Clustering

- **Review of K-means algorithm**

Algorithm: *k*-means. The *k*-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

Input:

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

Output: A set of *k* clusters.

Method:

(1) arbitrarily choose *k* objects from *D* as the initial cluster centers;
(2) **repeat**
(3) (re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster;
(4) update the cluster means, that is, calculate the mean value of the objects for each cluster;
(5) **until** no change;

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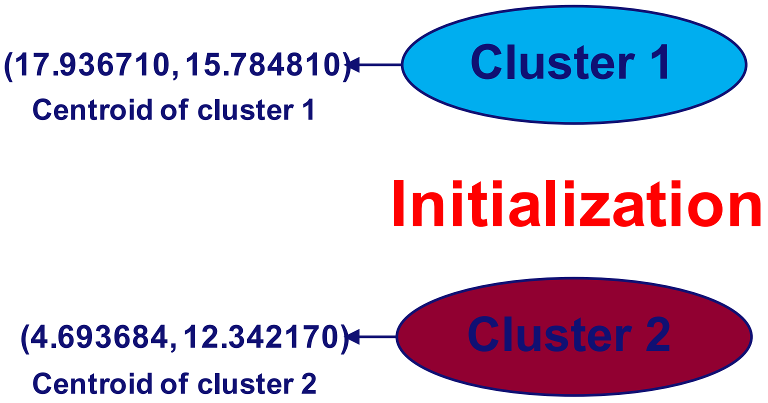
Clustering

- An example implementation of k-means algorithm



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
5	24.169930	32.024780
6	21.665780	4.892855
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Euclidean distance

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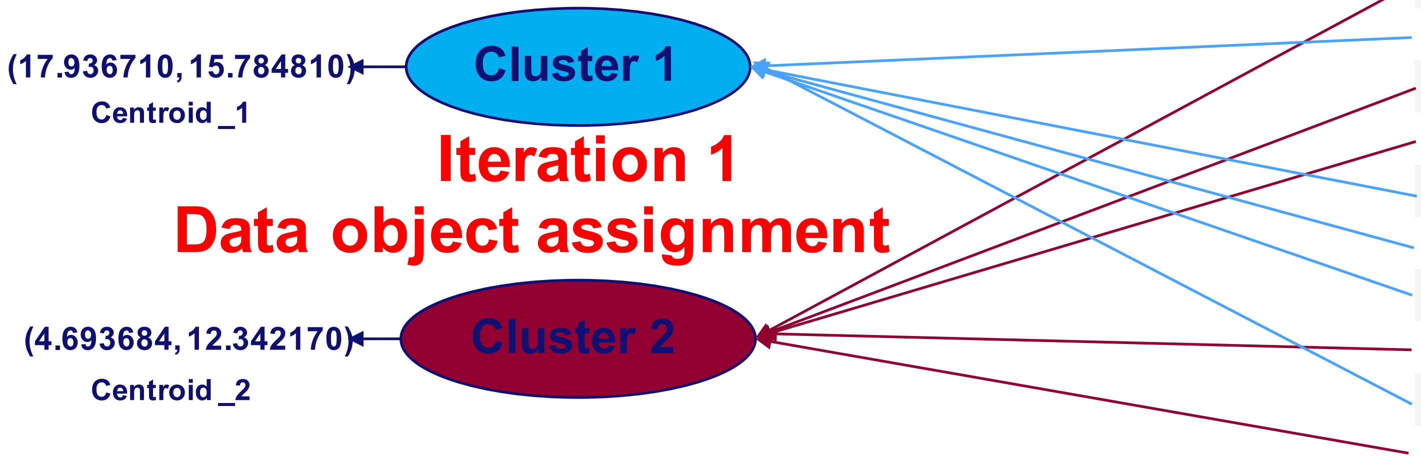
Clustering

- **An example implementation of k-means algorithm**



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
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Example data set

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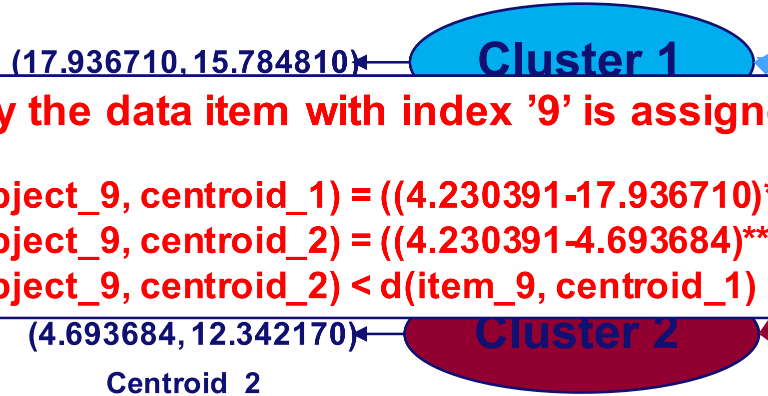
Clustering

