Lecture outline

- Density-based clustering (DB-Scan)
  - Reference: Martin Ester, Hans-Peter Kriegel, Jorg Sander, Xiaowei Xu: A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise. KDD 2006
- Co-clustering (or bi-clustering)
- References:
  - A. Anagnostopoulos, A. Dasgupta and R. Kumar: Approximation Algorithms for co-clustering, PODS 2008.
  - K. Puolamaki. S. Hanhijarvi and G. Garriga: An approximation ratio for biclustering, Information Processing Letters 2008.

Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise

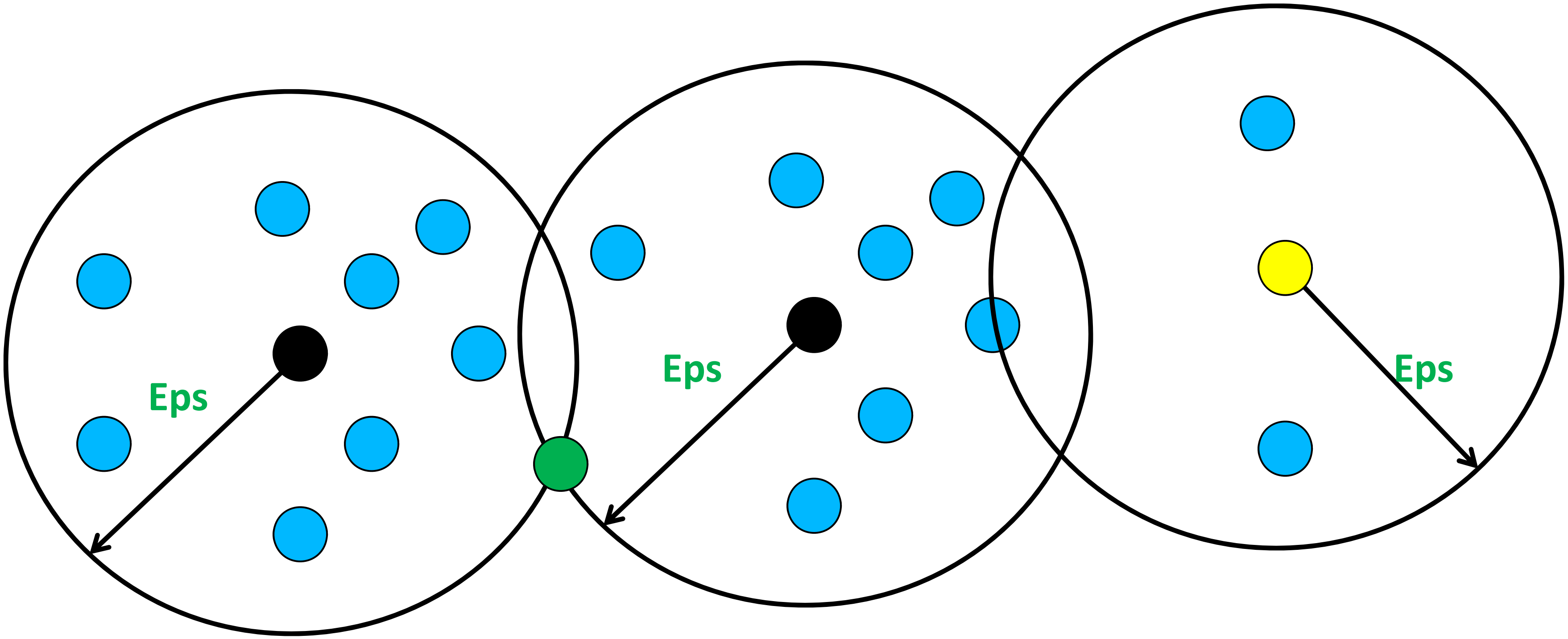
Classification of points in density-based clustering

- **Core points**: Interior points of a density-based cluster. A point **p** is a core point if for distance **Eps** :
  - **$|N_{Eps}(p)=\{q \mid dist(p,q) <= \varepsilon\}| \geq MinPts$**

- **Border points:** Not a core point but within the neighborhood of a core point (it can be in the neighborhoods of many core points)

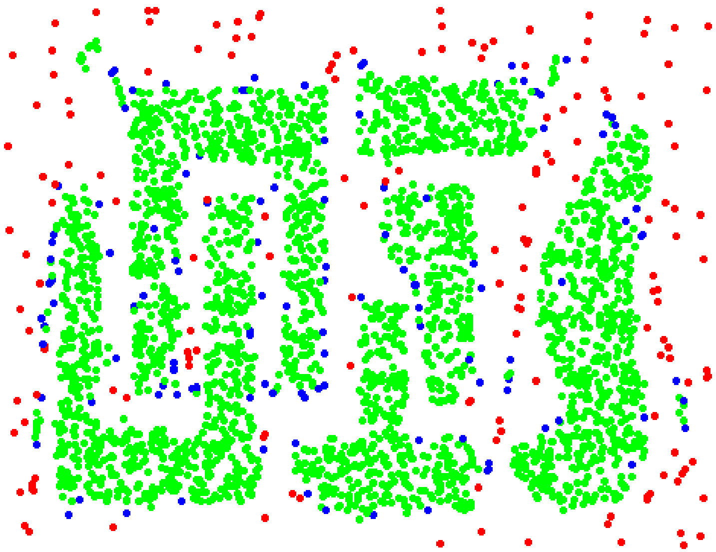
- **Noise points:** Not a core or a border point

