_2={6, 7, 8, 9, 10, 11}
    - C_3={14, 16, 17, 19, 20, 21, 23, 25, 27}
  - Re-calculated centroids: m_1=3, m_2=8.5, and m_3=20.2



Second Iteration: Calculating euclidean distance, determining the cluster membership and calculating new centroid.

D	5	19	25	21	4	1	17	23	8	7	6	10	2	20	14	11	27	9	3	16
d(m1, Di)	1.5	15.5	21.5	17.5	0.5	2.5	13.5	19.5	4.5	3.5	2.5	6.5	1.5	16.5	10.5	7.5	23.5	5.5	0.5	12.5
d(m2, Di)	2	12	18	14	3	6	10	16	1	0	1	3	5	13	7	4	20	2	4	9
d(m3, Di)	11.9	2.1	8.1	4.1	12.9	15.9	0.1	6.1	8.9	9.9	10.9	6.9	14.9	3.1	2.9	5.9	10.1	7.9	13.9	0.9

k-Means: Step-By-Step Example

- Clusters:
  - $C_1=\{1, 2, 3, 4, 5\}$
  - $C_2=\{6, 7, 8, 9, 10, 11\}$
  - $C_3=\{14, 16, 17, 19, 20, 21, 23, 25, 27\}$
- New centroids: $m_1=3$, $m_2=8.5$, and $m_3=20.2$
- **Third Iteration**
  - Clusters:
    - $C_1=\{1, 2, 3, 4, 5\}$
    - $C_2=\{6, 7, 8, 9, 10, 11, 14\}$
    - $C_3=\{16, 17, 19, 20, 21, 23, 25, 27\}$
  - Re-calculated centroids: $m_1=3$, $m_2=9.29$, and $m_3=21$

Third Iteration: Calculating euclidean distance, determining the cluster membership and calculating new centroid.

D	**5**	**19**	**25**	**21**	**4**	**1**	**17**	**23**	**8**	**7**	**6**	**10**	**2**	**20**	**14**	**11**	**27**	**9**	**3**	**16**
d(m1, Di)	2	16	22	18	1	2	14	20	5	4	3	7	1	17	11	8	24	6	0	13
d(m2, Di)	3.5	10.5	16.5	12.5	4.5	7.5	8.5	14.5	0.5	1.5	2.5	1.5	6.5	11.5	5.5	2.5	18.5	0.5	5.5	7.5
d(m3, Di)	15.2	1.2	4.8	0.8	16.2	19.2	3.2	2.8	12.2	13.2	14.2	10.2	18.2	0.2	6.2	9.2	6.8	11.2	17.2	4.2

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k-Means: Step-By-Step Example

- Clusters:
  - C_1={1, 2, 3, 4, 5}
  - C_2={6, 7, 8, 9, 10, 11, 14}
  - C_3={16, 17, 19, 20, 21, 23, 25, 27}
- New centroids: m_1=3, m_2=9.29, and m_3=21
- **Fourth Iteration**
  - Clusters:
    - C_1={1, 2, 3, 4, 5, 6}
    - C_2={7, 8, 9, 10, 11, 14}
    - C_3={16, 17, 19, 20, 21, 23, 25, 27}
  - Re-calculated centroids: m_1=3.5, m_2=9.83, and m_3=21

Fourth Iteration: Calculating euclidean distance, determining the cluster membership and calculating new centroid.

D	**5**	**19**	**25**	**21**	**4**	**1**	**17**	**23**	**8**	**7**	**6**	**10**	**2**	**20**	**14**	**11**	**27**	**9**	**3**	**16**
d(m1, Di)	2	16	22	18	1	2	14	20	5	4	3	7	1	17	11	8	24	6	0	13
d(m2, Di)	4.3	9.7	15.7	11.7	5.3	8.3	7.7	13.7	1.3	2.3	3.3	0.7	7.3	10.7	4.7	1.7	17.7	0.3	6.3	6.7
d(m3, Di)	16.0	2.0	4.0	0.0	17.0	20.0	4.0	2.0	13.0	14.0	15.0	11.0	19.0	1.0	7.0	10.0	6.0	12.0	18.0	5.0

