Unsupervised learning

Gosia Migut

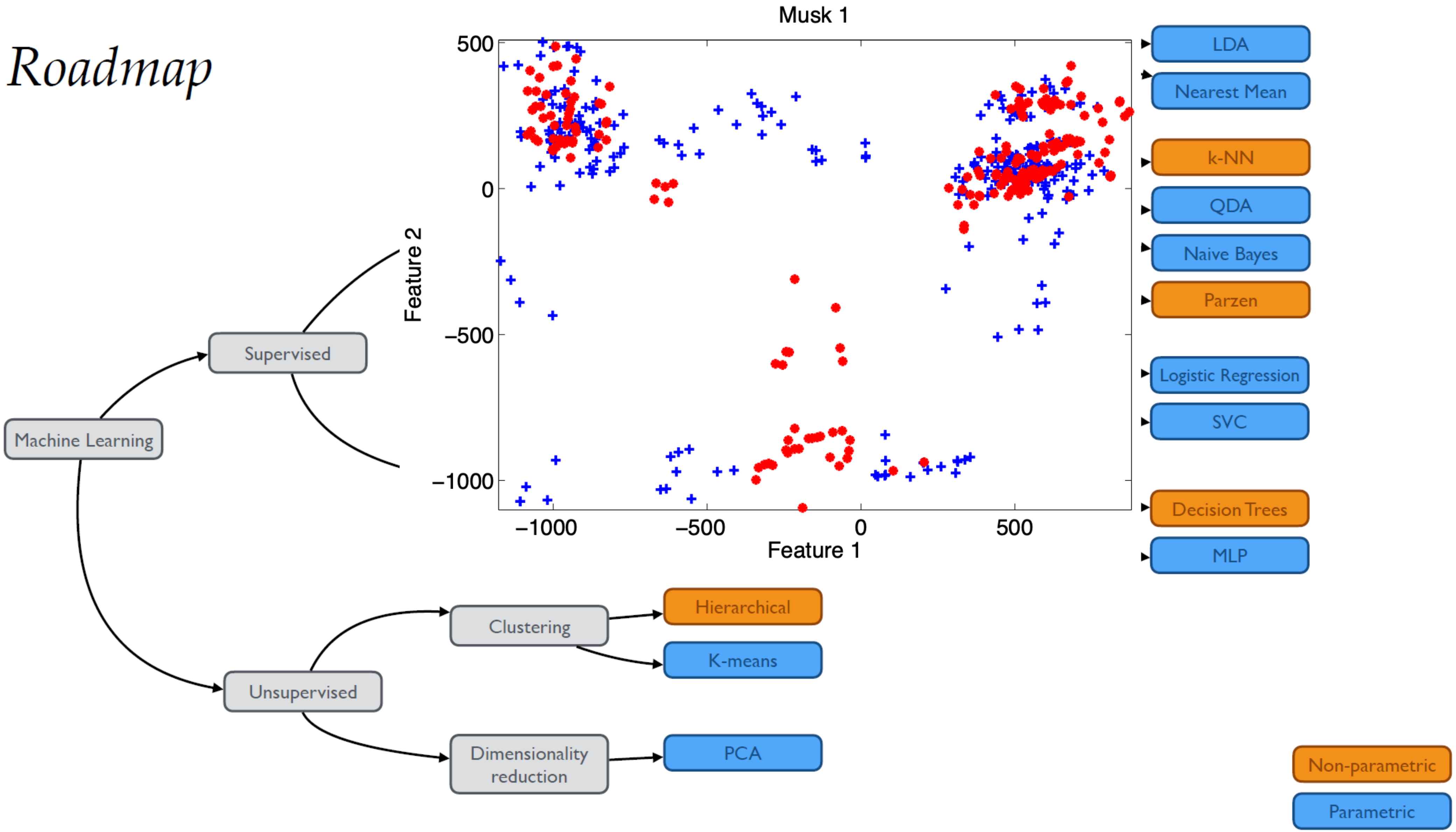
Admin stuff: schedule changes

7.1	18-10	Gosia Migut	Unsupervised Learning 1
7.2	20-10	Gosia Migut	Unsupervised Learning 2
8.1	25-10	Jesse Krijthe	Question & Answers lecture
8.2	27-10		No Lecture
9.1	**1-11**	Guest Lecturers	Convolutional Neural Networks & ML research in industry

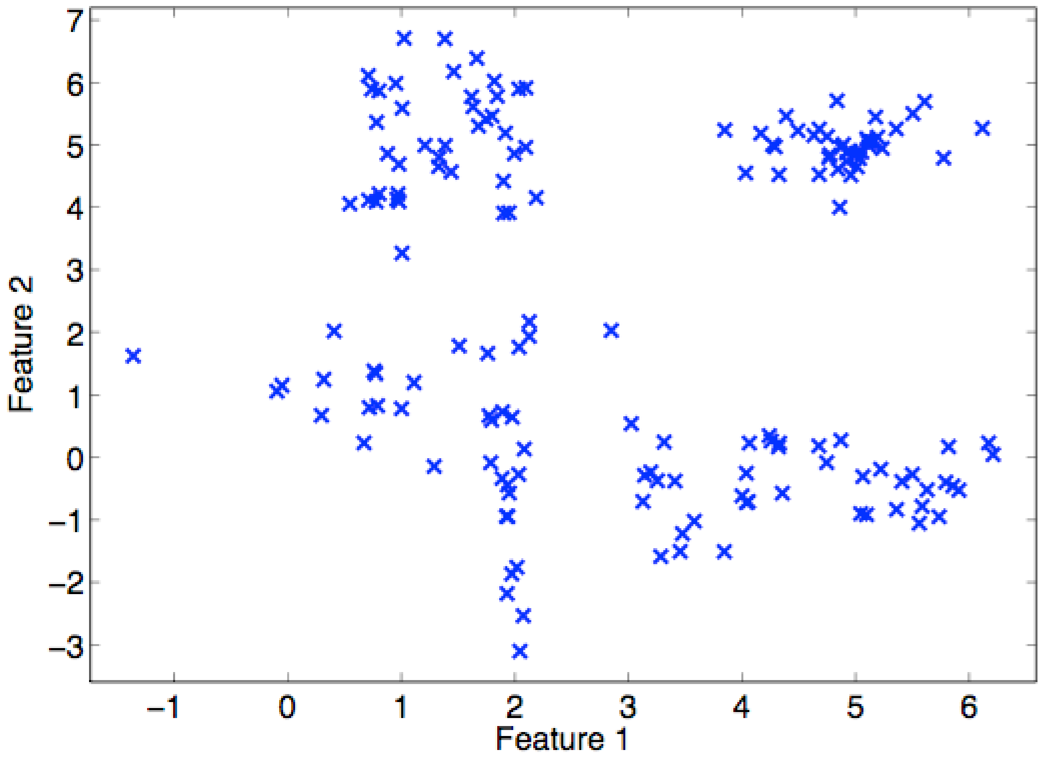
TU Delft

Machine learning

Roadmap



Unlabelled data: what now?



- Unsupervised learning: no labels/targets present

Unsupervised learning

- Clustering
  - Discover structures in unlabelled data

- Dimensionality reduction
  - does not use information about the labels

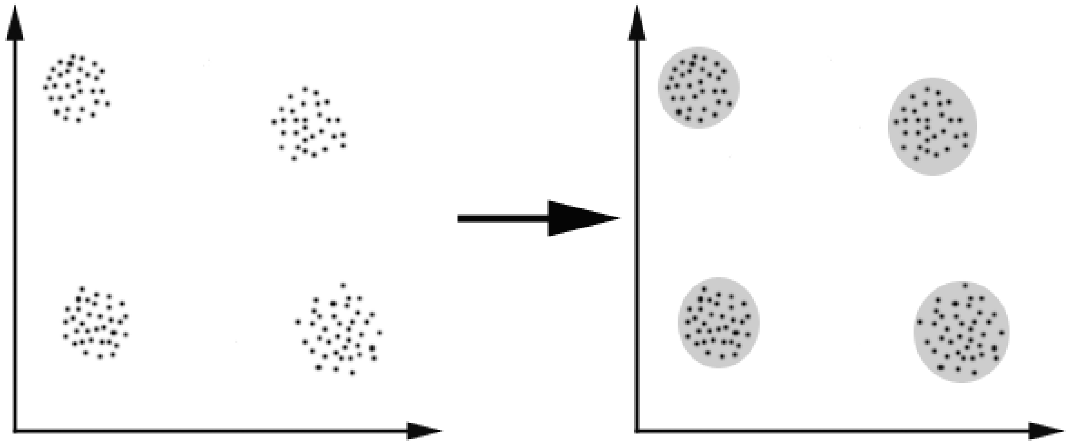
Clustering

Learning goals of today

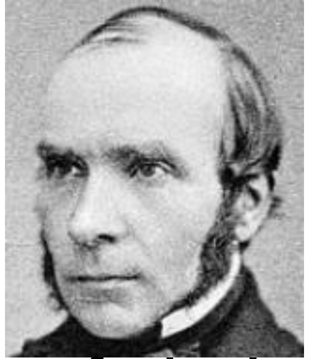
- Explain what clustering is and it’s applications
- Explain k-means algorithm
- Explain hierarchical clustering, single and complete link
- Pros and cons of k-means and hierarchical clustering
- Implement k-means

Clustering

- Finding natural groups in data where
  - Items within the group are close together
  - Items between groups are far apart



Historic application of clustering



- John Snow, a London physician plotted the locations of cholera deaths on a map during an outbreak in 1850s.

- The locations indicated that cases were clustered around certain intersections where there were polluted wells – exposing both the problem and the solution.

Clustering applications

- Market research: find groups of similar customers

- Social networks: find communities with similar interests / characteristics

- Recommender systems: find groups of users with similar ratings

What interesting clusterings / patterns can you find here? Take 3 minutes.

1

2

3

4

5

6

Clustering

- Clustering is best judged in context of application
  - Is the clustering good? If we can get some new / interesting insight from it
  - For one person a pattern is interesting, for another it's garbage

- In supervised learning: measure performance on test set, objective.
- In unsupervised learning: no clear performance measure, subjective.

What do we need for clustering?