Core, border and noise points



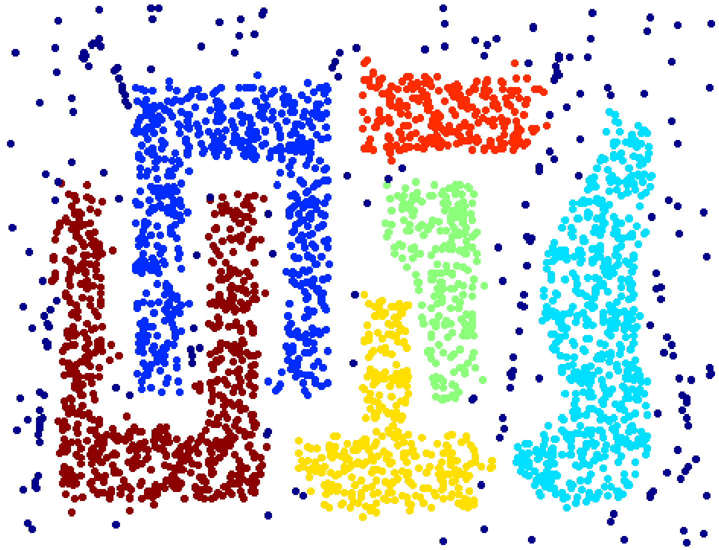
Core, Border and Noise points

Original Points



Point types: core border and noise

Clusters output by DBScan



- Resistant to Noise
- Can handle clusters of different shapes and sizes

Classification of points in density-based clustering

- **Core points**: Interior points of a density-based cluster. A point **p** is a core point if for distance **Eps** :
  - $|N_{Eps}(p)=\{q \mid dist(p,q) <= \varepsilon \}| \geq MinPts$

- **Border points:** Not a core point but within the neighborhood of a core point (it can be in the neighborhoods of many core points)

- **Noise points:** Not a core or a border point

DBSCAN: The Algorithm

– Label all points as ***core***, ***border***, or ***noise*** points

– Eliminate noise points

– Put an edge between all core points that are within ***Eps*** of each other

– Make each group of connected core points into a separate cluster

– Assign each border point to one of the cluster of its associated core points

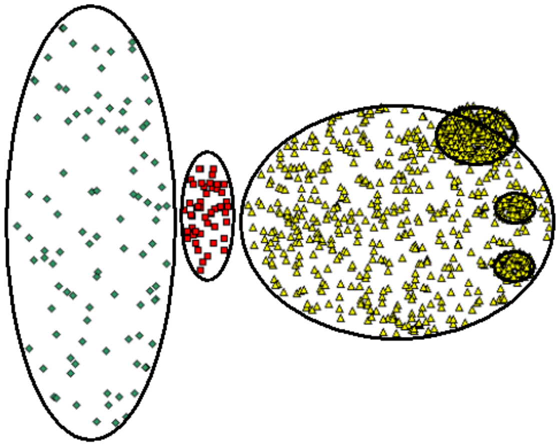
Time and space complexity of DBSCAN

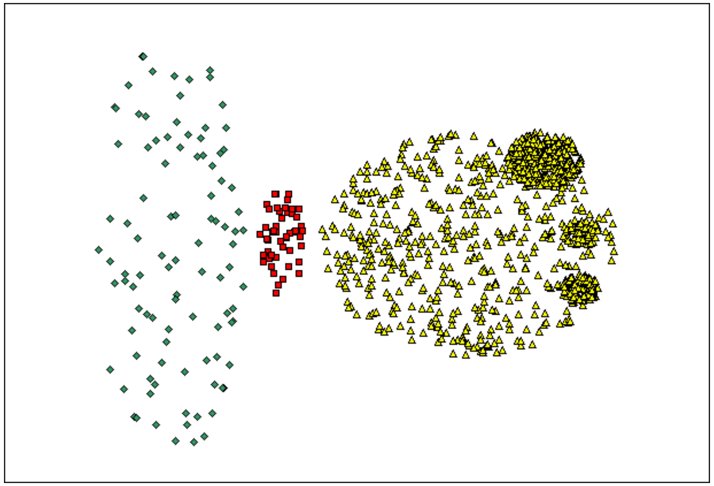
- For a dataset **X** consisting of **n** points, the time complexity of DBSCAN is **O(n x time to find points in the Eps-neighborhood)**

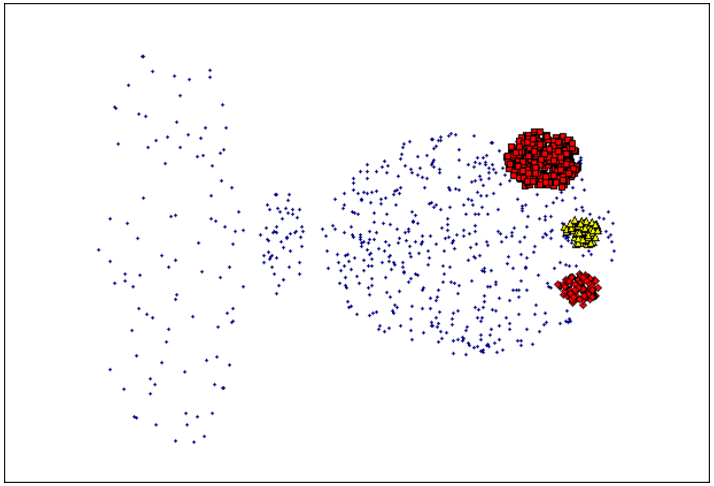
- Worst case **$O(n^2)$**

- In low-dimensional spaces **O(nlogn)**; efficient data structures (e.g., ***kd-trees***) allow for efficient retrieval of all points within a given distance of a specified point