- **An example implementation of k-means algorithm**



Why the data item with index '9' is assigned to cluster 2 ???

d(object_9, centroid_1) = ((4.230391-17.936710)**2 + (-4.441536-15.784810)**2)**0.5 = 24.43293378
d(object_9, centroid_2) = ((4.230391-4.693684)**2 + (-4.441536-12.342170)**2)**0.5 = 16.79009909
d(object_9, centroid_2) < d(item_9, centroid_1) => item with index 9 is assigned to cluster 2

	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
	4.693684	12.342170
	9.211910	-1.121366
9	4.230391	-4.441536

Example data set

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Euclidean distance

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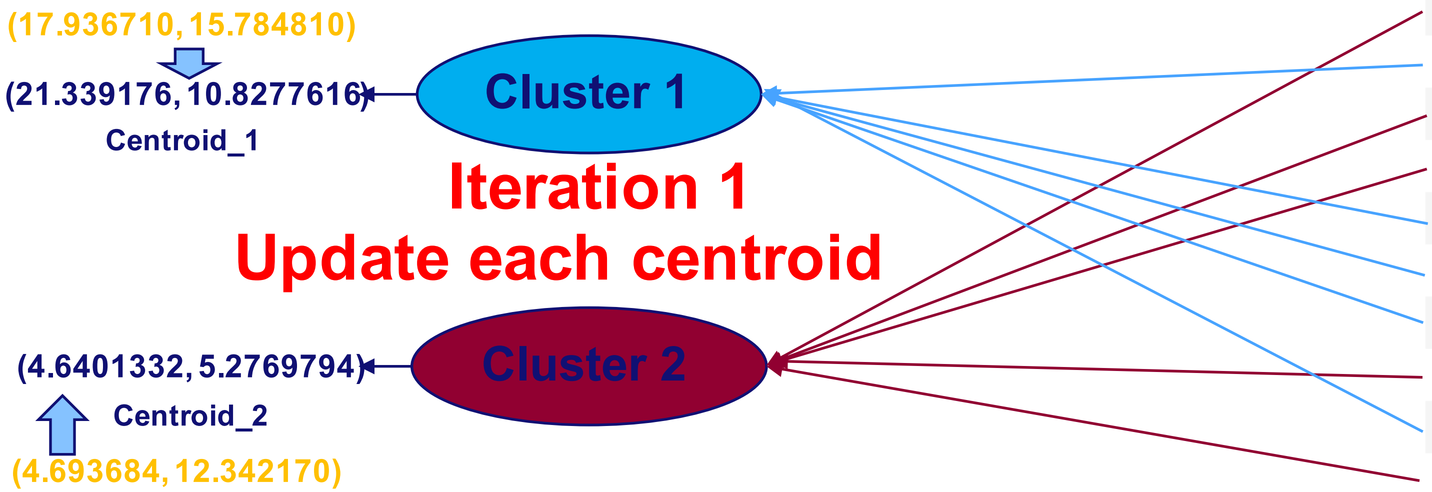
Clustering