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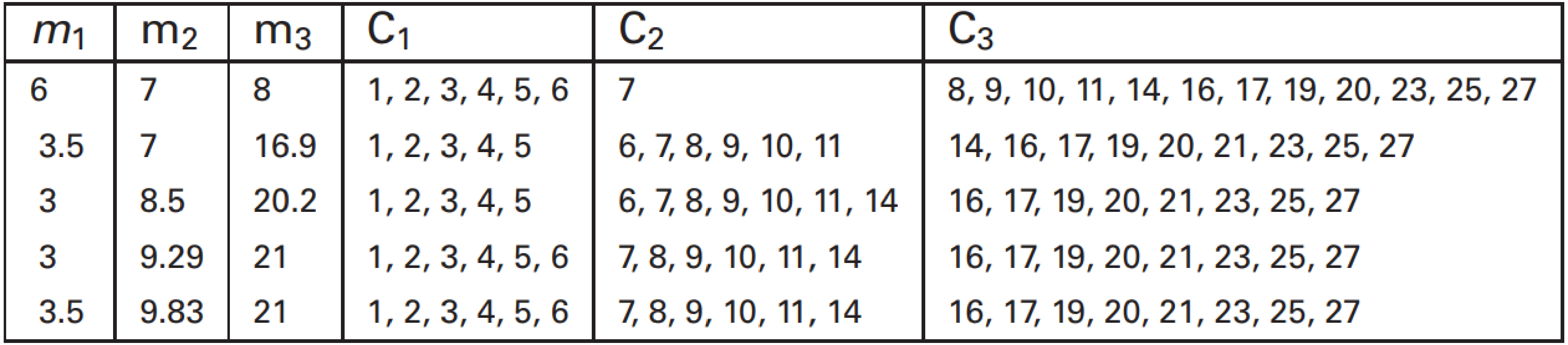
k-Means: Step-By-Step Example

- Clusters:
  - C_1={1, 2, 3, 4, 5, 6}
  - C_2={7, 8, 9, 10, 11, 14}
  - C_3={16, 17, 19, 20, 21, 23, 25, 27}
- New centroids: m_1=3.5, m_2=9.83, and m_3=21
- **Fifth Iteration**
  - No data movement from clusters (Process Terminated)



m_1	m_2	m_3	C_1	C_2	C_3
6	7	8	1, 2, 3, 4, 5, 6	7	8, 9, 10, 11, 14, 16, 17, 19, 20, 23, 25, 27
3.5	7	16.9	1, 2, 3, 4, 5	6, 7, 8, 9, 10, 11	14, 16, 17, 19, 20, 21, 23, 25, 27
3	8.5	20.2	1, 2, 3, 4, 5	6, 7, 8, 9, 10, 11, 14	16, 17, 19, 20, 21, 23, 25, 27
3	9.29	21	1, 2, 3, 4, 5, 6	7, 8, 9, 10, 11, 14	16, 17, 19, 20, 21, 23, 25, 27
3.5	9.83	21	1, 2, 3, 4, 5, 6	7, 8, 9, 10, 11, 14	16, 17, 19, 20, 21, 23, 25, 27

Evaluating K-Means Clusters

- One common measure is sum of squared error (SSE)

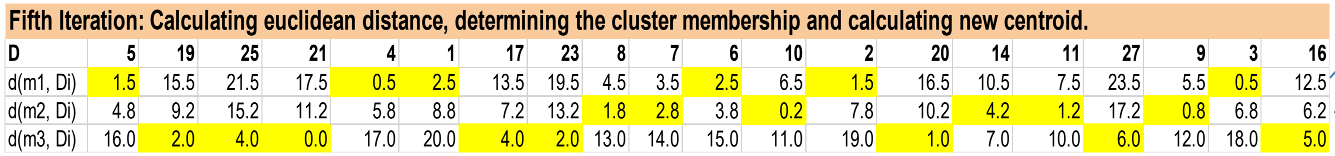
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

- x is a data point in cluster C_i
- m_i is the centroid of cluster C_i

SSE measures how close the assigned data points to centroids

- small value → maximized intra-cluster similarity

Example: How to calculate SSE?



Fifth Iteration: Calculating euclidean distance, determining the cluster membership and calculating new centroid.

D	5	19	25	21	4	1	17	23	8	7	6	10	2	20	14	11	27	9	3	16
d(m1, Di)	1.5	15.5	21.5	17.5	0.5	2.5	13.5	19.5	4.5	3.5	2.5	6.5	1.5	16.5	10.5	7.5	23.5	5.5	0.5	12.5
d(m2, Di)	4.8	9.2	15.2	11.2	5.8	8.8	7.2	13.2	1.8	2.8	3.8	0.2	7.8	10.2	4.2	1.2	17.2	0.8	6.8	6.2
d(m3, Di)	16.0	2.0	4.0	0.0	17.0	20.0	4.0	2.0	13.0	14.0	15.0	11.0	19.0	1.0	7.0	10.0	6.0	12.0	18.0	5.0

Clusters:
C_1={1, 2, 3, 4, 5, 6}
C_2={7, 8, 9, 10, 11, 14}
C_3={16, 17, 19, 20, 21, 23, 25, 27}
centroids: m_1=3.5, m_2=9.83, and m_3=21