When DBSCAN Does NOT Work Well



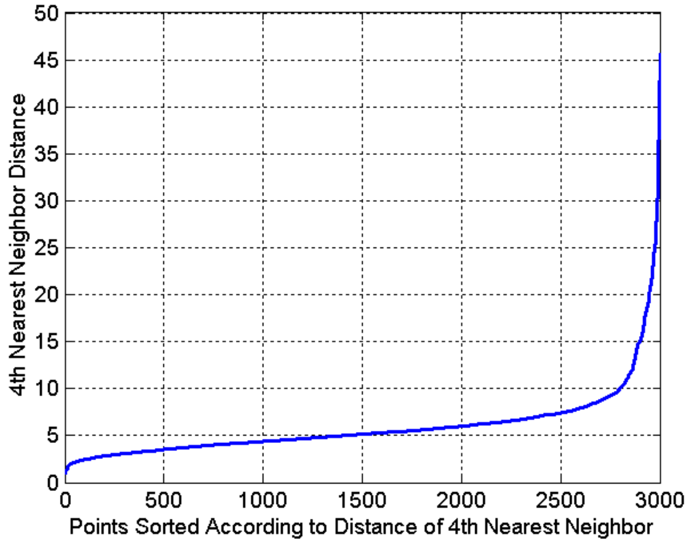




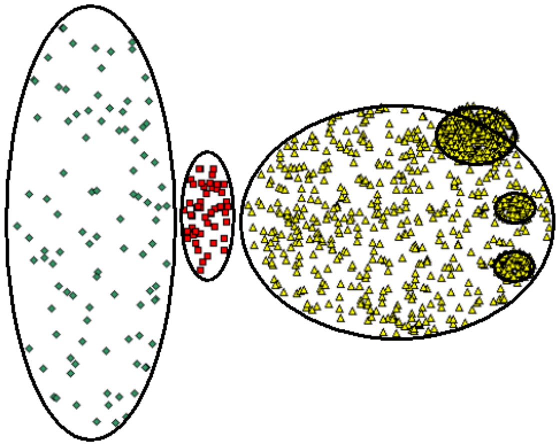
DBScan can fail to identify clusters of varying densities

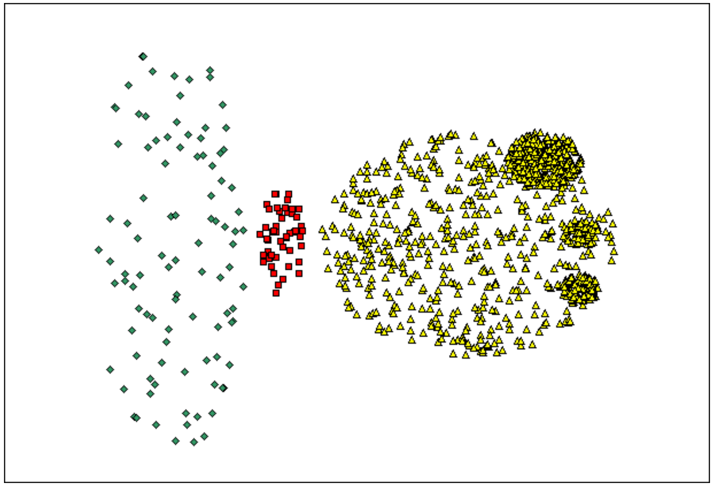
Determining EPS and MinPts

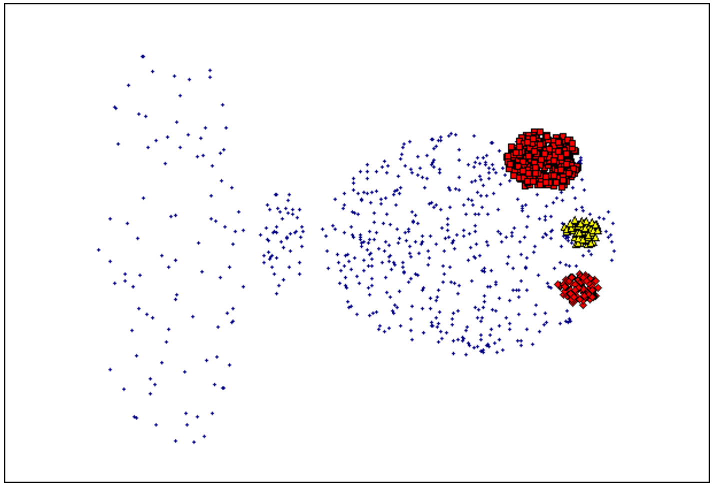
- Idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor



When DBSCAN Does NOT Work Well

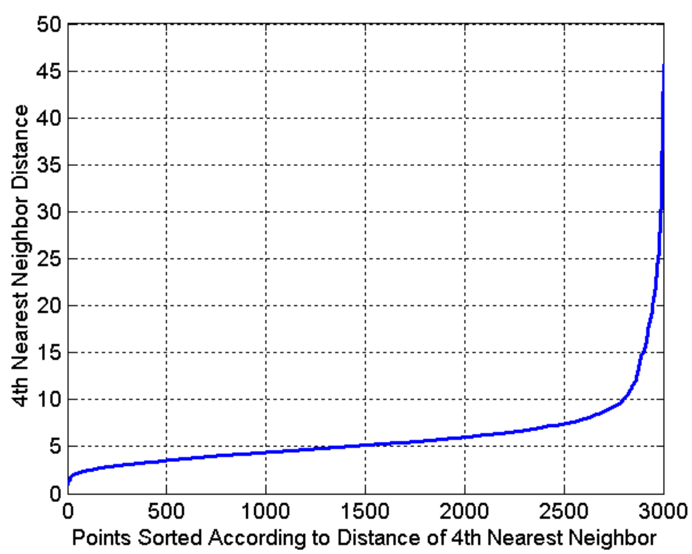






Determining EPS and MinPts

- Idea is that for points in a cluster, their **k**th nearest neighbors are at roughly the same distance
- Noise points have the **k**th nearest neighbor at farther distance
- So, plot sorted distance of every point to its **k**th nearest neighbor