1. Proximity measure, either
   - Similarity measure $s(x_i, x_k)$: large if $x_i \; and \; x_k$ are similar, or
   - Dissimilarity (distance) measure d(x_i, x_k): small if $x_i \; and \; x_k$ are similar

Distance measure

- Typically, we need to define a distance between objects first.
- Euclidean:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^{l} (x_i - y_i)^2}$$

- Manhattan:

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{l} |x_i - y_i|$$

More similarity measures

- Cosine similarity

$$s_{cos}(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}\| \|\mathbf{y}\|}$$

- Pearson's correlation coefficient

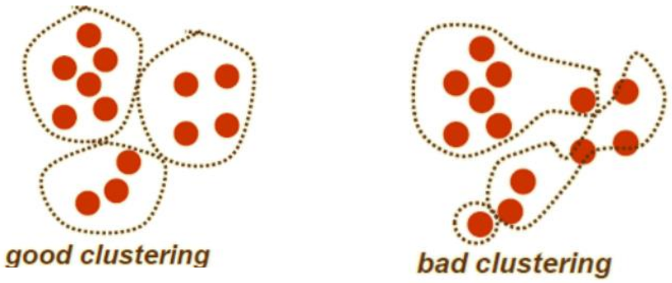
$$r_{Pearson}(\mathbf{x}, \mathbf{y}) = \frac{(\mathbf{x} - \mu_x)^T (\mathbf{y} - \mu_y)}{\|\mathbf{x} - \mu_x\| \|\mathbf{y} - \mu_y\|}$$

- and more... (for discrete features, mixed features, categorical features, ...)

What do we need for clustering?

1. Proximity measure, either
   - Similarity measure $s(x_i, x_k)$: large if x_i and x_k are similar, or
   - Dissimilarity (distance) measure d(x_i, x_k): small if x_i and x_k are similar

2. Method to evaluate a clustering



TU Delft

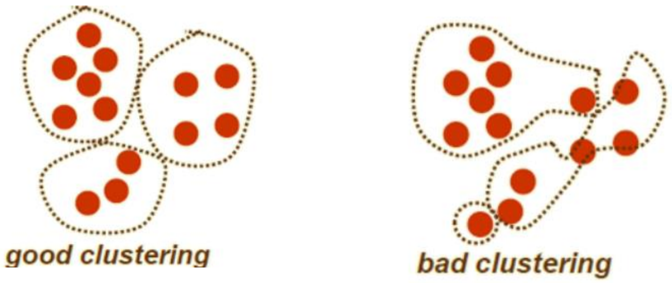
Cluster evaluation (a hard problem)

- Intra-cluster cohesion (compactness):
  - Cohesion measures how near the data points in a cluster are to the cluster's mean.
  - Sum of squared errors (SSE) is a commonly used measure.
- Inter-cluster separation (isolation):
  - Separation means that different cluster means should be far away from one another.
- In most applications, expert judgments are still the key

What do we need for clustering?

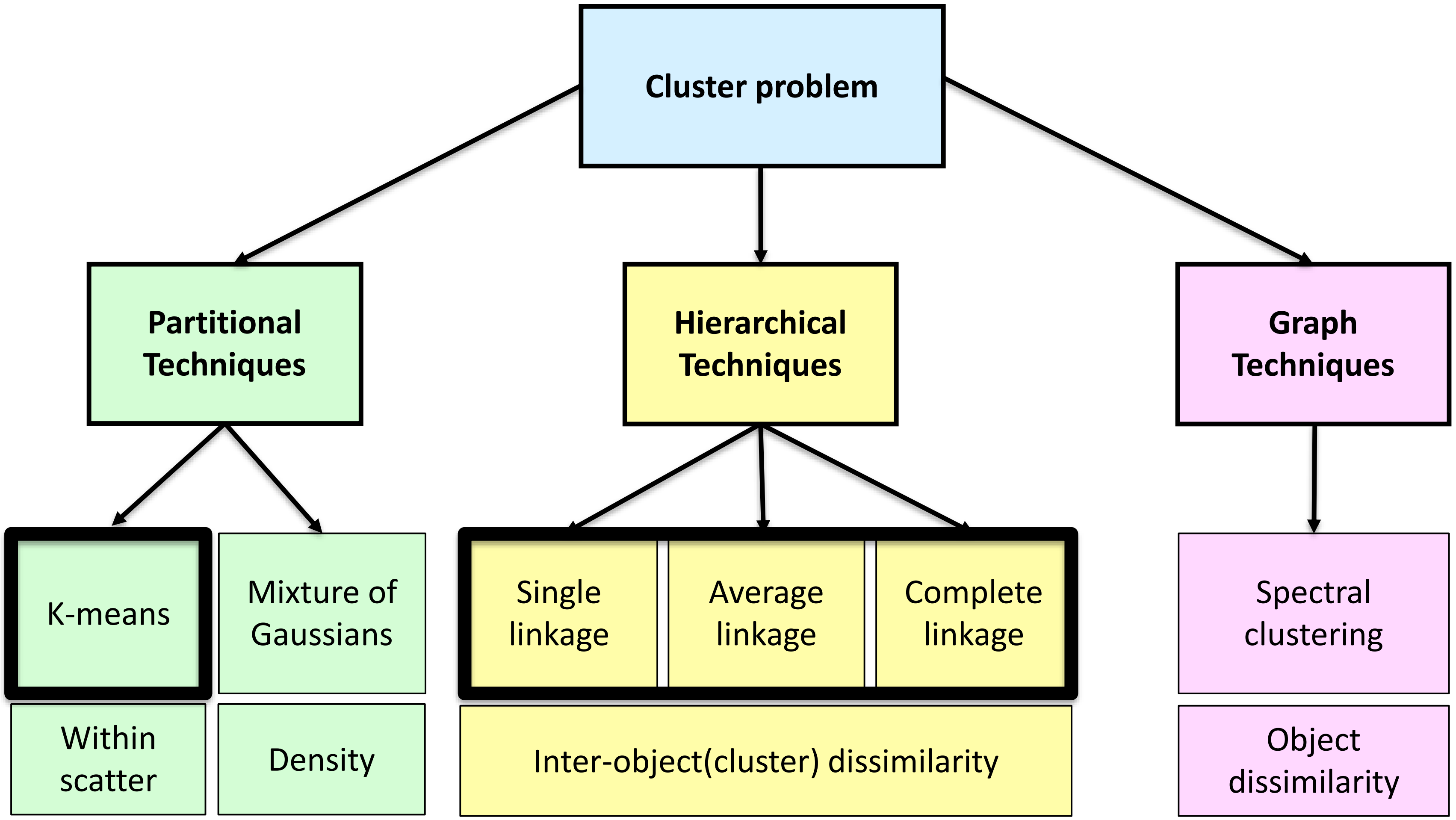
1. Proximity measure, either
   - Similarity measure $s(x_i, x_k)$: large if x_i and x_k are similar, or
   - Dissimilarity (distance) measure d(x_i, x_k): small if x_i and x_k are similar

2. Criterion function to evaluate a clustering



3. Algorithm to compute clustering
   - Eg. By optimizing the criterion function

Clustering techniques

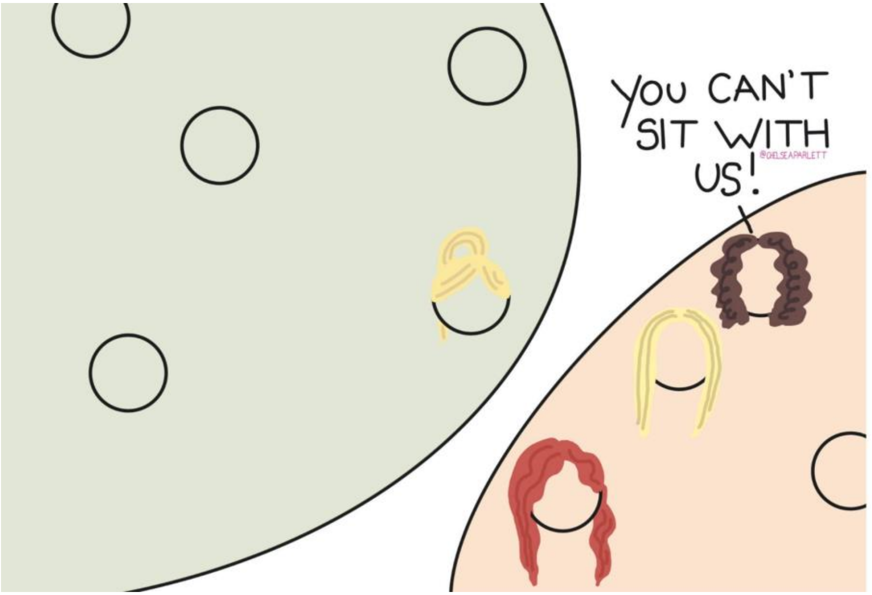


Hard vs. soft

- Hard assignments: each point assigned to 1 cluster
  - K-Means
  - Hierarchical clustering

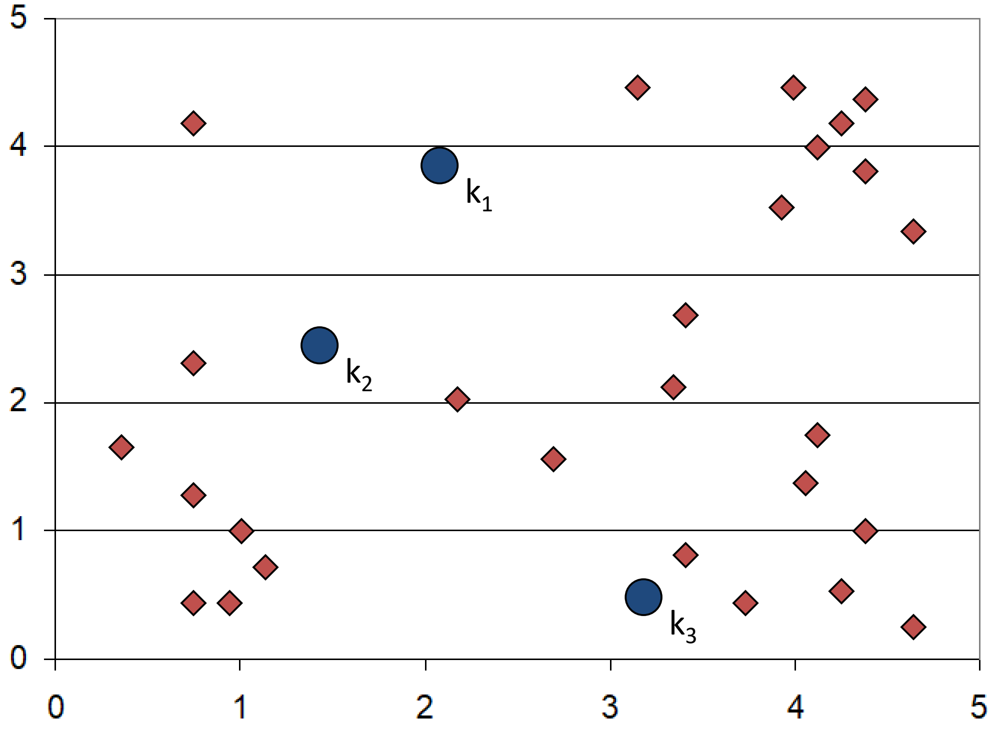
- Soft assignments: each point assigned cluster membership
  - Fuzzy C-means
  - Probabilistic mixture models