- An example implementation of k-means algorithm



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
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7	4.693684	12.342170
8	19.211910	-1.121366
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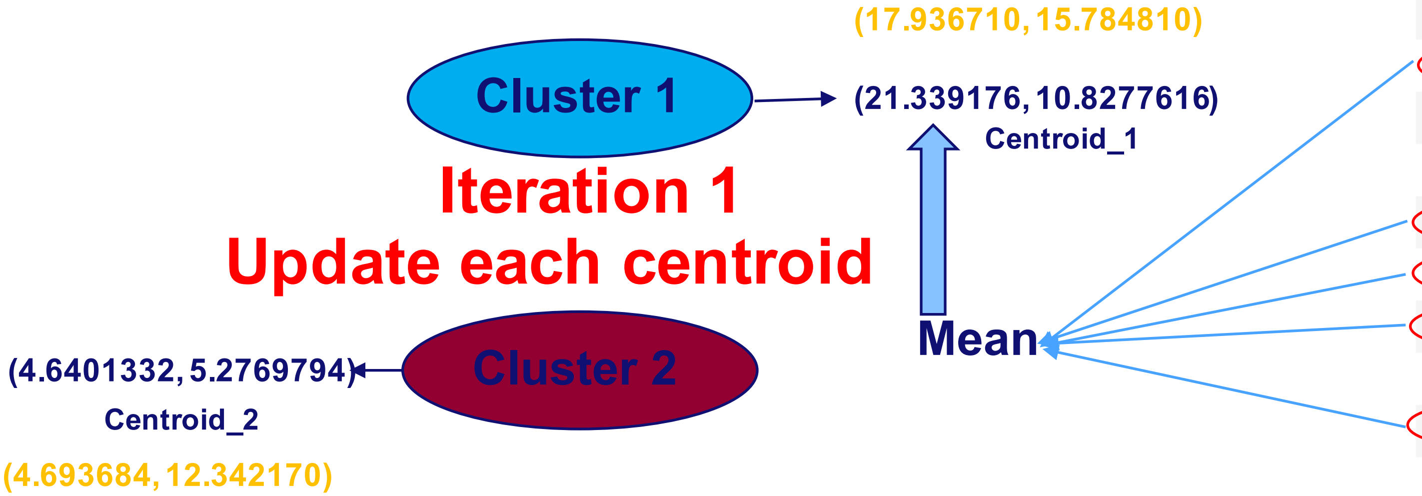
Example data set

Clustering

- An example implementation of k-means algorithm



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
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6	21.665780	4.892855
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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Clustering

- **An example implementation of k-means algorithm**

(17.936710, 15.784810)

Cluster 1 → (21.339176, 10.8277616)
Centroid_1

Iteration 1
Update each centroid

Mean

(4.6401332, 5.2769794) ← Cluster 2
Centroid_2

(4.693684, 12.342170)

	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
5	24.169930	32.024780
6	21.665780	4.892855
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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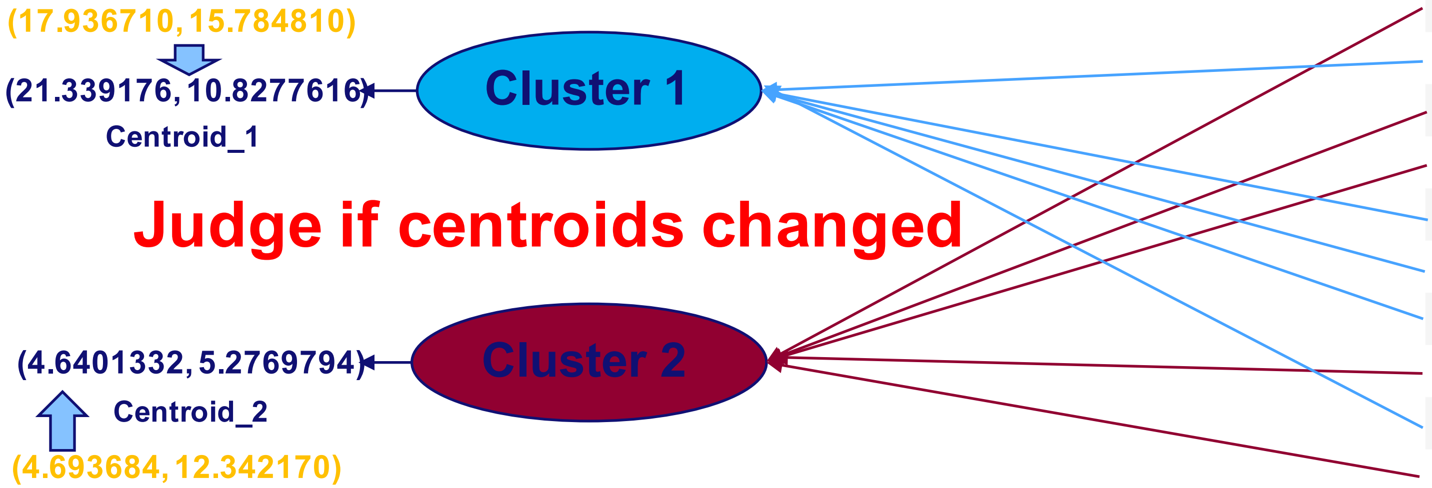
Clustering