Strengths and weaknesses of DBSCAN

- Resistant to noise
- Finds clusters of arbitrary shapes and sizes
- Difficulty in identifying clusters with varying densities
- Problems in high-dimensional spaces; notion of density unclear
- Can be computationally expensive when the computation of nearest neighbors is expensive

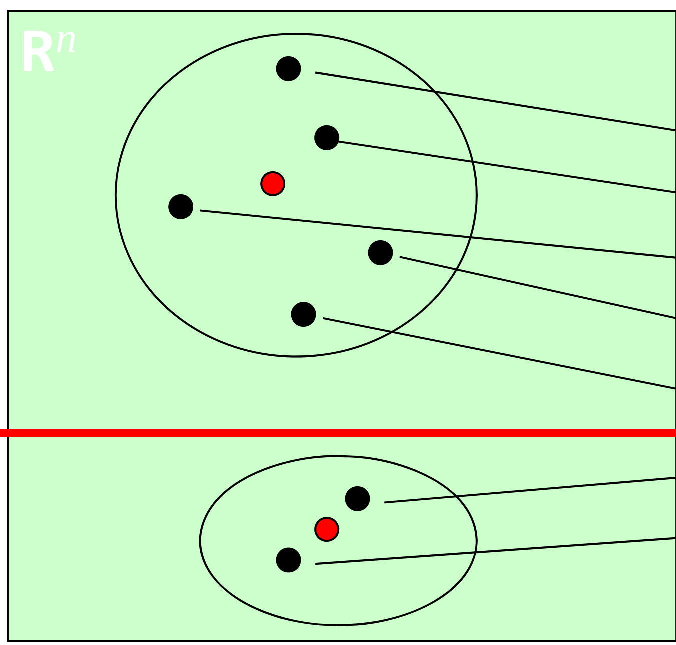
Lecture outline

- Density-based clustering

- Co-clustering (or bi-clustering)
- References:
  - A. Anagnostopoulos, A. Dasgupta and R. Kumar: Approximation Algorithms for co-clustering, PODS 2008.
  - K. Puolamaki. S. Hanhijarvi and G. Garriga: An approximation ratio for biclustering, Information Processing Letters 2008.

Clustering

- m points in $\mathbf{R}^n$
- Group them to k clusters
- Represent them by a matrix $A \in \mathbf{R}^{m \times n}$
  - A point corresponds to a row of A
- **Cluster:** Partition the rows to k

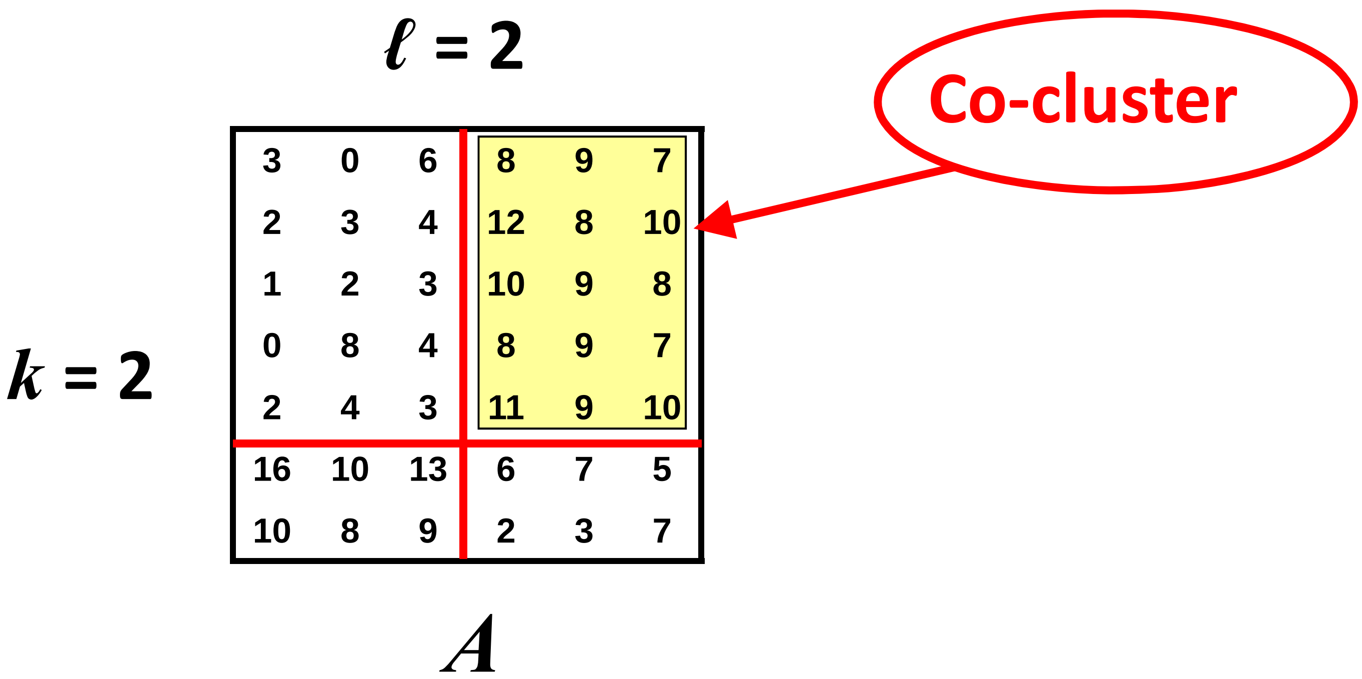


n (columns), m (rows)