K-means clustering



K-means: how it works

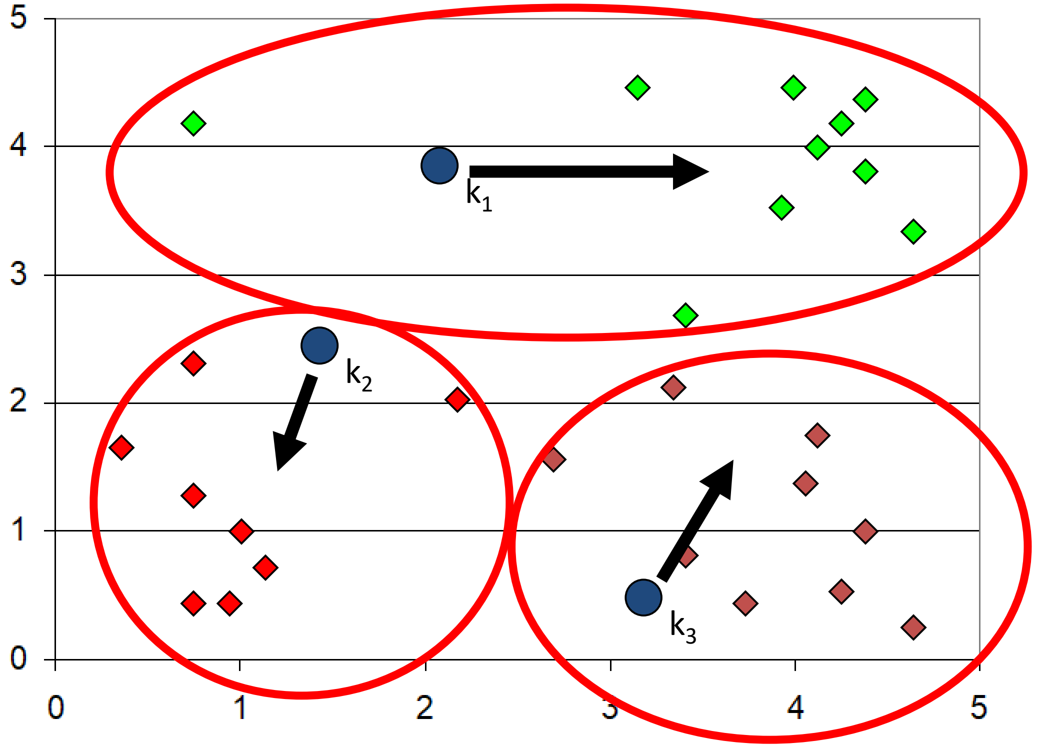
Choose k (random) seeds to be the initial centroids (cluster centers)



K-means: how it works

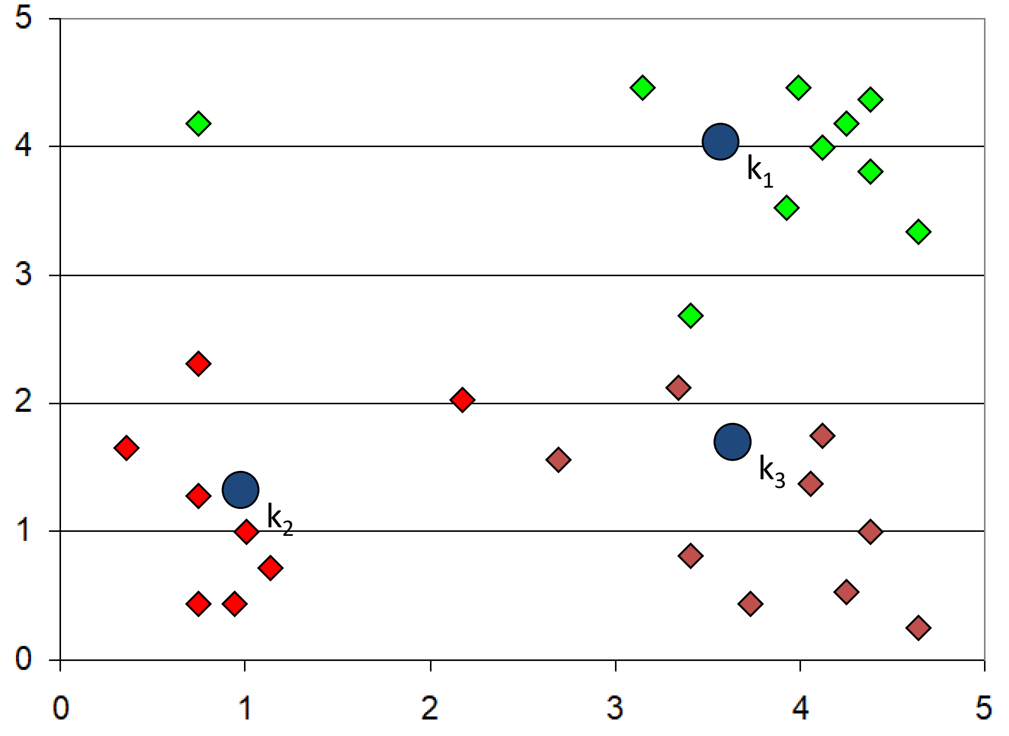
Assign each data point to the closest centroid

Re-compute the centroids using the current cluster memberships



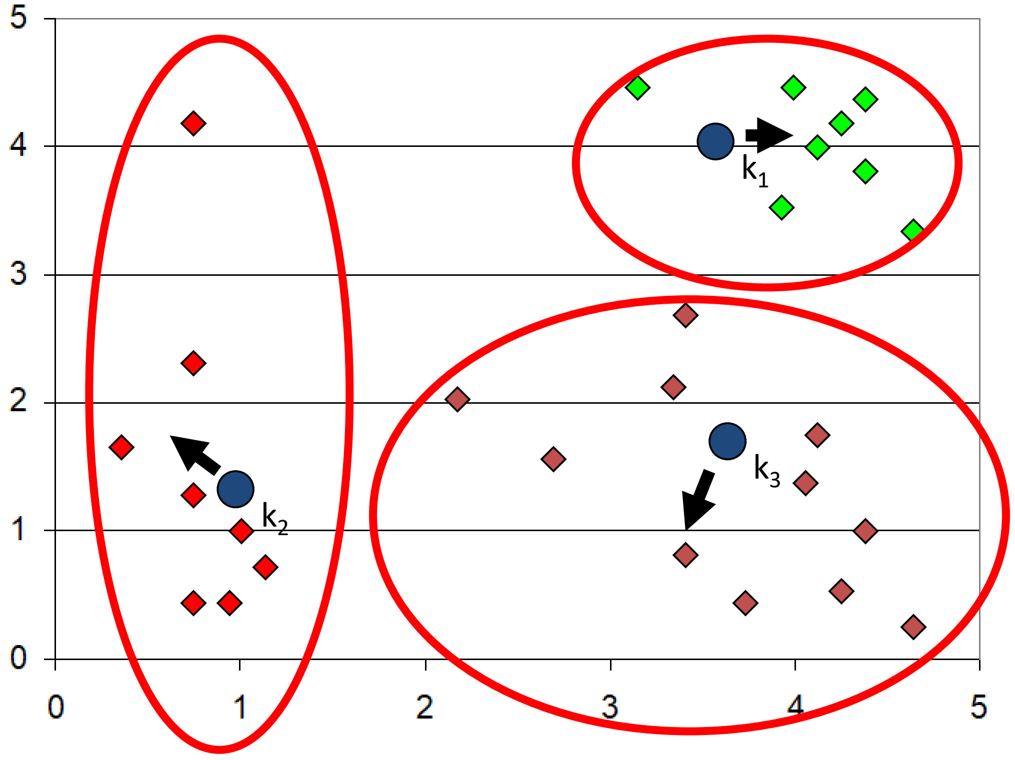
TU Delft

K-means: how it works



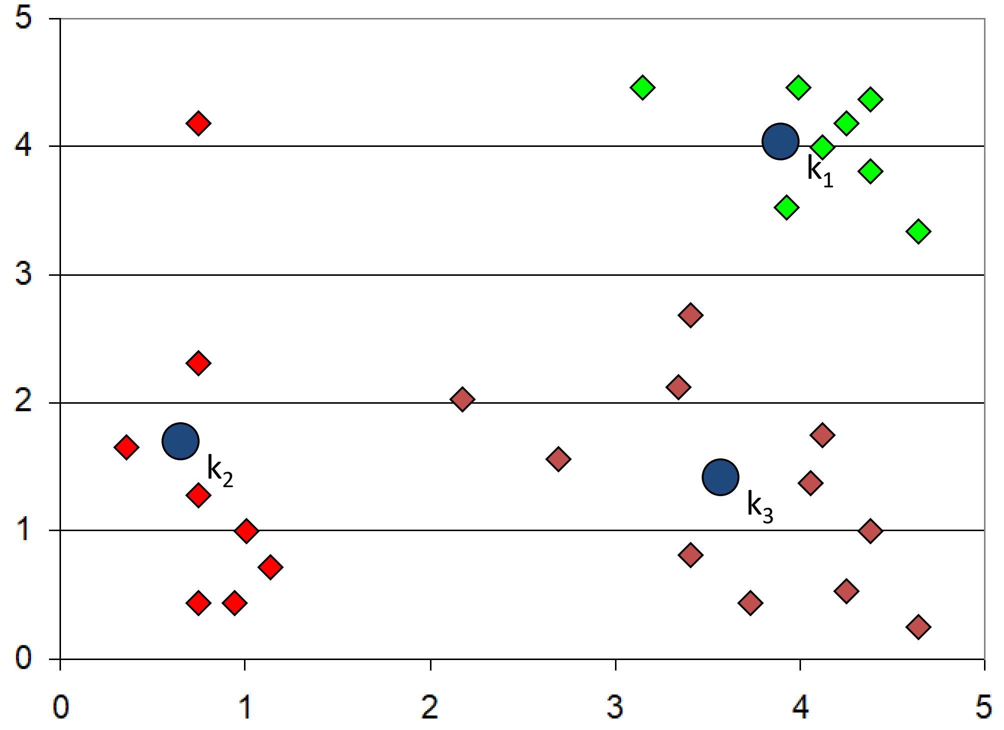
K-means: how it works

If a convergence criterion is not met, repeat steps 2 and 3



K-means: how it works

If a convergence criterion is not met, repeat steps



K-means algorithm

- Given k, the k-means algorithm works as follows:
  1. Choose k (random) data points (seeds) to be the initial centroids, cluster centers
  2. Assign each data point to the closest centroid
  3. Re-compute the centroids using the current cluster memberships
  4. If a convergence criterion is not met, repeat steps 2 and 3

K-means questions

- When do we know when to stop?
- What is it trying to optimize?
- How do we choose the number of centers (k)?
- Are we sure it will terminate?
- Are we sure it will find an optimal clustering?