$\sum_{x \in C_1} d^2(n$

+

$\sum_{x \in C_2} d^2(m$

+

$\sum_{x \in C_3} d^2(m$

K-Means Clustering

- The number of clusters *k* is predefined. The algorithm does not discover the ideal number of clusters. During the process, the number of clusters remains fixed – it does not shrink nor expand.
- The final composition of clusters is very sensitive to the choice of initial centroid values. Different initialisations may result in (

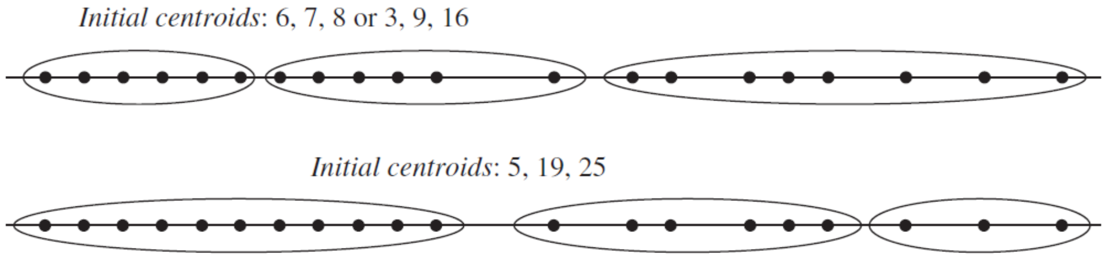

Initial centroids: 6, 7, 8 or 3, 9, 16
Initial centroids: 5, 19, 25

Figure 17.4 Different clustering results for different initial centroids

K-Means Clustering: Pros and Cons

Pros

- Simple and fast for low dimensional data (time complexity of K Means is linear i.e. O(n))
- Scales to large data sets
- Easily adapts to new data points

🕐 **Cons**

- 🕐 It will not identify outliers
- Restricted to data which has the notion of a centre (centroid)

K-means clustering

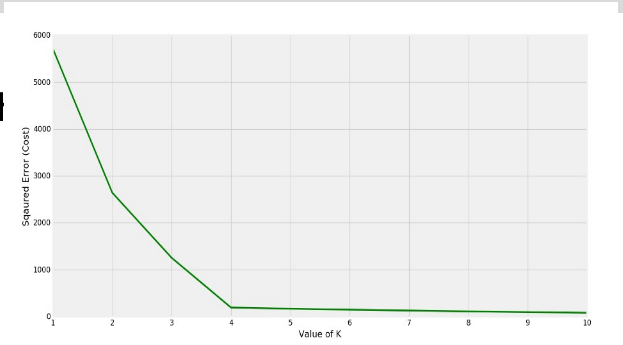
- **Exercise 1**
  - Data D = {8, 11, 12, 14, 16, 17, 24, 28}
  - Number of clusters: $k = 3$
  - Initial centroids: m_1=11, m_2=12, and m_3=28
  - Use the k-means *serial* algorithm to cluster the data in three clusters

Finding Optimal number of the clusters

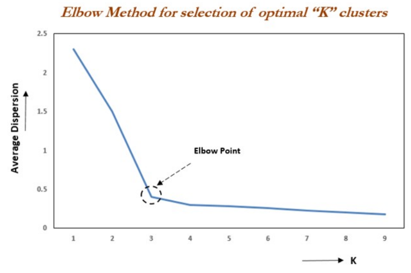
- As k increases, clusters become smaller.
- The neighbouring clusters become less distinct from one anot

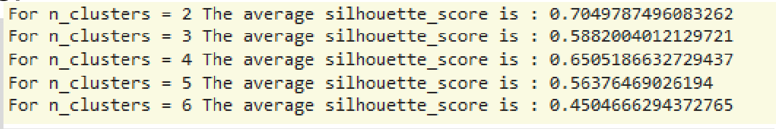
.

- **How to choose an optimal k?**
  - Elbow Method
    - Plot sum of squared errors as a function of k (a scree plot)
    - Select the value of k at the “elbow” ie the point after which the SSE start decreasing in a linear fashion.
  - Silhouette analysis
    - Measure of how close each point in one cluster is compared to points in the neighbouring clusters and provides a way to assess number of clusters.
    - If most points have a high silhouette value, then the clustering configuration is appropriate.
    - If many points have a low or negative value, then the clustering configuration may have too many or too few clusters.



optimal value for k = 4





```
For n_clusters = 2 The average silhouette_score is : 0.7049787496083262
For n_clusters = 3 The average silhouette_score is : 0.5882004012129721
For n_clusters = 4 The average silhouette_score is : 0.6505186632729437
For n_clusters = 5 The average silhouette_score is : 0.56376469026194
For n_clusters = 6 The average silhouette_score is : 0.4504666294372765
```