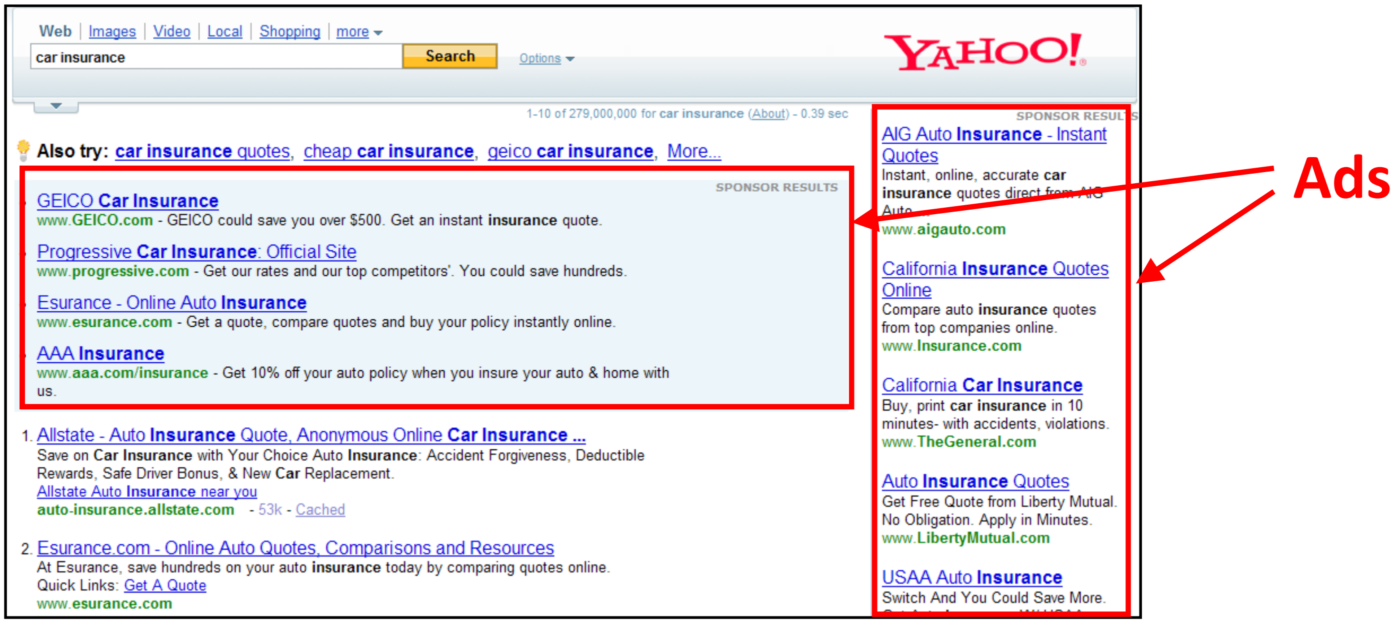
3	0	6	8	9	7
2	3	4	12	8	10
1	2	3	10	9	8
0	8	4	8	7	9
2	4	3	11	9	10
16	10	13	6	7	5
10	8	9	2	3	7