K-means convergence (stopping) criterion

- no (or minimum) re-assignments of data points to different clusters, or
- no (or minimum) change of centroids, or
- minimum decrease in the sum of squared errors (SSE)

Sum of squared errors

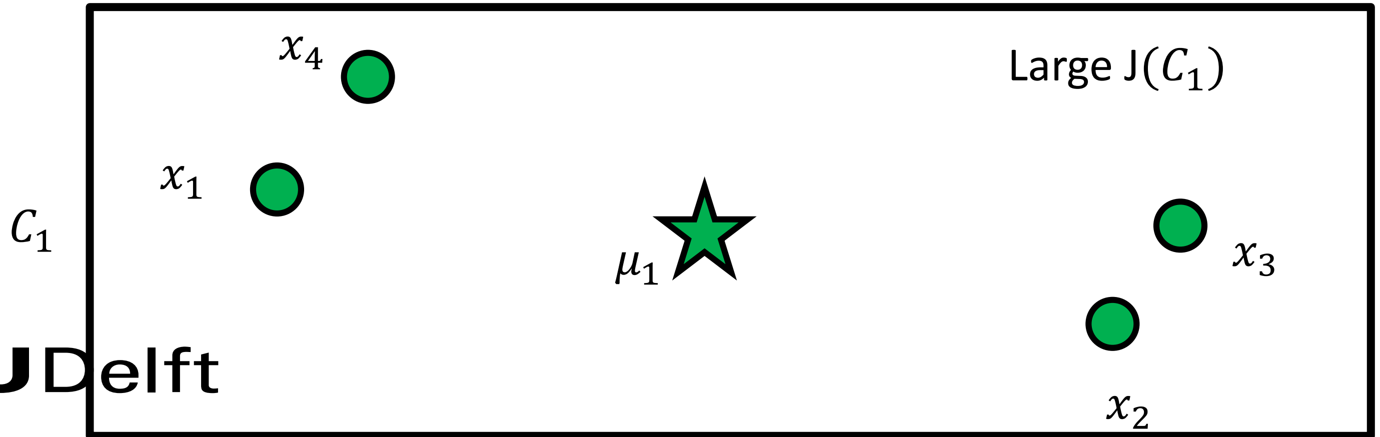
- Cost function (residual sum of squares, distortion, inertia, scatter, custer within variance): $\sum_k J(C_k)$

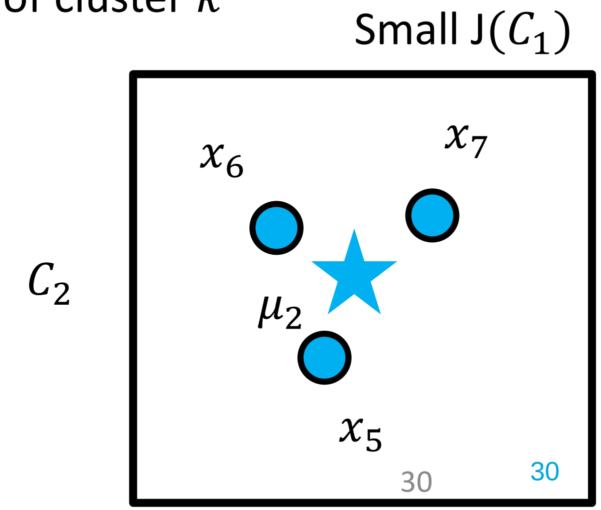
$$J(C_k) = \frac{1}{|C_k|}\sum_{i=1}^{m} ||x_i - \mu_{C_k}||^2$$

Sum over all objects x_i that belong to C_k

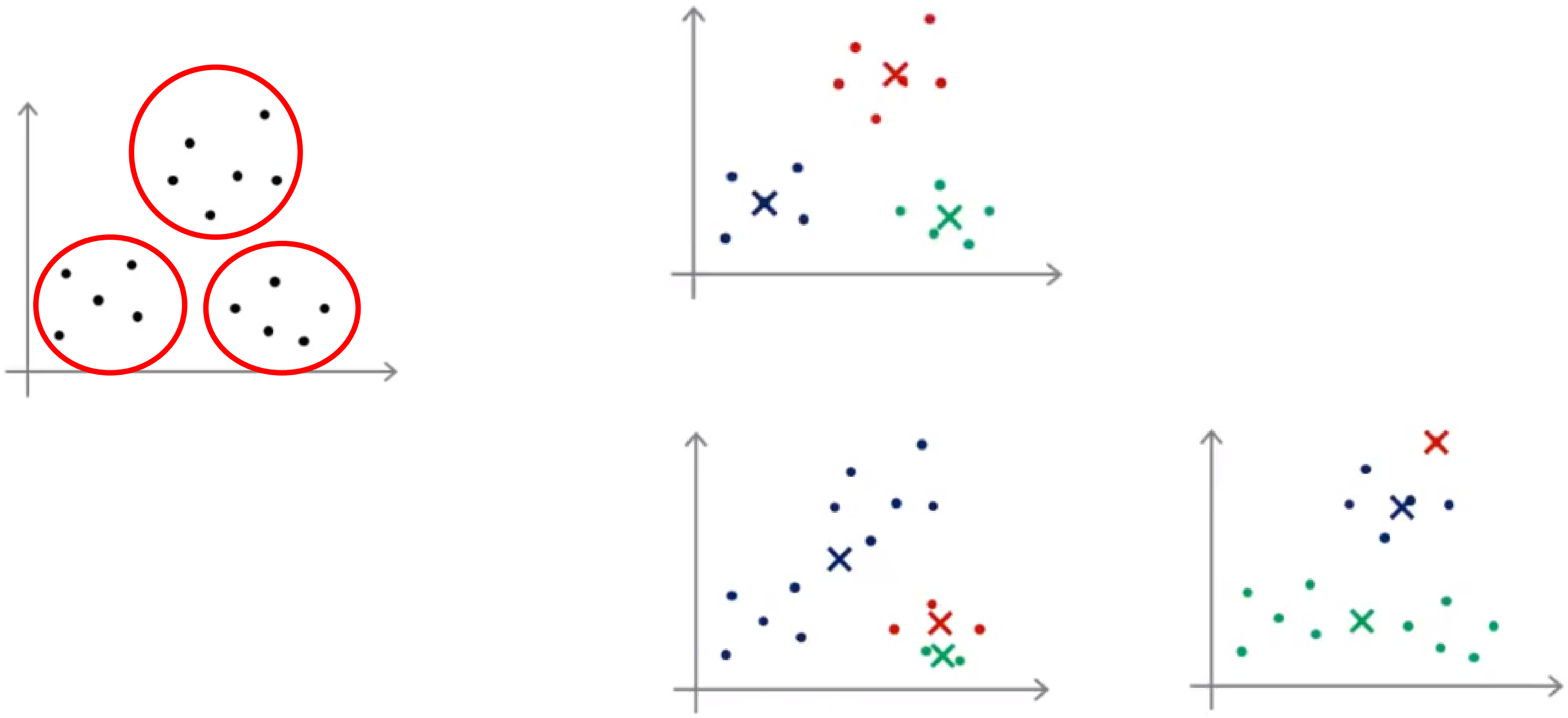
Cluster center of cluster k

objects in cluster C_k





Local optima



Random initialization

- For i=1 to 10000

  {

  Randomly initialize k means

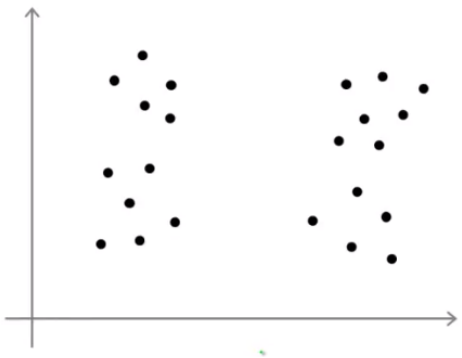
  Run k-means. Get centroids and means

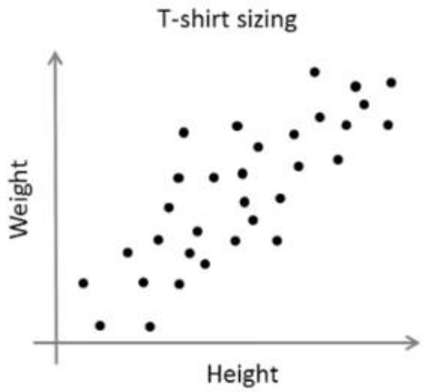
  Compute cost function J

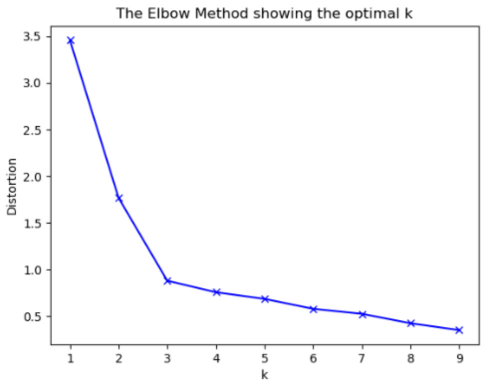
  }
- Pick clustering that gave lowest cost
- For high-dimensional data, many restarts are necessary (e.g. I = 10000)!

