

MONASH INFORMATION TECHNOLOGY

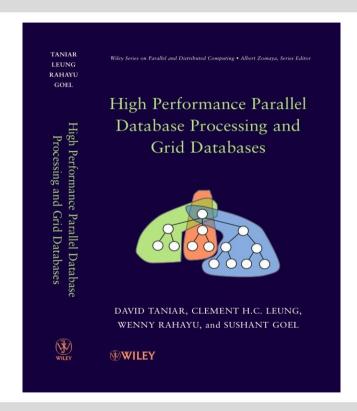
Machine Learning: Clustering

Prajwol Sangat





This week



Chapter 17 Parallel Clustering and Classification

- 17.1 Clustering and Classification
- 17.2 Parallel Clustering
- 17.3 Parallel Classification
- 17.4 Summary
- 17.5 Bibliographical Notes
- 17.6 Exercises



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.

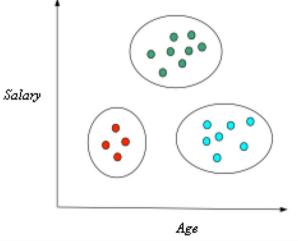


Clustering: an illustration

- 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

- Groups have no category or labe
- Unsupervised learning





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.

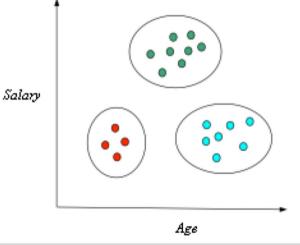


Clustering: an illustration

- Finds groups (or clusters) of data
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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



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, the more similar are the two objects (zero distance means identical objects)
- Euclidean Distance:

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



Clustering Techniques

Hierarchical clustering

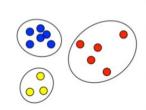
- Seeks to build a hierarchy of cluste
- Strategies:
 - *Agglomerative*: Bottom up approach
 - Divisive: Top down approach.

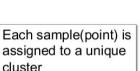
■ Partitional clustering

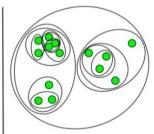
- Partitions the data objects based on a clustering criterion.
- Places the data objects into clusters to maximise intracluster similarity.

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Partitional vs Hierarchical







Creates a nested and hierarchical set of partitions/clusters

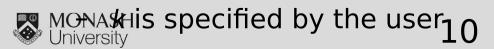
K-Means clustering (Partitional clustering)

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

$$\{\mathbf{x}_{1}, \mathbf{x}_{2}, ..., \mathbf{x}_{n}\},\$$

where $\mathbf{x}_i = (x_{i1}, x_{i2}, ..., x_{ir})$ 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.



K-Means clustering

Algorithm k-Means:

- Specifies k number of clusters, and guesses the k seed cluster centroid
- Iteratively looks at each data point and assigns it to the closest centroid
- Current clusters may receive or loose their members
- Each cluster must re-calculate the mean (centroid)
- The process is repeated until the clusters are stable (no

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change of members)
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Algorithm: k-means

Input:

D={x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>n</sub>} //Data objects

k //Number of desired clusters

Output:

K //Set of clusters

1. Assign initial values for means m<sub>1</sub>, m<sub>2</sub>, ..., m<sub>k</sub>

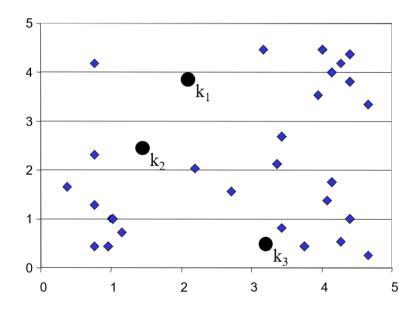
2. Repeat

3. Assign each data object x<sub>i</sub> to the cluster which has the closest mean

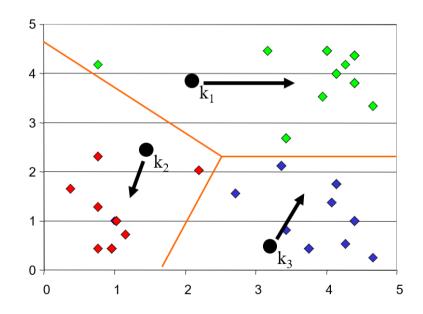
4. Calculate new mean for each cluster
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5. Until convergence criteria is met