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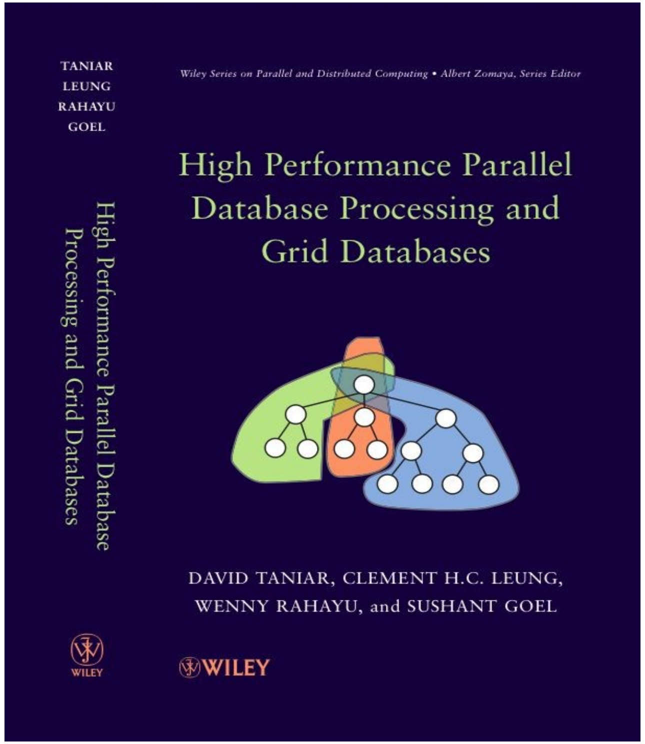
DEMO

https://instaview365.com/request-a-demo/

This week



Chapter 17 Parallel Clustering and Classification

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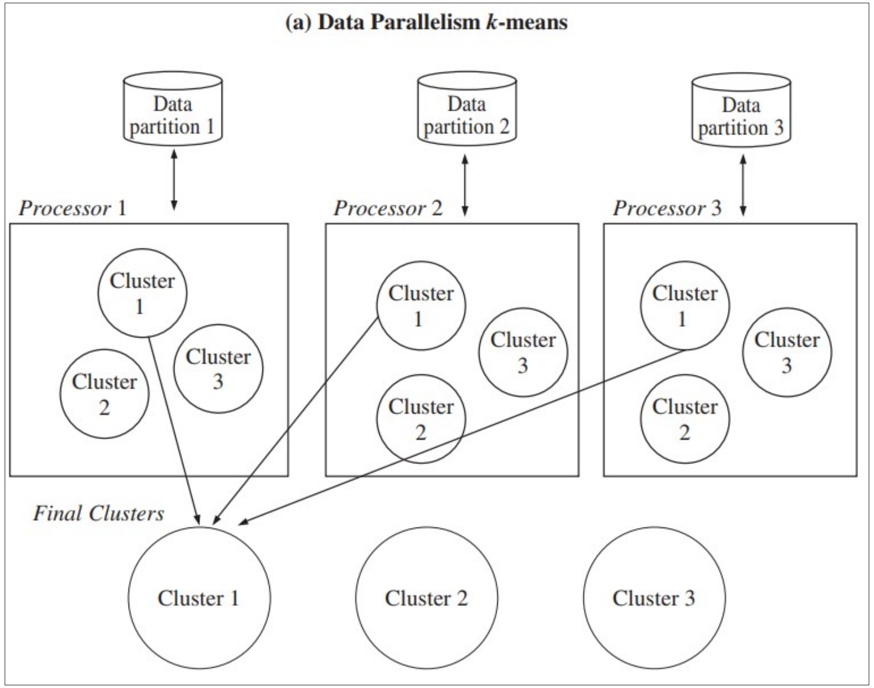
Parallel K-means clustering