Choosing the number of clusters

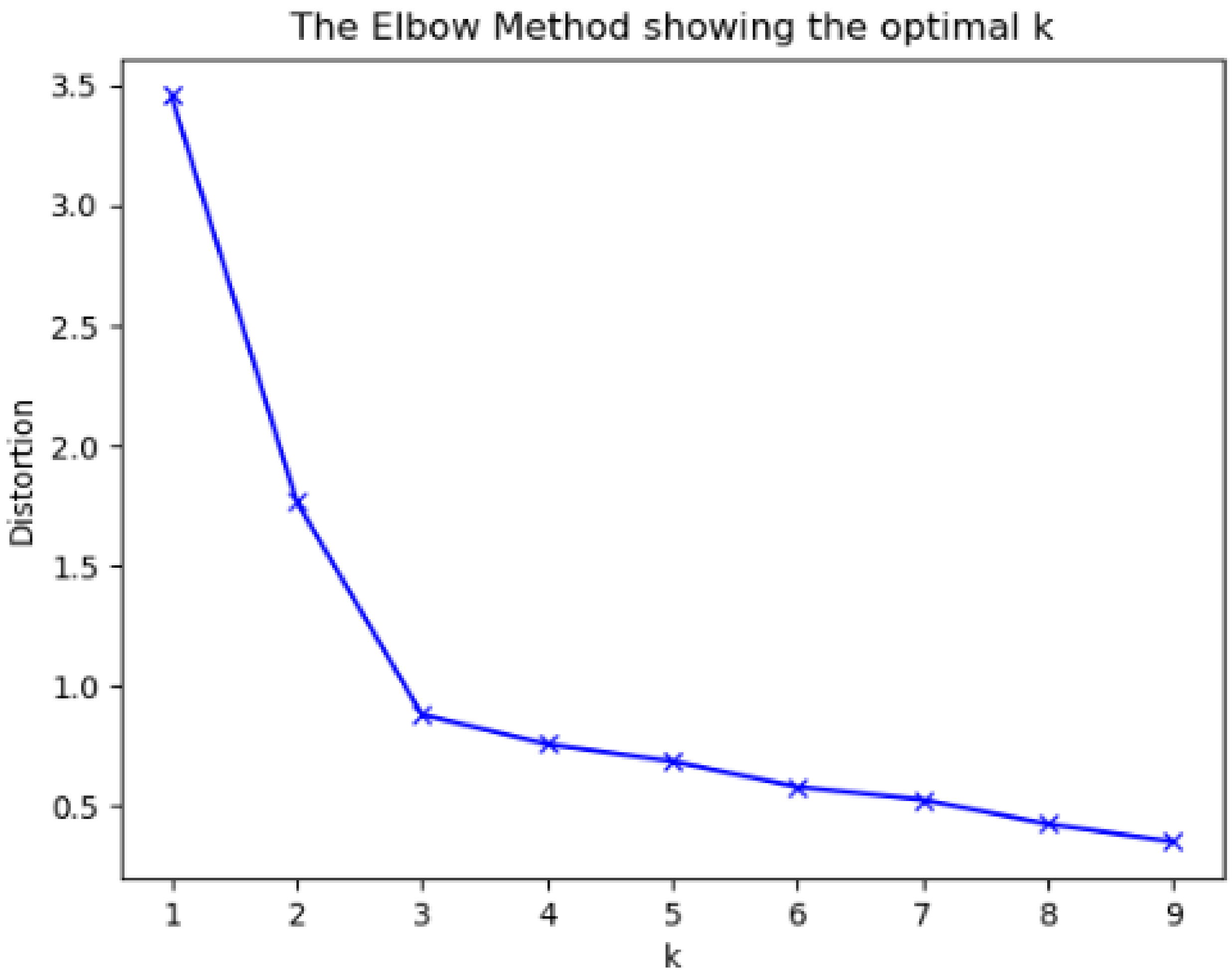
- Inspect visually
- Known purpose
- Elbow method





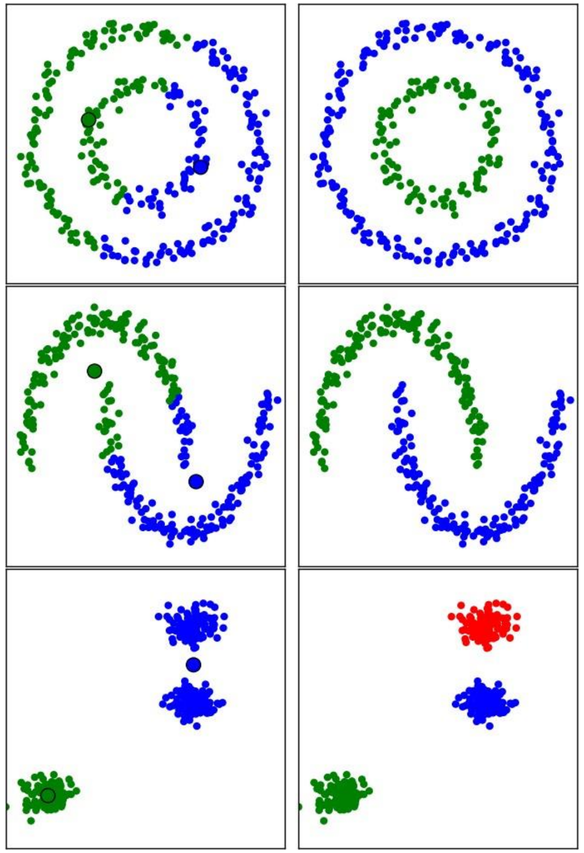


Elbow method



K-means summary

- Disadvantages:
  - Finds only convex clusters (“round shapes”)
  - doesn’t works for: non-spherical clusters, clusters of different sizes, different densities, outliers
  - Sensitive to initialization
  - Can get stuck in local minima
- Advantages:
  - Very simple
  - Fast



Interpret results carefully, ideally by hand (!) or with domain knowledge

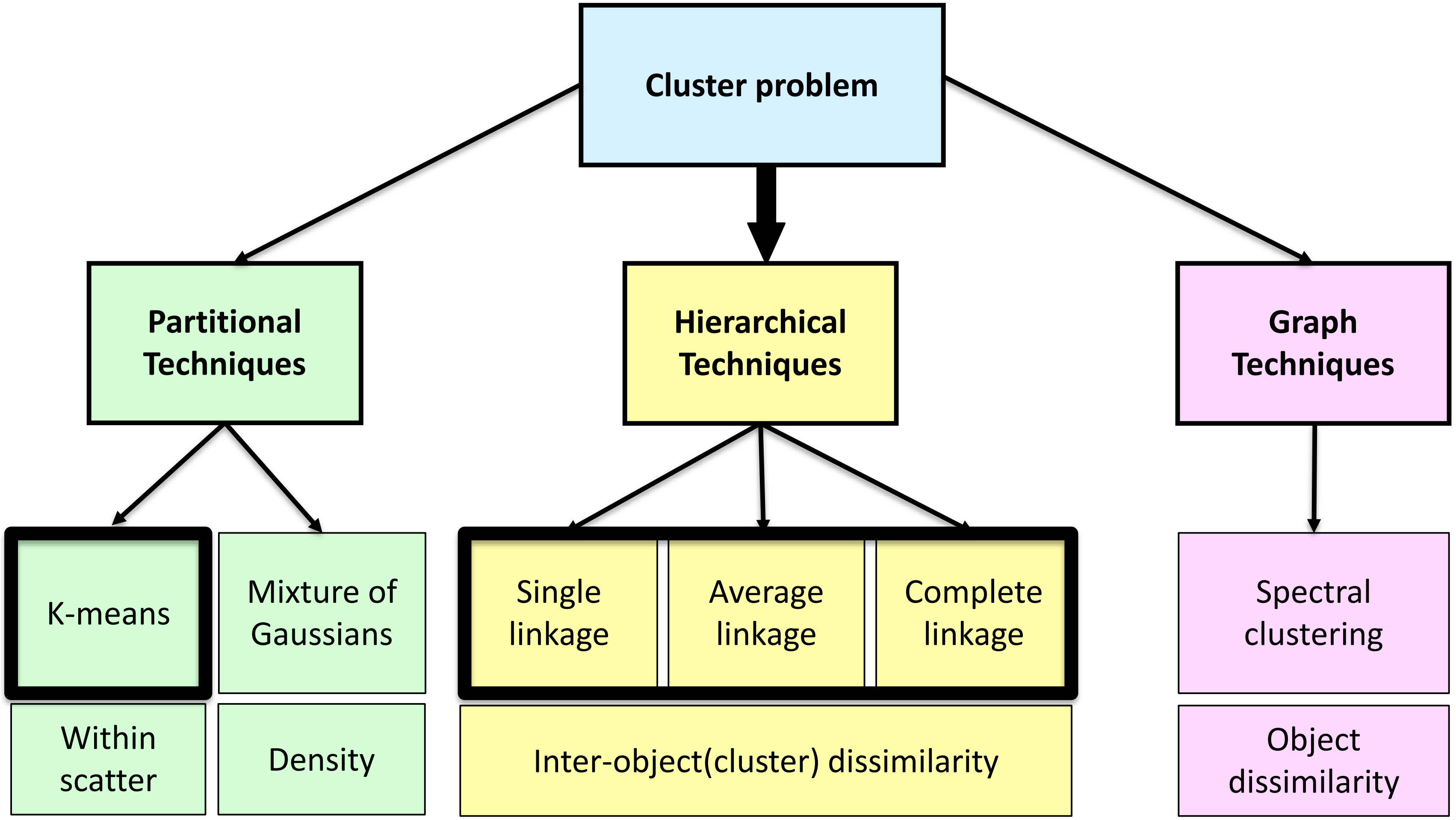
- Are the patterns found interesting? Subjective.

Example exercise

- Given are the following points:
  (1, 4), (2, 2), (5, 5), (4, 6),
  and two cluster centroids:
  $\mu_1 = (1, 2)$, $\mu_2 = (6, 6)$.

- What is the value of the k-means cost function (SSE)?