Co-Clustering

- **Co-Clustering:** **Cluster rows and columns of A simultaneously:**



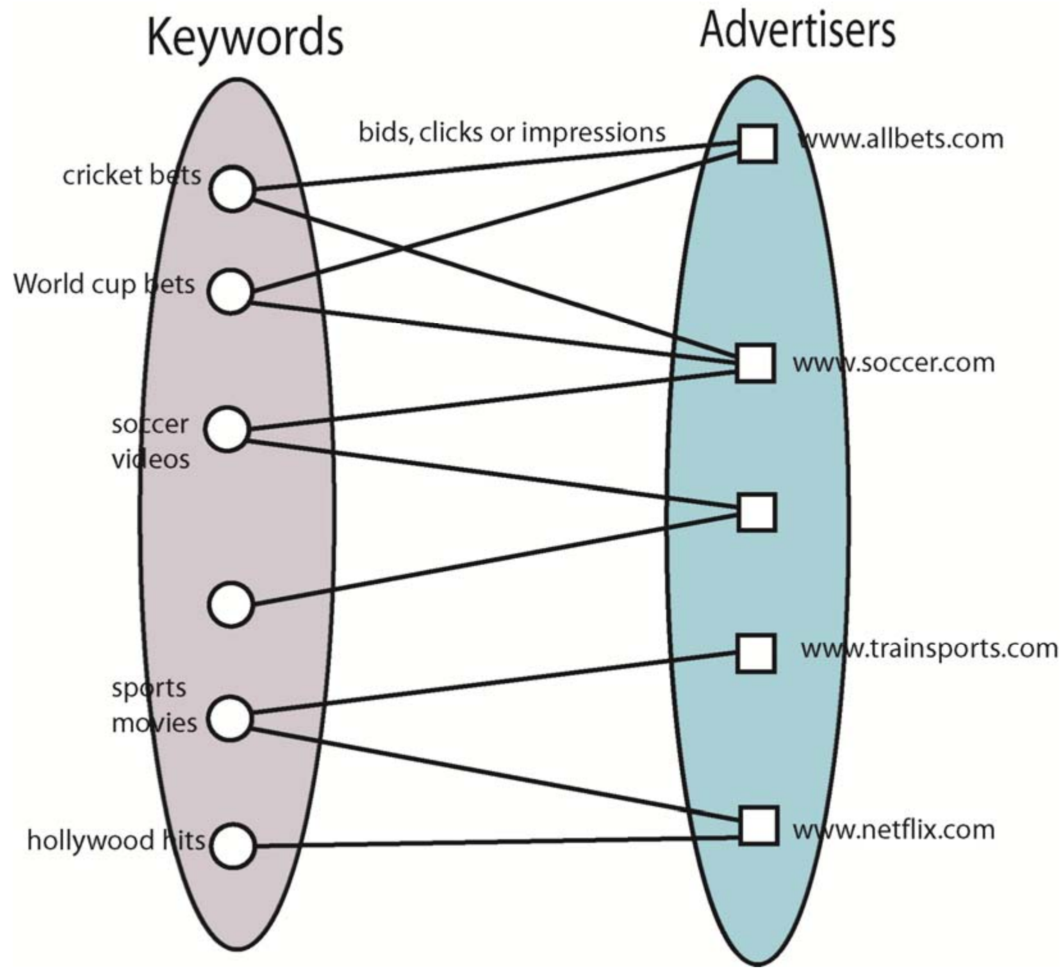
Motivation: Sponsored Search



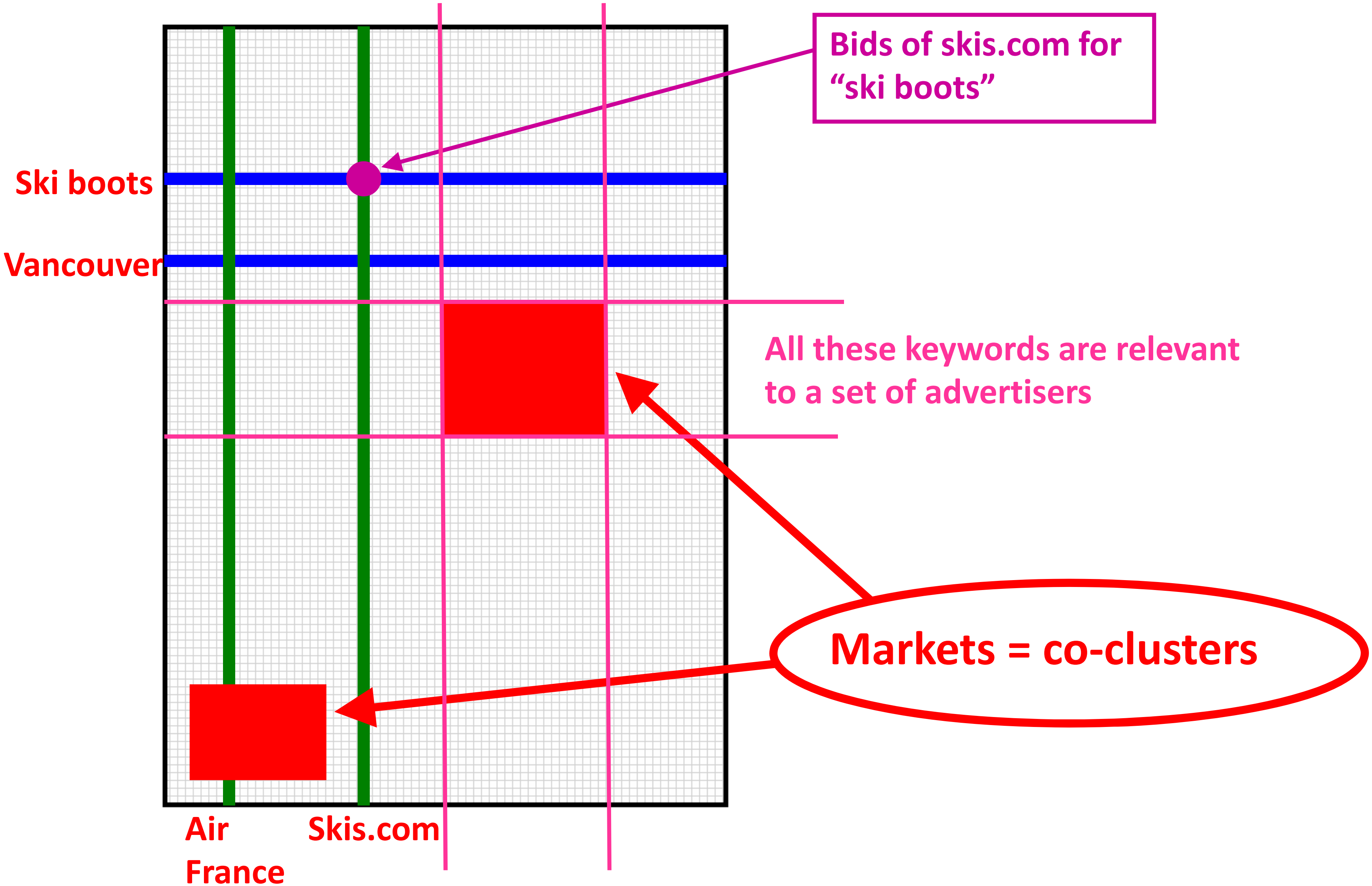
- Advertisers bid on keywords
- A user makes a query
- Show ads of advertisers that are relevant and have high bids
- User clicks or not an ad