- An example implementation of k-means algorithm



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
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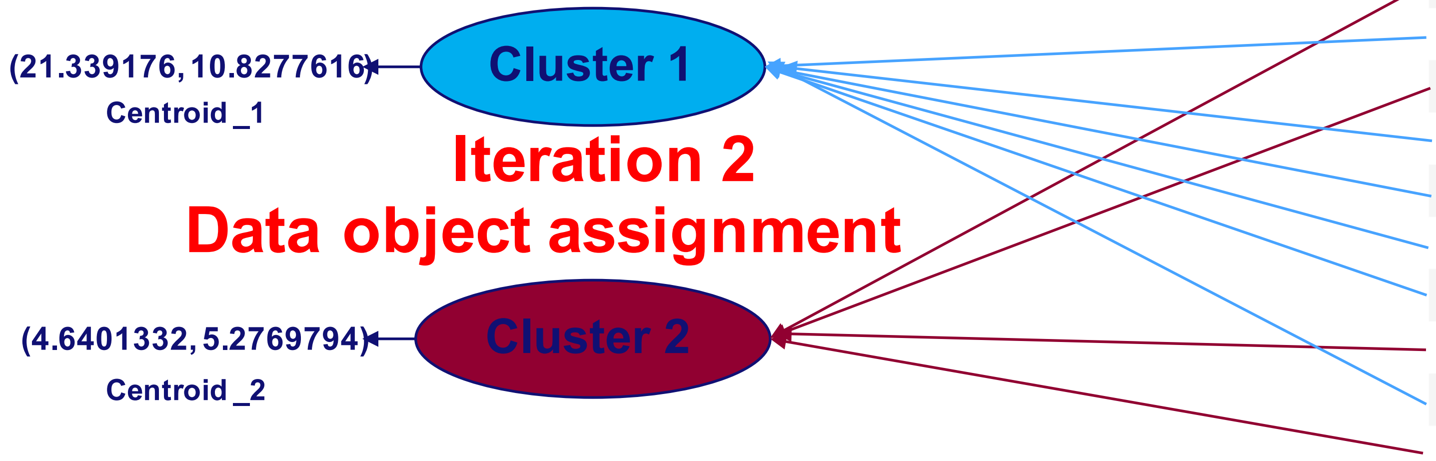
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

Clustering

- **An example implementation of k-means algorithm**



	x1	x2
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1	17.936710	15.784810
2	1.083576	7.319176
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8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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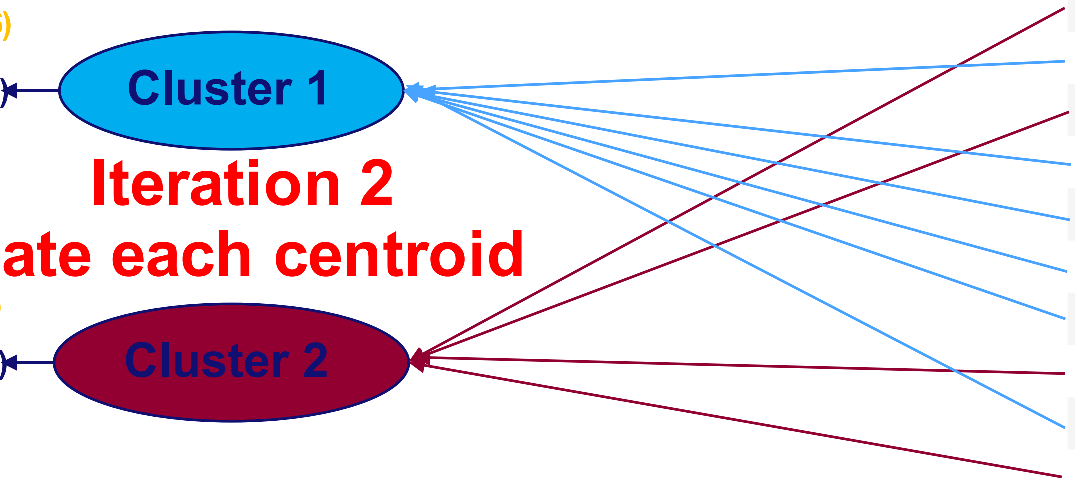
Clustering

- An example implementation of k-means algorithm

(21.339176, 10.8277616)

(19.636092, 11.4242647)

Centroid _1



Iteration 2

Update each centroid

(4.6401332, 5.2769794)

(3.019999, 2.99452925)

Centroid _2

	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
5	24.169930	32.024780
6	21.665780	4.892855
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

Chair of Process and Data Science

Clustering

- An example implementation of k-means algorithm

(21.339176, 10.8277616)