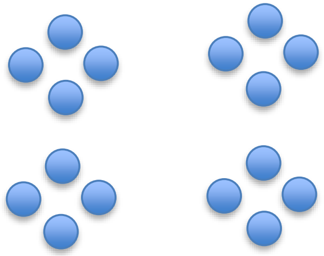
Clustering techniques



TUDelft

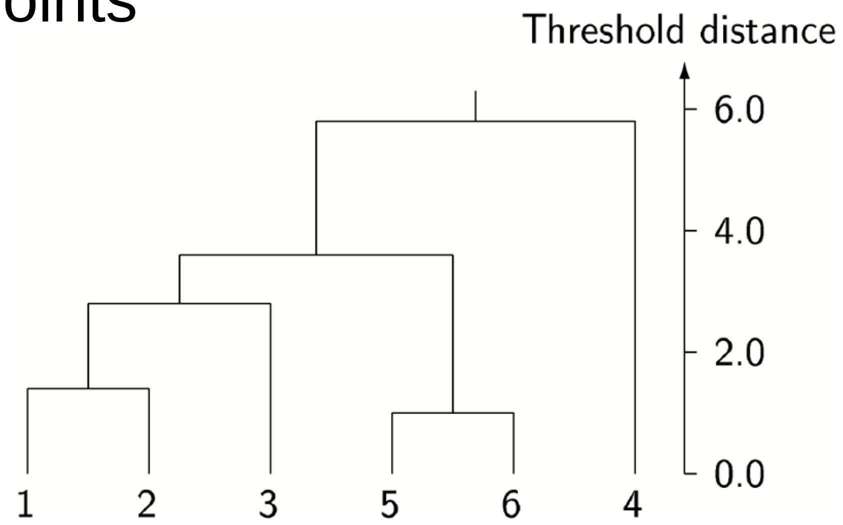
Hierarchical clustering

Hierarchical clustering



- Selecting k is a problem of granularity
  - How course or fine-grained is the structure in the data?
  - No cluster algorithm able to pick k

- Instead of picking k find a hierarchy of structure
  - Course effects: top level contains all points
  - Fine-grained: bottom level
    one cluster per data point



Hierarchical clustering approaches

- Agglomerative (bottom-up):
  - each point starts as cluster
  - group two closest clusters
  - stop at some point

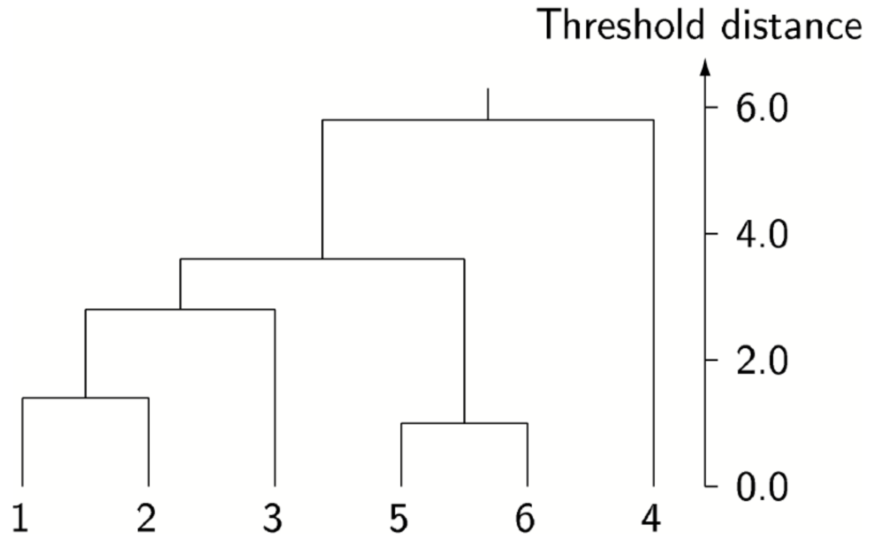


Figure 11.1 Dendrogram.

Hierarchical clustering approaches

- Divisive (top-down):
  - all points start in one cluster
  - split cluster in some sensible way
  - stop at some point

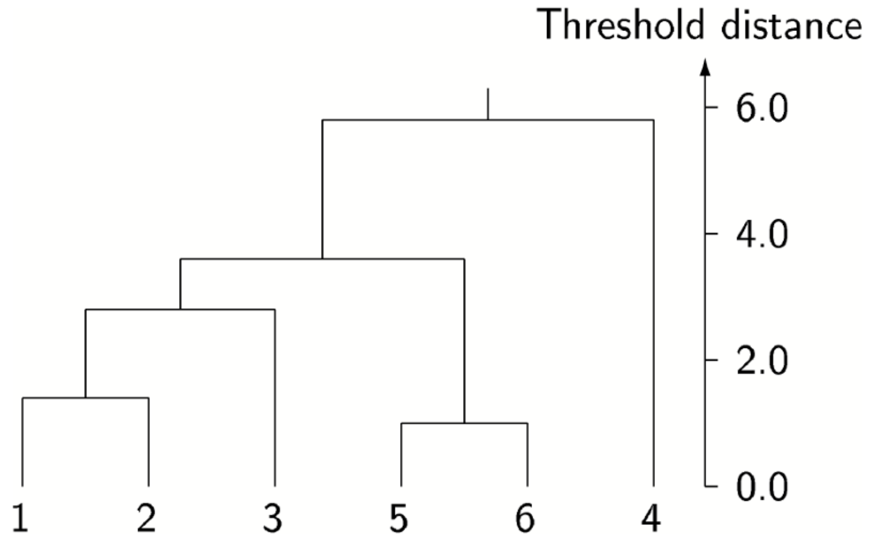
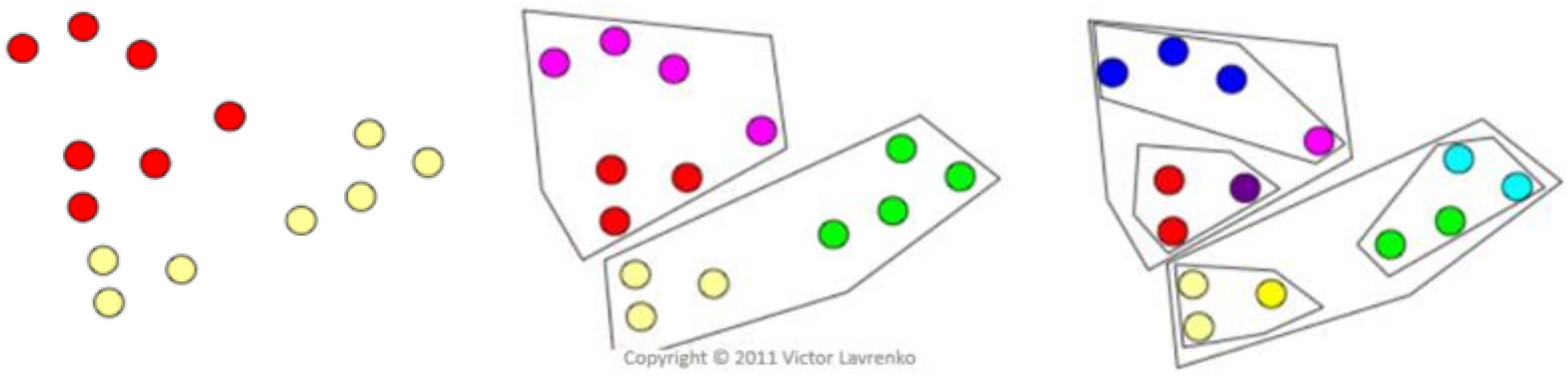


Figure 11.1 Dendrogram.

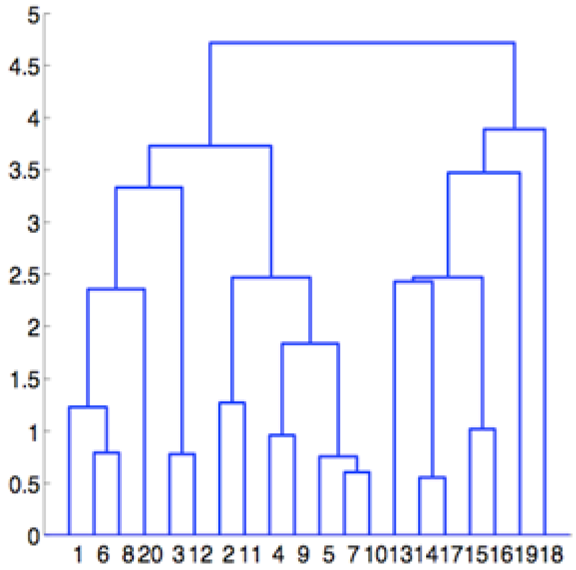
Divisive: hierarchical k-means

- Apply k-means recursively:
  - Run k-mean on the original data for k=2
  - For each of the resulting clusters run k-means with k=2



Agglomerative clustering

- Starting from individual observations, produce sequence of clusterings of increasing size
- At each level, two clusters chosen by criterion are merged



dendrogram

TU Delft

Agglomerative clustering

1. Determine distances between all clusters
2. Merge clusters that are closest
3. IF #clusters>1 THEN GOTO 1

- Which clusters to start with?
- What is the distance between clusters?
- Final number of clusters?

Different merging rules

- **Single linkage:** two nearest objects in the clusters :

$$g(R,S) = min_{ij}\{d(x_i, x_j): x_i \in R, x_j \in S\}$$

- **Complete linkage**: two most remote objects in the clusters :

$$g(R,S) = max_{ij}\{d(x_i, x_j): x_i \in R, x_j \in S\}$$

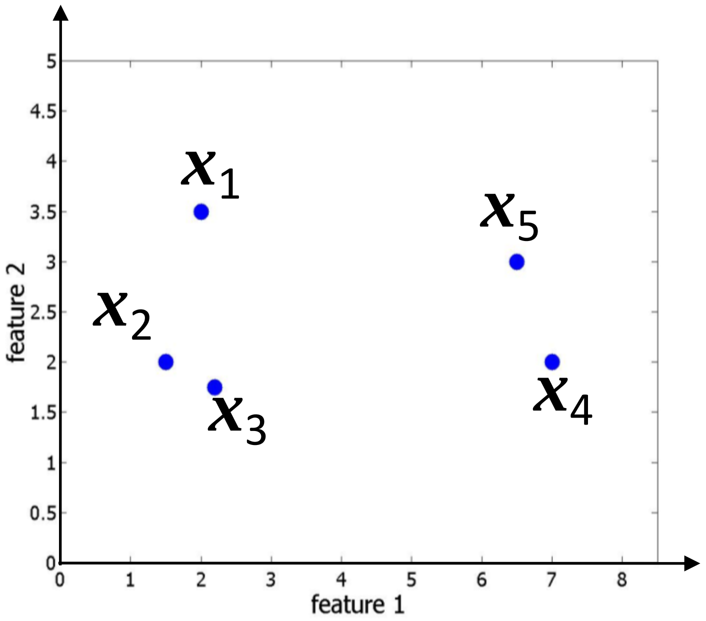
- **Average linkage**: cluster centres :

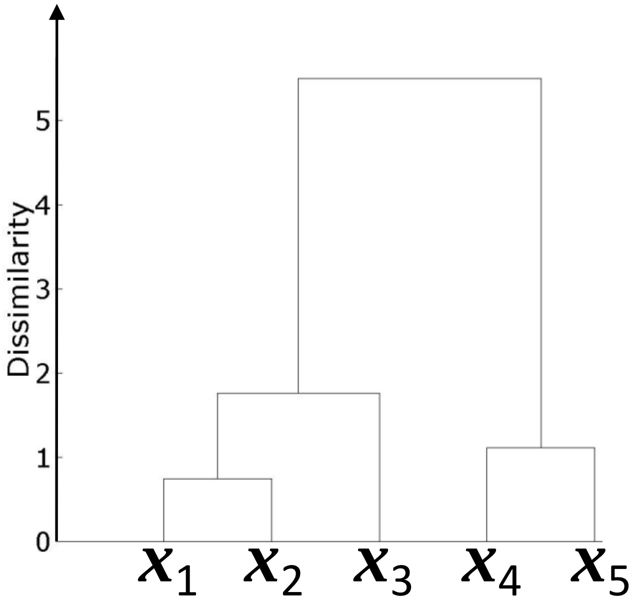
$$g(R,S) = \frac{1}{|R||S|}\sum_{ij}\{d(x_i, x_j): x_i \in R, x_j \in S\}$$