Motivation: Sponsored Search

- For every (*advertiser, keyword*) pair we have:
  - Bid amount
  - Impressions
  - # clicks
- Mine information at query time
  - Maximize # clicks / revenue



Co-Clusters in Sponsored Search



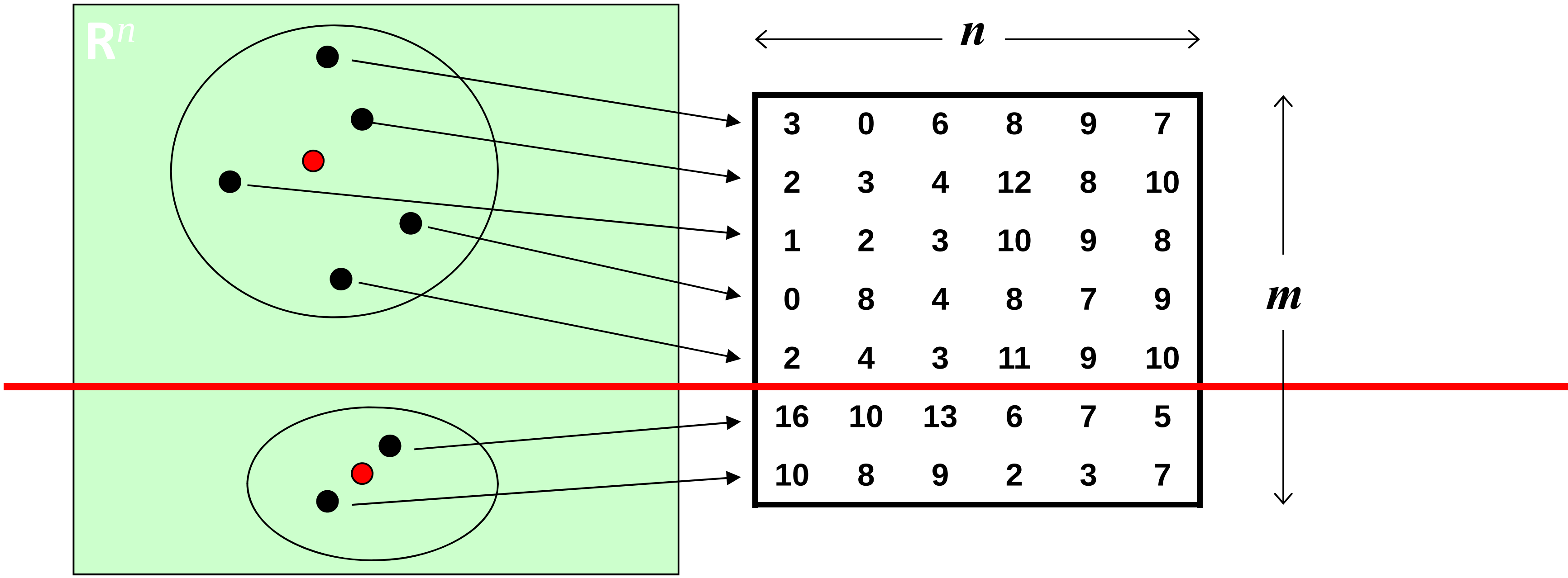
Co-Clustering in Sponsored Search

Applications:

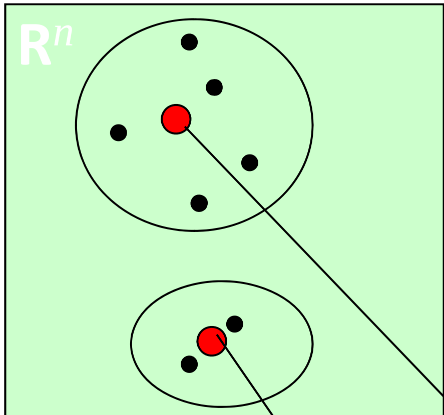
- Keyword suggestion
  - Recommend to advertisers other relevant keywords
- Broad matching / market expansion
  - Include more advertisers to a query
- Isolate submarkets
  - Important for economists
  - Apply different advertising approaches
- Build taxonomies of advertisers / keywords

Clustering of the rows

- m points in $\mathbf{R}^n$
- Group them to k clusters
- Represent them by a matrix $A \in \mathbf{R}^{m \times n}$
  - A point corresponds to a row of A
- **Clustering:** Partitioning of the rows into k groups



Clustering of the columns



- n points in $\mathbf{R}^m$
- Group them to k clusters
- Represent them by a matrix $A \in \mathbf{R}^{m \times n}$
  - A point corresponds to a column of A
- **Clustering:** Partitioning of the columns into k groups

3	0	6	8	9	7
2	3	4	12	8	10
1	2	3	10	9	8
0	8	4	8	7	9
2	4	3	11	9	10
16	10	13	6	7	5
10	8	9	2	3	7

m n

3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
11	11	11	5	5	5
11	11	11	5	5	5

Cost of clustering

3	0	6	8	9	7
2	3	4	12	8	10
1	2	3	10	9	8
0	8	4	8	7	9
2	4	3	11	9	10
16	10	13	6	7	5
10	8	9	2	3	7

Original data points **A**

1.6	3.4	4	9.8	8.4	8.8
1.6	3.4	4	9.8	8.4	8.8
1.6	3.4	4	9.8	8.4	8.8
1.6	3.4	4	9.8	8.4	8.8
1.6	3.4	4	9.8	8.4	8.8
13	9	11	4	5	6
13	9	11	4	5	6

Data representation **A'**

- In **A'** every point in **A** (row or column) is replaced by the corresponding representative (row or column)
- The quality of the clustering is measured by computing distances between the data in the cells of **A** and **A'**.