- ***Data parallelism*** of k-means

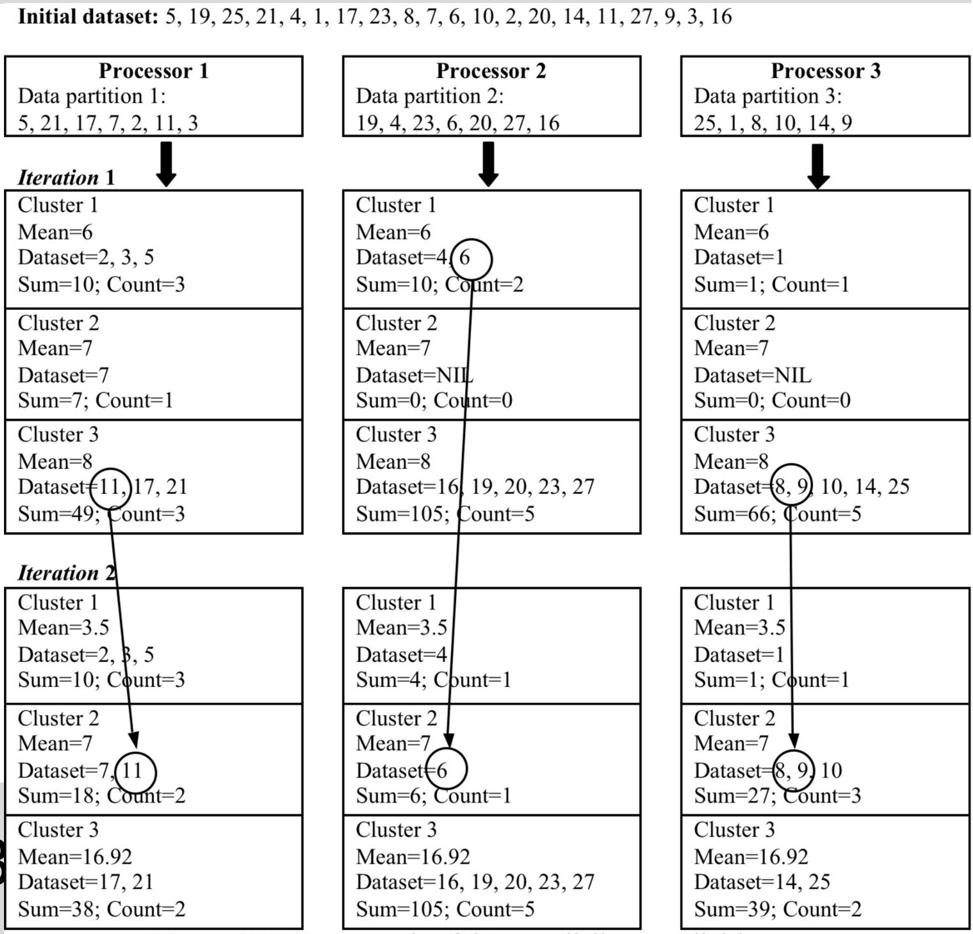
- ❑ Create parallelism from the beginning because of partitioning of the dataset.
- ❑ Data is partitioned into multiple partition
- ❑ Each processor will work independently to create three clusters
- ❑ The final clusters from each processor are respectively united



Parallel K-means

■ *Data parallelism*

- ❑ Example: Data partitioning using round-robin
- ❑ Initial centroids: 6, 7, 8
- ❑ Each processor will run k_Means locally
- ❑ At the end of each iteration, info about sum & count of data points in each local cluster is shared to calculate new centroid/mean
- ❑ Data does not move among processors (it stays where it was allocated initially)
- ❑ Data move across clusters within same processor



Initial dataset: 5, 19, 25, 21, 4, 1, 17, 23, 8, 7, 6, 10, 2, 20, 14, 11, 27, 9, 3, 16

Processor 1	**Processor 2**	**Processor 3**
Data partition 1: 5, 21, 17, 7, 2, 11, 3	Data partition 2: 19, 4, 23, 6, 20, 27, 16	Data partition 3: 25, 1, 8, 10, 14, 9

***Iteration* 1**

Cluster 1 Mean=6 Dataset=2, 3, 5 Sum=10; Count=3	Cluster 1 Mean=6 Dataset=4, 6 Sum=10; Count=2	Cluster 1 Mean=6 Dataset=1 Sum=1; Count=1
Cluster 2 Mean=7 Dataset=7 Sum=7; Count=1	Cluster 2 Mean=7 Dataset=NIL Sum=0; Count=0	Cluster 2 Mean=7 Dataset=NIL Sum=0; Count=0
Cluster 3 Mean=8 Dataset=11, 17, 21 Sum=49; Count=3	Cluster 3 Mean=8 Dataset=16, 19, 20, 23, 27 Sum=105; Count=5	Cluster 3 Mean=8 Dataset=8, 9, 10, 14, 25 Sum=66; Count=5

***Iteration* 2**

Cluster 1 Mean=3.5 Dataset=2, 3, 5 Sum=10; Count=3	Cluster 1 Mean=3.5 Dataset=4 Sum=4; Count=1	Cluster 1 Mean=3.5 Dataset=1 Sum=1; Count=1
Cluster 2 Mean=7 Dataset=7, 11 Sum=18; Count=2	Cluster 2 Mean=7 Dataset=6 Sum=6; Count=1	Cluster 2 Mean=7 Dataset=8, 9, 10 Sum=27; Count=3
Cluster 3 Mean=16.92 Dataset=17, 21 Sum=38; Count=2	Cluster 3 Mean=16.92 Dataset=16, 19, 20, 23, 27 Sum=105; Count=5	Cluster 3 Mean=16.92 Dataset=14, 25 Sum=39; Count=2