TU Delft

Agglomerative clustering: how it works

- Input:
  - dataset, $\boldsymbol{X}$: [n x p], or directly:
  - dissimilarity matrix, $\boldsymbol{D}$: [n x n]
  - linkage type
- Output:
  - dendrogram

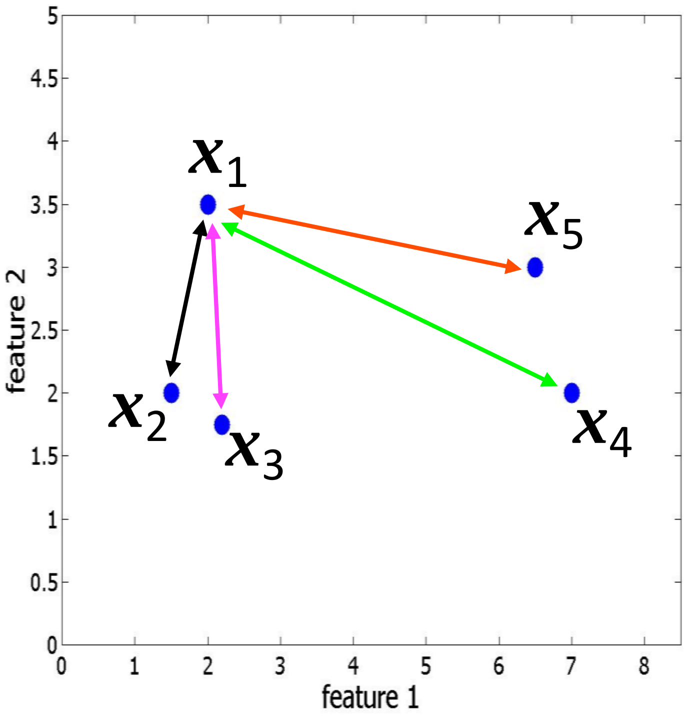




Agglomerative clustering

- **Step 0:** each object is a cluster:

Dataset

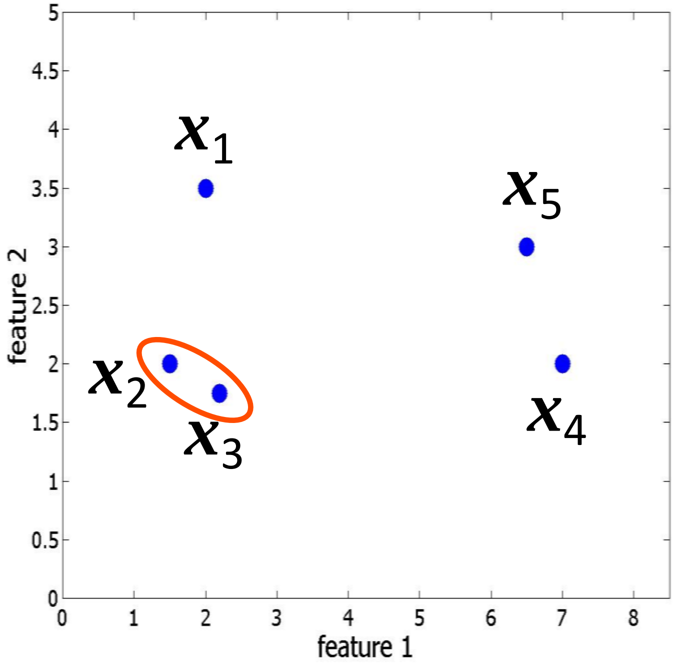


(Euclidean) distance matrix, $\boldsymbol{D}$

	x_1	x_2	x_3	x_4	x_5
x_1	0.00	$\boxed{1.58}$	$\boxed{1.76}$	$\boxed{5.22}$	$\boxed{4.53}$
x_2		0.00	0.74	5.50	5.10
x_3			0.00	4.81	4.48
x_4				0.00	1.12
x_5					0.00

Agglomerative clustering

- **Step 1:**
  Find the most similar pair: $\min_{(i,j)}\{d(i,j)\} = d(2,3)$

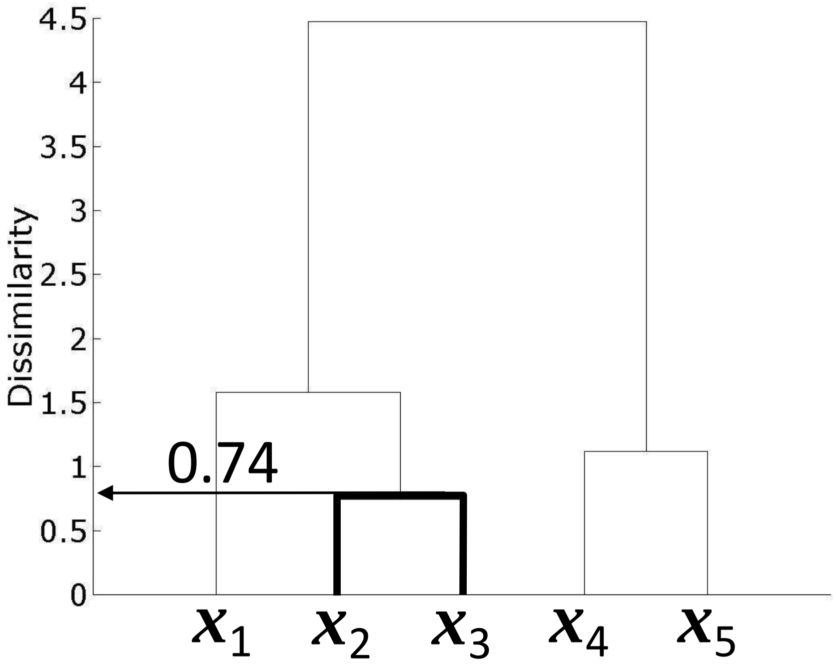


	x_1	x_2	x_3	x_4	x_5
x_1	0.00	1.58	1.76	5.22	4.53
x_2		0.00	$\boxed{0.74}$	5.50	5.10
x_3			0.00	4.81	4.48
x_4				0.00	1.12
x_5					0.00

TUDelft

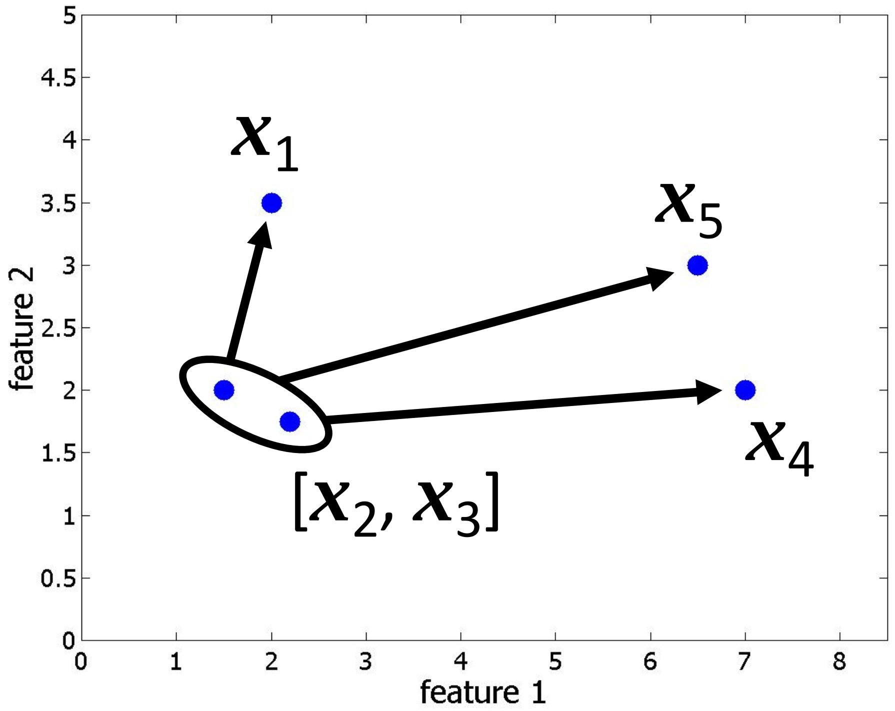
Agglomerative clustering

- **Step 2:**
  Merge $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$ into a single object, $[\boldsymbol{x}_2, \boldsymbol{x}_3]$;



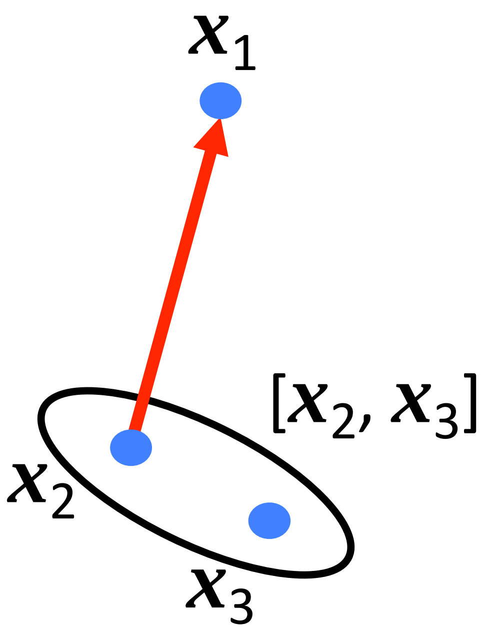
Agglomerative clustering

- **Step 3:**
  Recompute $\boldsymbol{D}$ – what is the distance between $[\boldsymbol{x}_2, \boldsymbol{x}_3]$ and the rest?