- **k-means clustering**: cost = $\sum_{i=1\ldots n} \sum_{j=1\ldots m} (A(i,j)-A'(i,j))^2$
- **k-median clustering**: cost = $\sum_{i=1\ldots n} \sum_{j=1\ldots m} |A(i,j)-A'(i,j)|$

Co-Clustering

- **Co-Clustering:** Cluster rows and columns of $A \in \mathbf{R}^{m \times n}$ simultaneously
- k row clusters, ℓ column clusters
- Every cell in **A** is represented by a cell in **A'**
- All cells in the same co-cluster are represented by the same value in the cells of **A'**

3	0	6	8	9	7
2	3	4	12	8	10
1	2	3	10	9	8
0	8	4	8	9	7
2	4	3	11	9	10
16	10	13	6	7	5
10	8	9	2	3	7

Original data **A**

3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
11	11	11	5	5	5
11	11	11	5	5	5

Co-cluster representation **A'**

Co-Clustering Objective Function

3	0	6	8	9	7
2	3	4	12	8	10
1	2	3	10	9	8
0	8	4	8	7	9
2	4	3	11	9	10
16	10	13	6	7	5
10	8	9	2	3	7

3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
3	3	3	9	9	9
11	11	11	5	5	5
11	11	11	5	5	5

- In **A'** every point in **A** (row or column) is replaced by the corresponding representative (row or column)
- The quality of the clustering is measured by computing distances between the data in the cells of **A** and **A'**.

- **k-means Co-clustering**: cost = $\sum_{i=1\ldots n} \sum_{j=1\ldots m} (A(i,j)-A'(i,j))^2$
- **k-median Co-clustering**: cost = $\sum_{i=1\ldots n} \sum_{j=1\ldots m} |A(i,j)-A'(i,j)|$

Some Background

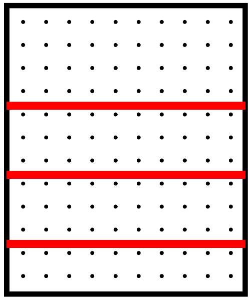
- A.k.a.: biclustering, block clustering, …

- Many objective functions in co-clustering
  - This is one of the easier
  - Others factor out row-column average (priors)
  - Others based on information theoretic ideas (e.g. KL divergence)

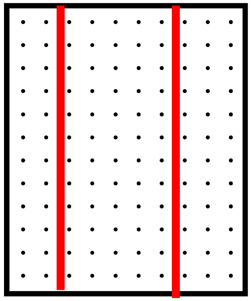
- A lot of existing work, but mostly heuristic
  - k-means style, alternate between rows/columns
  - Spectral techniques

Algorithm

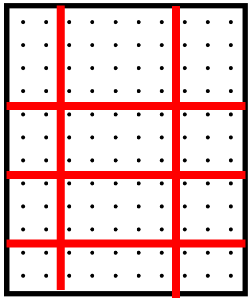
1. Cluster rows of A



2. Cluster columns of A



3. Combine



Properties of the algorithm

Theorem 1. Algorithm with optimal row/column clusterings is 3-approximation to co-clustering optimum.

Theorem 2. For L_2 distance function, the algorithm with optimal row/column clusterings is a 2-approximation.

Algorithm--details

- Clustering of the **n** rows of **A** assigns every row to a cluster with cluster name **{1,…,k}**
  - $R(i)= r_i$ with $1 \leq r_i \leq k$
- Clustering of the **m** columns of **A** assigns every column to a cluster with cluster name **{1,…,ℓ}**
  - $C(j)=c_j$ with $1 \leq c_j \leq \ell$
- $A'(i,j) = \{r_i,c_j\}$
- **(i,j)** is in the same co-cluster as **(i',j')** if $A'(i,j)=A'(i',j')$

From distance to points: Multi-dimensional scaling

Multi-Dimensional Scaling (MDS)

- So far we assumed that we know both data points **X** and distance matrix **D** between these points

- What if the original points **X** are not known but only distance matrix **D** is known?

- Can we reconstruct **X** or some approximation of **X**?

Problem

- Given distance matrix **D** between **n** points

- Find a **k**-dimensional representation of every x_i point **i**

- So that $d(x_i,x_j)$ is as close as possible to $D(i,j)$

Why do we want to do that?

How can we do that? (Algorithm)

High-level view of the MDS algorithm

- Randomly initialize the positions of **n** points in a **k**-dimensional space
- Compute pairwise distances **D'** for this placement
- Compare **D'** to **D**
- Move points to better adjust their pairwise distances (make **D'** closer to **D**)
- Repeat until **D'** is close to **D**

The MDS algorithm

- ***Input:*** **n×n** distance matrix **D**
- Random **n** points in the **k**-dimensional space **($x_1,\ldots,x_n$)**
- **stop = false**
- **while not stop**
  - **totalerror = 0.0**
  - For every **i,j** compute
    - **$D'(i,j)=d(x_i,x_j)$**
    - **error = $(D(i,j)-D'(i,j))/D(i,j)$**
    - **totalerror +=error**
    - **For** every dimension **m**: **$grad_{im} = (x_{im}-x_{jm})/D'(i,j)*error$**
  - **If totalerror** small enough, **stop = true**
  - **If(!stop)**
    - **For every point i and every dimension m: $x_{im}= x_{im} - rate*grad_{im}$**

Questions about MDS

- Running time of the MDS algorithm
  - **$O(n^2 I)$,** where **I** is the number of iterations of the algorithm

- MDS does not guarantee that metric property is maintained in **D'**