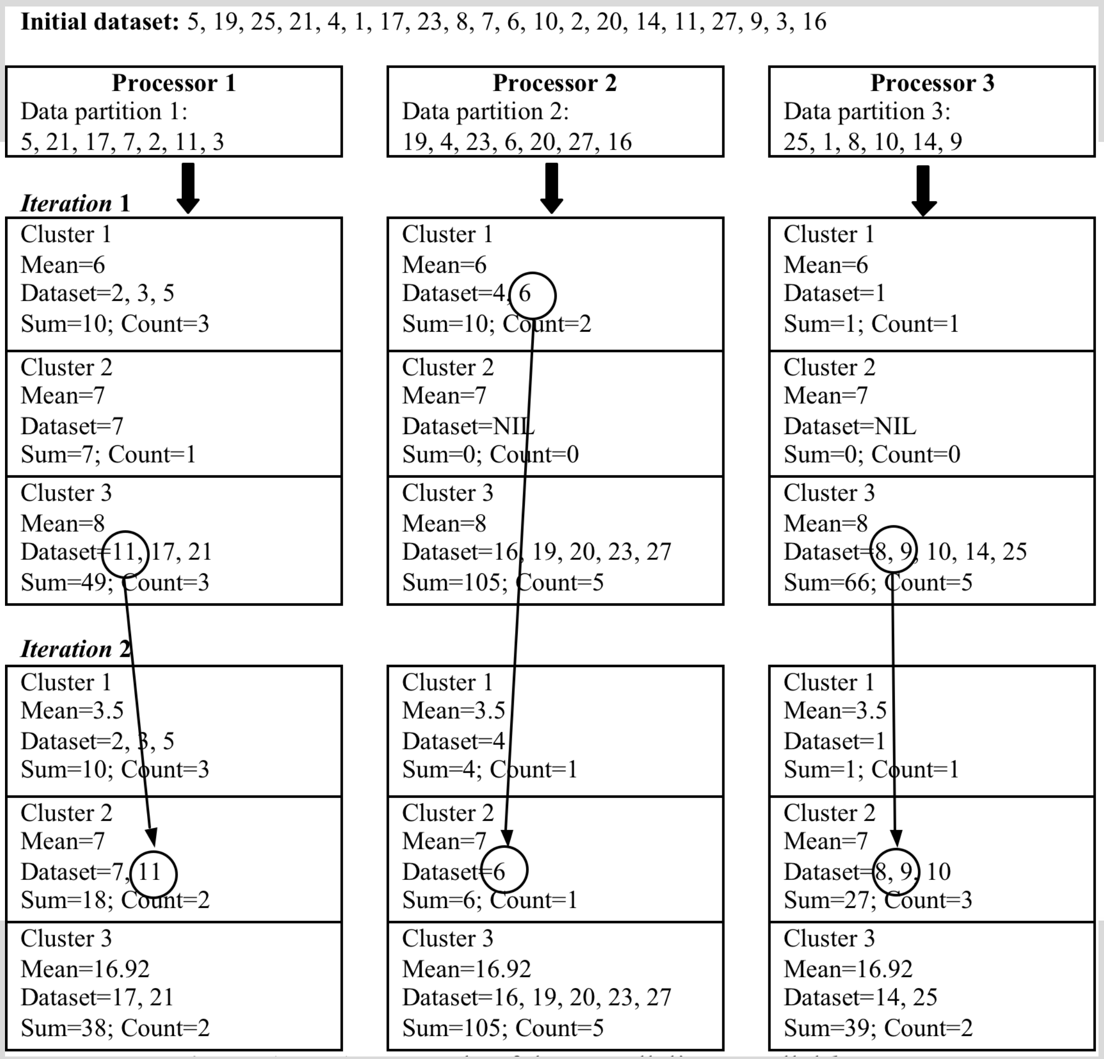
Parallel K-means

- ***Data parallelism***

k-means

Processor 1: Cluster 1 = 2, 3, 5
Cluster 2 = 7, 11
Cluster 3 = 17, 21
Processor 2: Cluster 1 = 4, 6
Cluster 2 = NIL
Cluster 3 = 16, 19, 20, 23, 27
Processor 3: Cluster 1 = 1
Cluster 2 = 8, 9, 10, 14
Cluster 3 = 25

Cluster 1 = 1, 2, 3, 4, 5, 6
Cluster 2 = 7, 8, 9, 10, 11, 14
Cluster 3 = 16, 17, 19, 20, 21, 23, 25, 27



Initial dataset: 5, 19, 25, 21, 4, 1, 17, 23, 8, 7, 6, 10, 2, 20, 14, 11, 27, 9, 3, 16