(19.636092, 11.4242647)

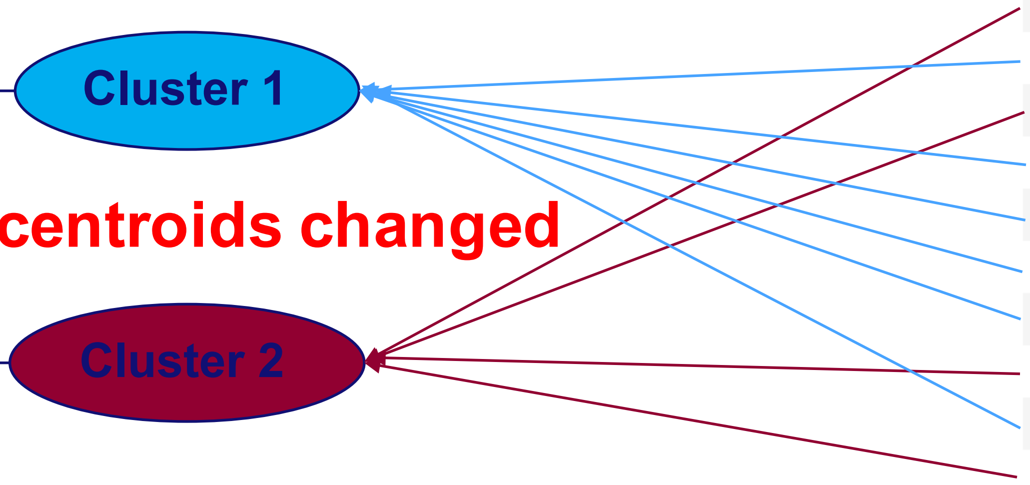
Centroid _1

Judge if centroids changed

(4.6401332, 5.2769794)

(3.019999, 2.99452925)

Centroid _2



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
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7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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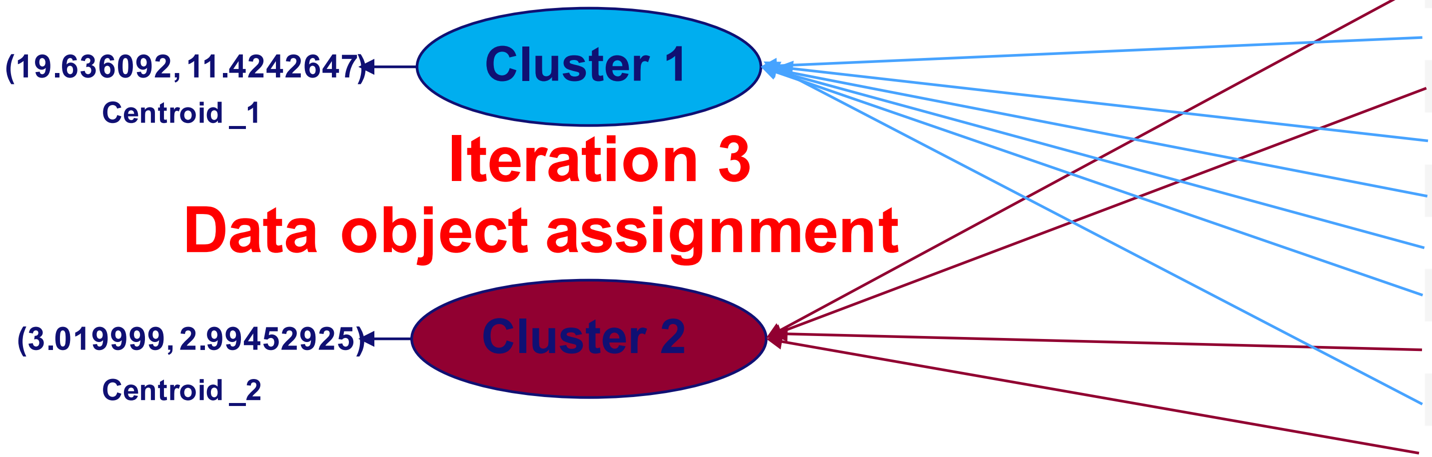
Clustering

- An example implementation of k-means algorithm



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
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7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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Clustering

- **An example implementation of k-means algorithm**

(19.636092, 11.4242647)

(19.636092, 11.4242647)