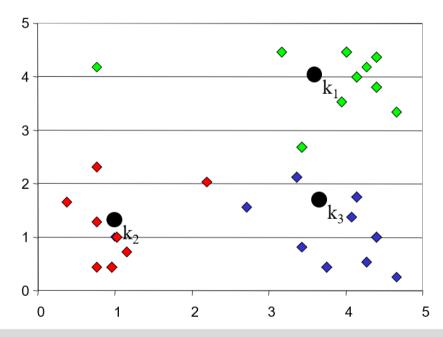




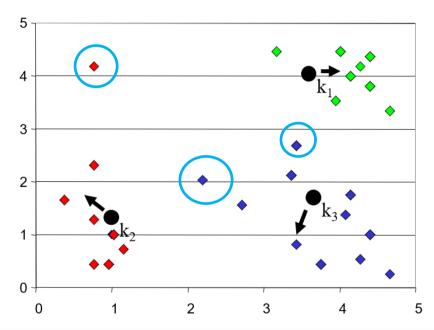




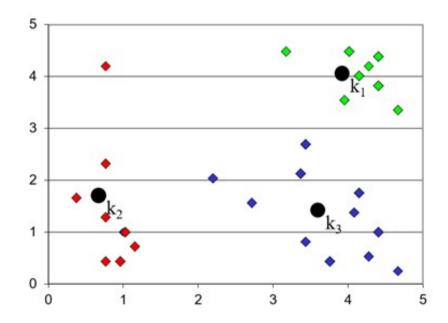














- Data $D = \{5, 19, 25, 21, 4, 1, 17, 23, 8, 7, 6, 10, 2, 20, 14, 11, 27, 9, 3, 16\}$
- Number of clusters: k = 3
- Initial centroids: $m_1=6$, $m_2=7$, and $m_3=8$

First Iteration

- 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}
- Re-calculated centroids: m_1 =3.5, m_2 =7, and m_3 =16.9



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First Iteration

- Clusters:
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- 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



- 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



- 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



- Clusters:

$$C_1 = \{1, 2, 3, 4, 5, 6\}$$

$$C_2 = \{7, 8, 9, 10, 11, 14\}$$

- 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

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

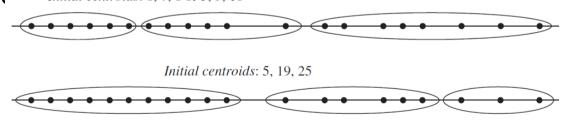


Figure 17.4 Different clustering results for different initial centroids



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

(P) Cons

- ② 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 for one another.

How to choose an optimal k?

- Elbow Method
 - Sum of squared errors as a function of k (a scree plot)

optimal value for k

- Silhouette analysis
 - Measure of how close each point in one cluster is to points in the neighbouring clusters and thus provides a way to assess number of clusters = 2 The average silhouette_score is : 0.7049787496083262

```
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
```

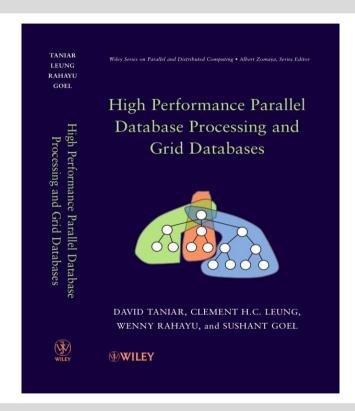


DEMO





This week



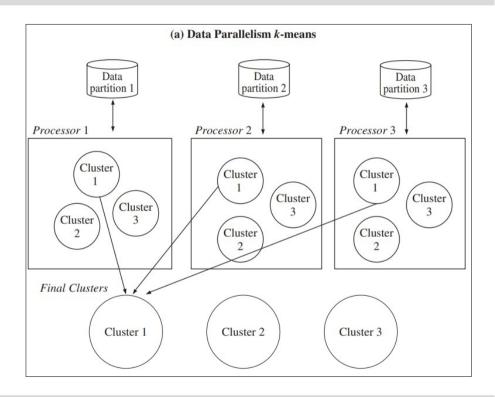
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Parallel K-means clustering

Data parallelism of k-means





Parallel K-means

Data parallelism

k-means

5, 21, 17, 7, 2, 11, 3 Iteration 1 Cluster 1 Mean=6 Dataset=2, 3, 5Sum=10: Count=3

Processor 1

Data partition 1:

Cluster 2 Mean=7 Dataset=7

Sum=7: Count=1 Cluster 3 Mean=8 Dataset 11, 17, 21 Sum=49: Count=3

Iteration 2 Cluster 1 Mean=3.5Dataset=2, 3, 5Sum=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 Cluster 1 Mean=6 Dataset=4/6 Sum=10: Count=2

Processor 2

Data partition 2:

Mean=3.5

Dataset=4

Cluster 2

Mean=7

Cluster 3

Mean=16.92

Dataset €6

Sum=6: Count=1

Sum=105: Count=5

19, 4, 23, 6, 20, 27, 16

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

Cluster 2 Mean=7 Dataset=NII Sum=0: Count=0 Cluster 3

Mean=8 Dataset=16, 19, 20, 23, 27 Sum=105; Count=5 Cluster 1

Sum=4; Cbunt=1

Mean=7 Dataset=(8, 9) 10 Sum=27: Count=3 Cluster 3

Processor 3

Data partition 3:

25, 1, 8, 10, 14, 9

Sum=1: Count=1

Sum=0: Count=0

Sum=66: Count=5

Dataset=(8, 9) 10, 14, 25

Cluster 1

Mean=6

Dataset=1

Cluster 2

Mean=7

Cluster 3

Mean=8.