Processor 1
Data partition 1:
5, 21, 17, 7, 2, 11, 3

Processor 2
Data partition 2:
19, 4, 23, 6, 20, 27, 16

Processor 3
Data partition 3:
25, 1, 8, 10, 14, 9

***Iteration* 1**

Processor 1:
Cluster 1
Mean=6
Dataset=2, 3, 5
Sum=10; Count=3
Cluster 2
Mean=7
Dataset=7
Sum=7; Count=1
Cluster 3
Mean=8
Dataset=11, 17, 21
Sum=49; Count=3

Processor 2:
Cluster 1
Mean=6
Dataset=4, 6
Sum=10; Count=2
Cluster 2
Mean=7
Dataset=NIL
Sum=0; Count=0
Cluster 3
Mean=8
Dataset=16, 19, 20, 23, 27
Sum=105; Count=5

Processor 3:
Cluster 1
Mean=6
Dataset=1
Sum=1; Count=1
Cluster 2
Mean=7
Dataset=NIL
Sum=0; Count=0
Cluster 3
Mean=8
Dataset=8, 9, 10, 14, 25
Sum=66; Count=5

***Iteration* 2**

Processor 1:
Cluster 1
Mean=3.5
Dataset=2, 3, 5
Sum=10; Count=3
Cluster 2
Mean=7
Dataset=7, 11
Sum=18; Count=2
Cluster 3
Mean=16.92
Dataset=17, 21
Sum=38; Count=2

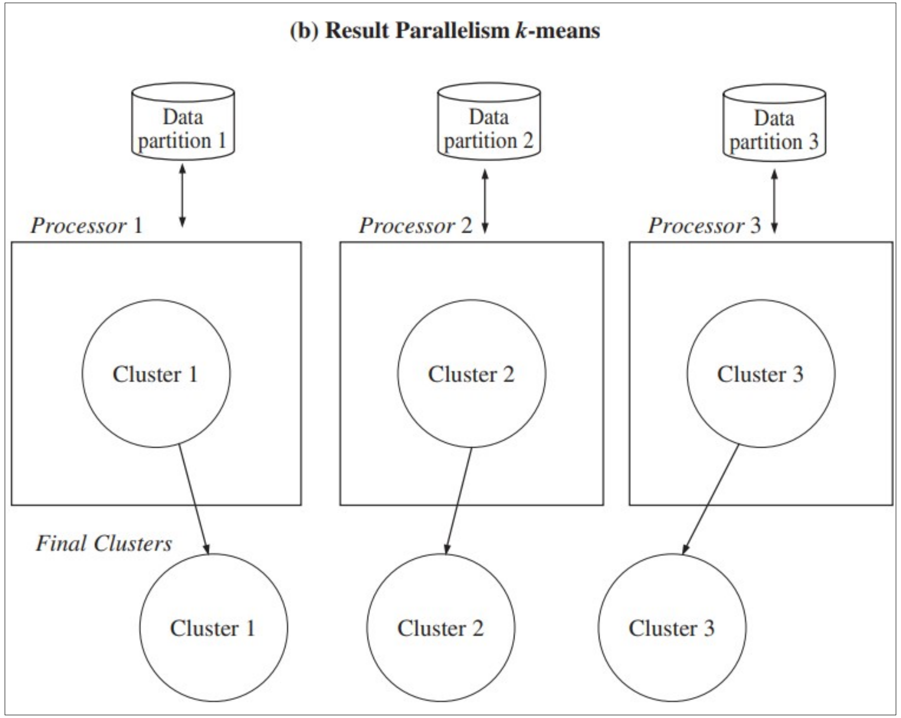
Processor 2:
Cluster 1
Mean=3.5
Dataset=4
Sum=4; Count=1
Cluster 2
Mean=7
Dataset=6
Sum=6; Count=1
Cluster 3
Mean=16.92
Dataset=16, 19, 20, 23, 27
Sum=105; Count=5

Processor 3:
Cluster 1
Mean=3.5
Dataset=1
Sum=1; Count=1
Cluster 2
Mean=7
Dataset=8, 9, 10
Sum=27; Count=3
Cluster 3
Mean=16.92
Dataset=14, 25
Sum=39; Count=2