Centroid _1

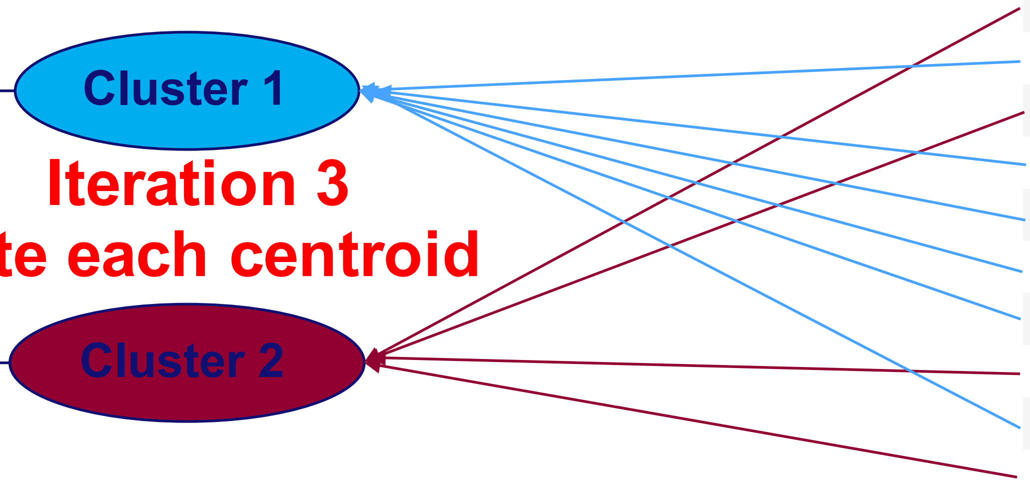
Iteration 3

Update each centroid

(3.019999, 2.99452925)

(3.019999, 2.99452925)

Centroid _2



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729
5	24.169930	32.024780
6	21.665780	4.892855
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8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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Clustering

- An example implementation of k-means algorithm

(19.636092, 11.4242647)

(19.636092, 11.4242647)

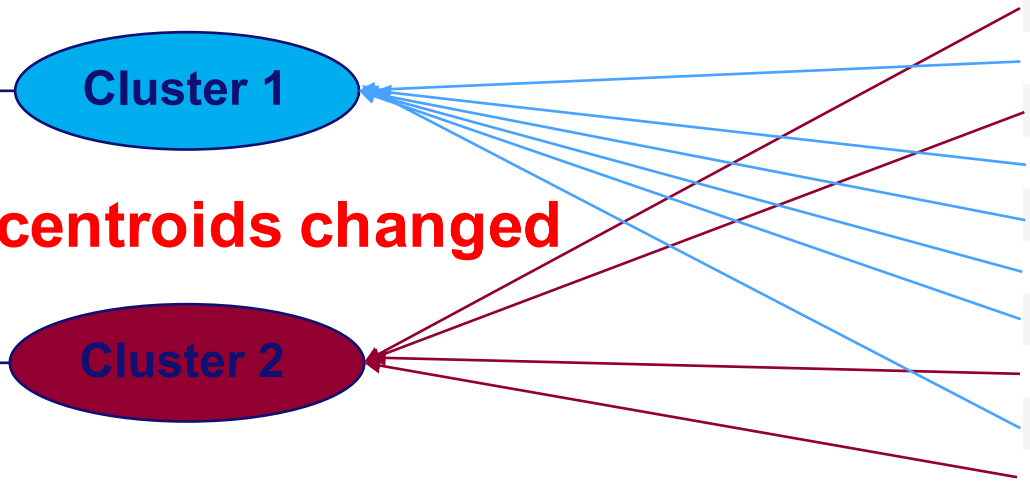
Centroid _1

Judge if centroids changed

(3.019999, 2.99452925)

(3.019999, 2.99452925)

Centroid _2



	x1	x2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
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6	21.665780	4.892855
7	4.693684	12.342170
8	19.211910	-1.121366
9	4.230391	-4.441536

Example data set

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Clustering

- **Exercise 1: cluster data objects from data set 1 manually**
- **Conditions**
  - **K = 2 :– cluster 1 and cluster 2**
  - **Data object with index '4' as initial centroid for cluster 1**
  - **Data object with index '8' as initial centroid for cluster 2**
  - **Use Euclidean distance**
- **You should calculate and output**
  - **Centroids of the found clusters**
  - **Data objects for each of the two final clusters**

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Euclidean distance

	x1	x2
0	0.407503	15.297050
1	7.314846	3.309312
2	-3.438403	-12.025270
3	17.639350	-3.212345
$\boxed{\textbf{4}}$	4.415292	22.815550
5	11.941220	8.122487
6	0.725853	1.806819
7	8.185273	28.132600
$\boxed{\textbf{8}}$	-5.773587	1.024800
9	18.769430	24.169460