Cluster 1

Mean=3.5

Dataset=1

Cluster 2

Sum=1; Count=1

Dataset=NIL

Mean=16.92 Dataset=16, 19, 20, 23, 27 Dataset=14, 25Sum=39: Count=2



Parallel K-means

Data parallelism

k-means

Processor 1: Cluster 1 = 2, 3, 5Cluster 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 = 1Cluster 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,



5, 21, 17, 7, 2, 11, 3 Iteration 1 Cluster 1 Mean=6 Dataset=2, 3, 5Sum=10: Count=3 Cluster 2

Processor 1

Data partition 1:

Mean=7 Dataset=7 Sum=7: Count=1 Cluster 3 Mean=8

Dataset 11, 17, 21 Sum=49: Count=3 Iteration 2

Cluster 1

Mean=3.5Dataset=2, 3, 5Sum=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 Data partition 2: 19, 4, 23, 6, 20, 27, 16 Cluster 1

Processor 2

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

Mean=6 Dataset=4(6) Sum=10: Count=2 Cluster 2 Mean=7

Dataset=NII Sum=0: Count=0 Cluster 3 Mean=8

Dataset=16, 19, 20, 23, 27 Sum=105: Count=5

Cluster 1

Mean=3.5

Dataset=4

Cluster 2

Mean=7

Dataset €6

Cluster 3

Mean=16.92

Sum=105; Count=5

Sum=4; Cbunt=1

Sum=6; Count=1

Dataset=16, 19, 20, 23, 27

Cluster 2 Mean=7 Dataset=(8, 9) 10

Sum=39: Count=2

Sum=1; Count=1

Processor 3

Data partition 3:

25, 1, 8, 10, 14, 9

Sum=1: Count=1

Sum=0: Count=0

Sum=66: Count=5

Dataset=(8, 9) 10, 14, 25

Cluster 1

Mean=6

Dataset=1

Cluster 2

Mean=7

Cluster 3

Mean=8.

Cluster 1

Mean=3.5

Dataset=1

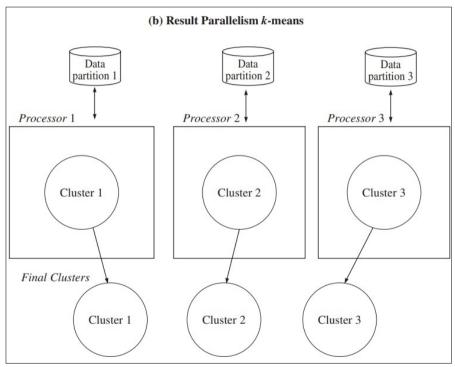
Dataset=NIL

Sum=27: Count=3 Cluster 3

Mean=16.92 Dataset=14, 25

Parallel K-means clustering

Result Parallelism of k-means

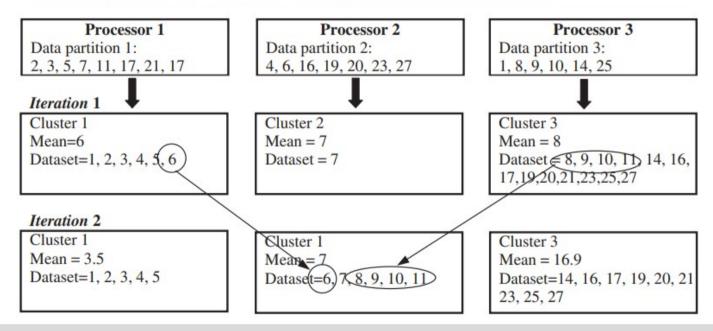




Parallel K-means

Result parallelism k-means

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

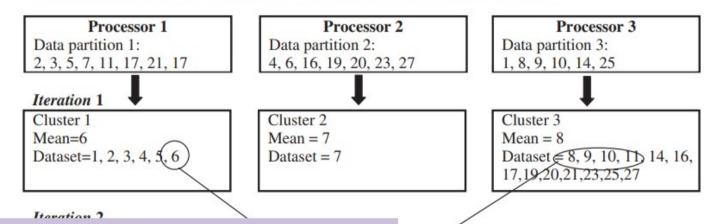




Parallel K-means

Result parallelism k-means

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



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,



Cluster 3 Mean = 16.9 Dataset=14, 16, 17, 19, 20, 21 23, 25, 27





What have we learnt today?

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