Parallel K-means clustering

- ***Result Parallelism*** of k-means

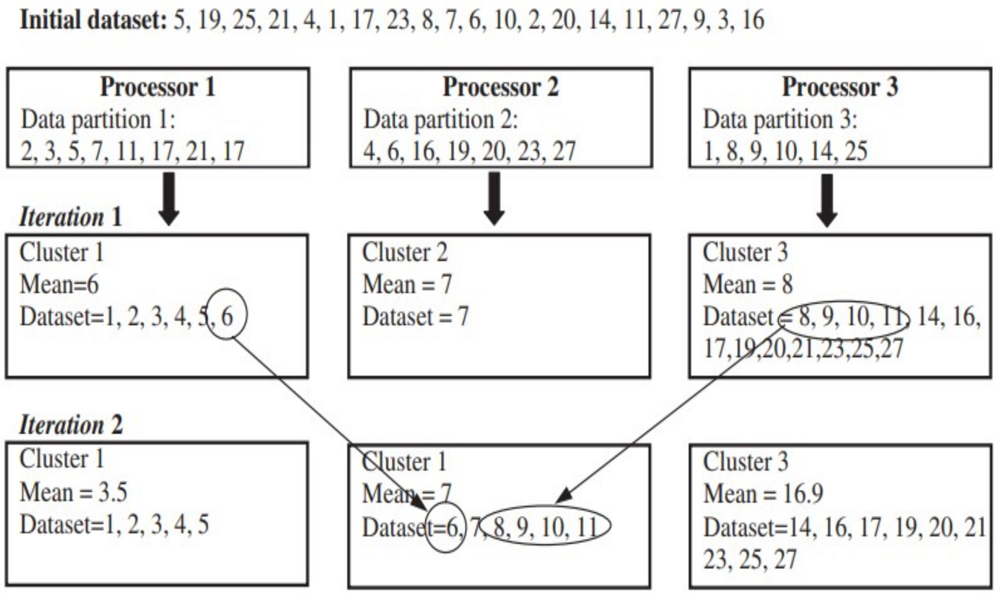
- Focuses on clusters partitioning
- Each processor will work on a particular target cluster
- For example, from the very beginning, processor 1 will produce only one cluster assigned to it, that is cluster 1.
- During the iteration, the memberships of cluster can change. -→ data movement across processors



Parallel K-means

- ***Result parallelism*** k-means

- Example: Data partitioning using round-robin
- Each processor is allocated only one cluster.
- Three initial means are distributed among the three processors,
- Data points may move from one processor to another at each iteration to join a cluster in a different processor
- Since a cluster is processed by one processor, calculating the mean is straightforward because all the data points within a cluster are located at the same processor

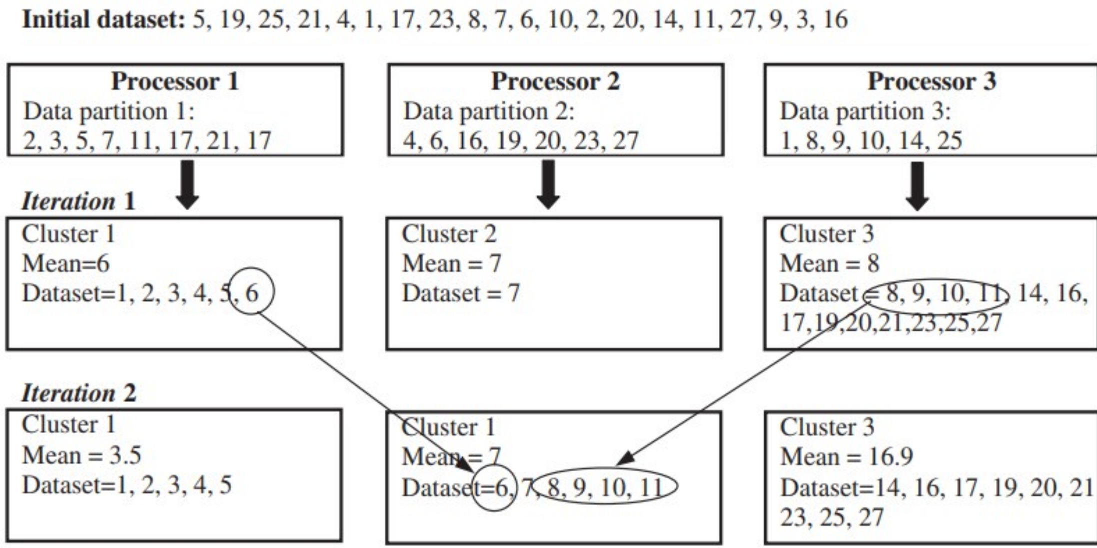


Parallel K-means

- ***Result parallelism*** k-means

At the end, the final cluster result is basically the union of all local clusters from each processor.

Processor 1 cluster 1 = 1, 2, 3, 4, 5, 6
Processor 2 cluster 2 = 7, 8, 9, 10, 11, 14
Processor 3 cluster 3 = 16, 17, 19, 20, 21, 23, 25, 27



Data parallelism vs Result parallelism

Data parallelism

- Parallelism is created due to the fragmentation of initial input data
- Each processor focuses on its partition of the dataset
- Final results are formed by combining all local results produced by individual processors.

Result parallelism

- Focuses on the fragmentation of the results, not necessarily the input data.
- Each processor focuses on its target result partition.

What have we learnt today?

- Partitional (k-means) to attain meaningful groups of data
- Algorithmic examples for clustering of data