Data set 1

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Clustering

- Some weaknesses of k-means algorithm
  - Number of clusters needs to be decided beforehand
  - Can only discover spherical clusters (compare to density-based methods)
  - Sensitive to outliers (show this to you later)

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Frequent Itemsets

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

Minimum support$_{count}$ = 2

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

Frequent itemsets

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Frequent Itemsets

- Basic ideas of Apriori algorithm
  - Apriori rule: all the non-empty sub-itemsets of frequent itemsets must be frequent.

Frequent Itemsets

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

Minimum support$_{count}$ = 2

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

Frequent itemsets

Itemset {bread, meat, wine} is frequent

Sub-item set	Support	
{bread}	3	frequent
{meat}	3	frequent
{wine}	3	frequent
{bread, meat}	3	frequent
{bread, wine}	2	frequent
{meat, wine}	2	frequent

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Frequent Itemsets

- Basic ideas of Apriori algorithm
  - **Apriori rule**: all the non-empty **sub-itemsets** of **frequent itemsets** should **be frequent**.
  - Use the set L_k of frequent itemsets with **length k** to search for both candidate set C_{k+1} of itemsets and the set L_{k+1} of frequent itemsets with length **k+1**

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_1

Frequent itemsets

First, Scan D to generate L_1

Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_1

Frequent itemsets

First, Scan D to generate L_1

min_sup represents minimum support_{count}

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

Scan, compare support to min_sup

remove infrequent ones

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3

L_1

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Frequent Itemsets

- **Exercise 2: manually generate L_1 from set S**
  - **Set minimum support_{count} to 2**

Item set	Support
?	

L_1

TID	Data items
1	A, B, E
2	C, A, D
3	C, B, D
4	C, A, B, E

Example data set S

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, when $k >= 2$?

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, when $k >= 2$?

1. Keep items in itemsets in L_{k-1} in an ascending order according to their dictionary order

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, when $k >= 2$?

1. Keep items in itemsets in L_{k-1} in an ascending order according to their dictionary order

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

For generating C_3

bread < meat

bread < wine

meat < wine

pizza < wine

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, when $k >= 2$?

2. Merge each possible pair of items from L_{k-1}

Let $(\{p_1, p_2, \ldots, p_{k-2}, p_{k-1}\}, \{q_1, q_2, \ldots, q_{k-2}, q_{k-1}\})$ be a pair of two itemsets from L_{k-1}.

-- if: $\{p_1, p_2, \ldots, p_{k-2}\} = \{q_1, q_2, \ldots, q_{k-2}\}$ and $p_{k-1} < q_{k-1}$

-- then merge them into: $\{p_1, p_2, \ldots, p_{k-2}, p_{k-1}, q_{k-1}\}$

-- else: not merge them

Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, where $k >= 2$?

2. Merge each possible pair of items from L_{k-1}

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

({bread, meat}, {bread, wine})
=> {bread, meat, wine}

Because {bread} = {bread} and
meat < wine

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, where $k >= 2$?

2. Merge each possible pair of items from L_{k-1}

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

({bread, wine}, {bread, meat}) ≠> {bread, meat, wine}

Because wine > meat

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, where $k >= 2$?

2. Merge each possible pair of items from L_{k-1}

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

({bread, wine}, {meat, wine}) $\not\Rightarrow$ {bread, meat, wine}

Because {bread} $\neq$ {meat}

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

How to generate C_k from L_{k-1}, where $k >= 2$?

2. Merge each possible pair of items from L_{k-1}

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

merge itemsets in L_2

Item set
{bread, meat, wine}

C_3

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

Pre-pruning for C_k when k >= 2 before scanning D

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

Pre-pruning for C_k when k >= 2 before scanning D

Pruning rule: given an itemset $i_k \subseteq C_k$, if not all sub-itemsets of length $k-1$ of i_k are contained in L_{k-1}, then remove i_k from C_k

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

Pre-pruning for C_k when k >= 2 before scanning D

Set of items	Support
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2

L_2

Item set
{bread, meat, wine}

C_3

The sub-itemsets of length 2 for {bread, meat, wine} include: {bread, meat}, {bread, wine}, {meat, wine}, which are all Included in L_2. So keep {bread, meat, wine}.

Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

Pre-pruning for C_k when k >= 2 before scanning D

Item set
{bread, meat, wine}

C_3

Pre-pruning

Item set
{bread, meat, wine}

C_3

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	L_2 2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	L_3 2

Frequent itemsets

Scan D to add supports for itemsets in C_k

Item set
{bread, meat, wine}

C_3

scan →

item set	support
{bread, meat, wine}	2

C_3

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Frequent Itemsets

Item set	Support
{bread}	3
{meat}	3
{pizza}	2
{wine}	3
{bread, meat}	3
{bread, wine}	2
{meat, wine}	2
{pizza, wine}	2
{bread, meat, wine}	2

L_2

L_3

Frequent itemsets

Remove infrequent itemsets and generate L_k

item set	support
{bread, meat, wine}	2

C_3

compare support to min_sup

remove infrequent ones

item set	support
{bread, meat, wine}	2

L_3

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Frequent Itemsets

- Exercise 3: given L_2 for set S, show the three C_3 and L_3
  - Set minimum support$_{count}$ to 2

TID	Data items
1	A, B, E
2	C, A, D
3	C, B, D
4	C, A, B, E

Data set S

Item set	Support
{A, B}	2
{A, C}	2
{A, E}	2
{B, C}	2
{B, E}	2
{C, D}	2

L_2

merge itemsets in L_2 →

Item set	Support

?

C_3

pruning →

Item set	Support

?

C_3

Scan S →

Item set	Support

?

C_3

compare support to min_sup

remove infrequent ones →

Item set	Support

?

L_3

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Association Rules

- T is a set of transactions
- I is the set of all possible itemsets composed by items in T
- A ⊆ I and B ⊆ I are two itemsets/sub-itemsets from T
- A => B is an association rule

Association Rules

- Usually, we would like to discover the association rule A => B of which the support and confidence are above certain levels.

Association Rules

- $support(A \Rightarrow B) = support(A \cup B) = \frac{support_{count}(A \cup B)}{|T|}$
- $confidence(A \Rightarrow B) = \frac{support(A \cup B)}{support(A)} = \frac{support_{count}(A \cup B)}{support_{count}(A)}$

- min_sup represents minimum support and min_conf represents minimum confidence

- A => B is a desired association rule if:
- $support(A \Rightarrow B)$ >= min_sup and $confidence(A \Rightarrow B)$ >= min_conf

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Association Rules

- Set min_sup to 0.5, min_conf to 0.7, is {bread} => {meat} from D a desired association rule?

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

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Association Rules

- Set min_sup to 0.5, min_conf to 0.7, is {bread} => {meat} from D a desired association rule?

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

$$support(\{\text{bread}\} \Rightarrow \{\text{meat}\}) = \frac{support_{count}(\{\text{bread,meat}\})}{|D|} = \frac{3}{4} = 0.75 > \text{min\_sup}$$

$$\text{confidence}(\{\text{bread}\} \Rightarrow \{\text{meat}\}) = \frac{support_{count}(\{\text{bread,meat}\})}{support_{count}(\{\text{bread}\})} = \frac{3}{3} = 1 > \text{min\_conf}$$

{bread} => {meat} is a desired association rule

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Association Rules

- Usually, we use **lift** to evaluate the quality of the discovered association rule **A => B**

$$lift(A \Rightarrow B) = \frac{support(A \cup B)}{support(A) \cdot support(B)} = \frac{P(A \cup B)}{P(A) \cdot P(B)}$$

If $lift(A \Rightarrow B) \approx 1$ then A and B are independent

If $lift(A \Rightarrow B) \ll 1$ then A and B are negatively correlated

If $lift(A \Rightarrow B) \gg 1$ then A and B are positively correlated

Association Rules

- Evaluate the quality of the association rule {bread} => {meat} by using lift

TID	Set of items
0	bread, meat, wine
1	bread, meat
2	pizza, wine
3	bread, meat, pizza, wine

Set of transactions D

$$lift(\{bread\} \Rightarrow \{meat\}) = \frac{support(\{bread, meat\})}{support(\{bread\}) \cdot support(\{meat\})} = \frac{(3/4)}{(3/4) \cdot (3/4)} = 1.33$$

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Association Rules

- **Exercise 3: judge if {A, B} => {E}, {A} => {B} and {A} => {C} are the desired association rules under minimum support 0.5 and minimum confidence 0.75? Also evaluate the quality of the desired rules.**

TID	Data items
1	A, B, E
2	C, A, D
3	C, B, D
4	C, A, B, E

Example data set S

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