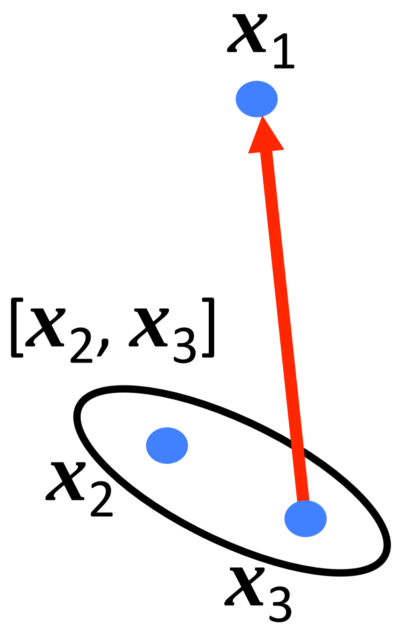
Agglomerative clustering

- **Step 3:**
  Recompute $\boldsymbol{D}$ – **single linkage:** $d([\mathbf{x}_2,\mathbf{x}_3],\mathbf{x}_1) = \min(d(\mathbf{x}_1,\mathbf{x}_2),d(\mathbf{x}_1,\mathbf{x}_3))$



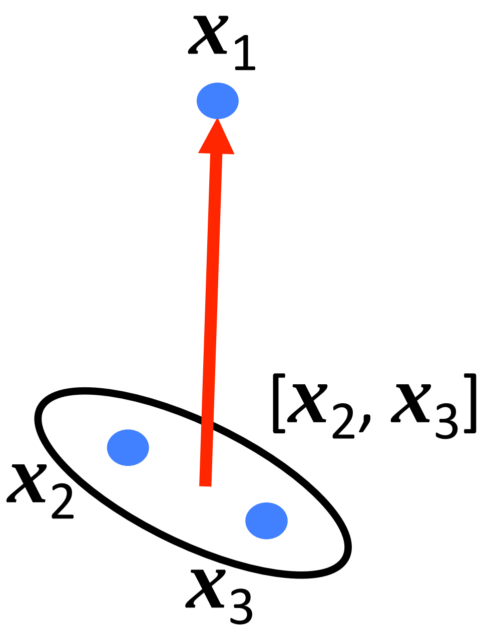
Agglomerative clustering

- **Step 3:**
  Recompute $\boldsymbol{D}$ – **complete linkage:** $d([\mathbf{x}_2,\mathbf{x}_3],\mathbf{x}_1) = \max(d(\mathbf{x}_1,\mathbf{x}_2),d(\mathbf{x}_1,\mathbf{x}_3))$



Agglomerative clustering

- **Step 3:**
  Recompute $\boldsymbol{D}$ – **average linkage:** $d([\boldsymbol{x}_2,\boldsymbol{x}_3],\boldsymbol{x}_1) = \text{mean}(d(\boldsymbol{x}_1,\boldsymbol{x}_2),d(\boldsymbol{x}_1,\boldsymbol{x}_3))$



Agglomerative clustering

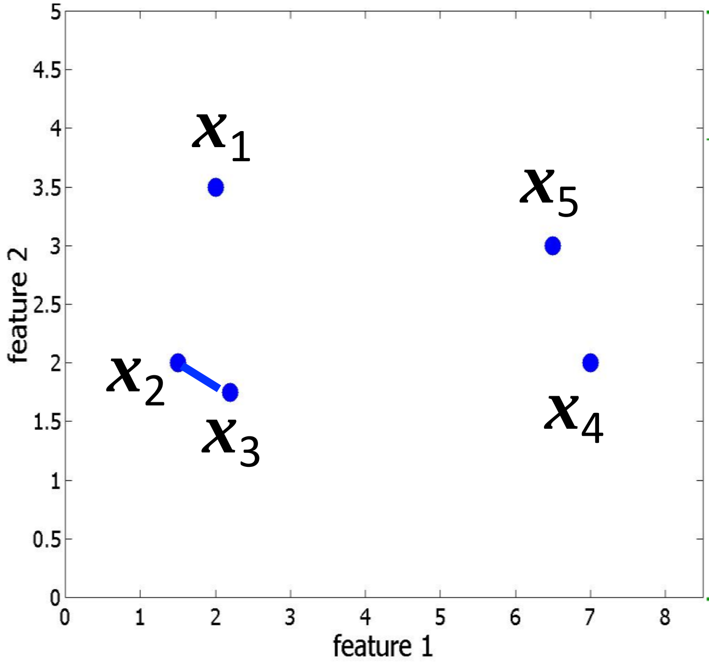
- **Step 3:**
  Recompute $\boldsymbol{D}$ – **single linkage:**

	x_1	$[x_2,x_3]$	x_4	x_5
x_1	0.00	1.58	5.22	4.53
$[x_2,x_3]$		0.00	4.81	4.48
x_4			0.00	1.12
x_5				0.00

TUDelft

Agglomerative clustering

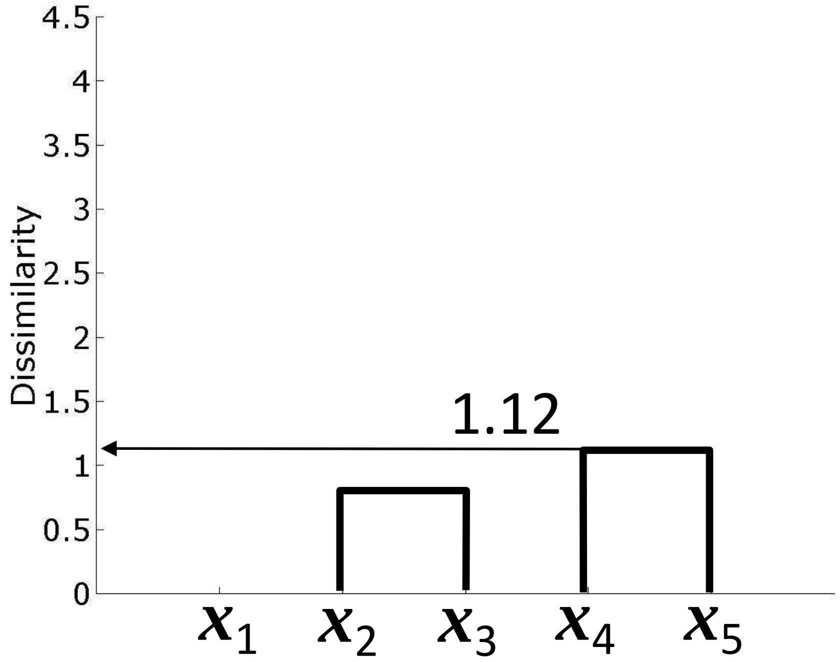
- **Repeat, step 1:**
  Find the most similar pair of objects: $\min_{(i,j)}\{d(i,j)\} = d(4,5)$



	x_1	$[x_2,x_3]$	x_4	x_5
x_1	0.00	1.58	5.22	4.53
$[x_2,x_3]$	1.58	0.00	4.81	4.48
x_4	5.22	4.81	0.00	$\boxed{1.12}$
x_5	4.53	4.48	1.12	0.00

Agglomerative clustering

- **Repeat, step 2:**
  Merge $\boldsymbol{x}_4$ and $\boldsymbol{x}_5$ into a single object, $[\boldsymbol{x}_4,\boldsymbol{x}_5]$;



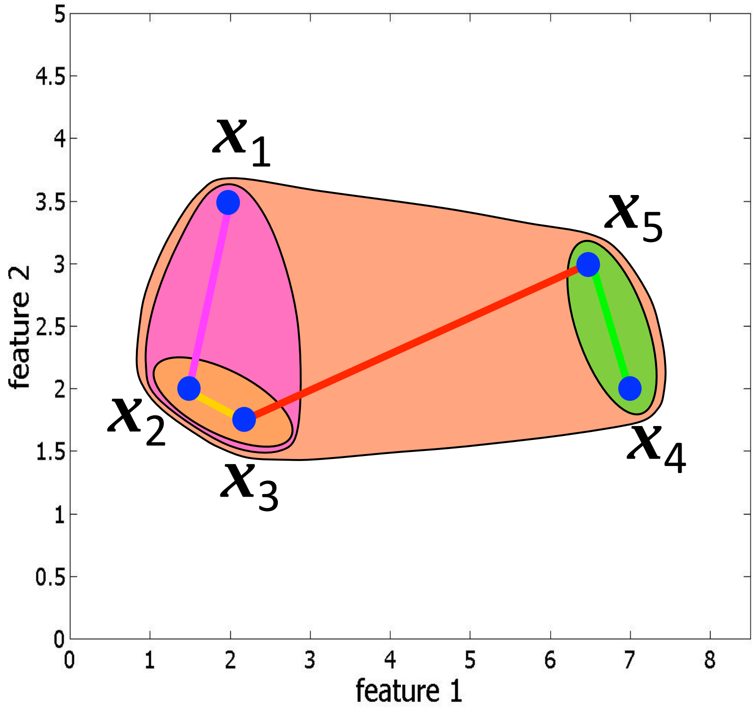
Agglomerative clustering

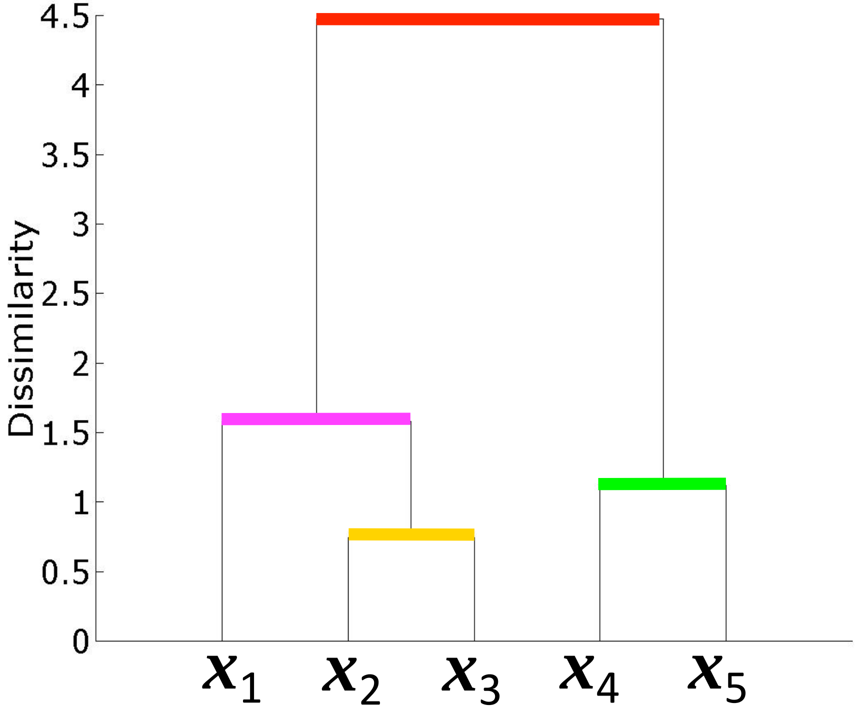
- **Repeat, step 3:**
  Recompute $\boldsymbol{D}$ (single linkage):

	x_1	$[x_2,x_3]$	$[x_4,x_5]$
x_1	0.00	1.58	4.53
$[x_2,x_3]$		0.00	4.48
$[x_4,x_5]$			0.00

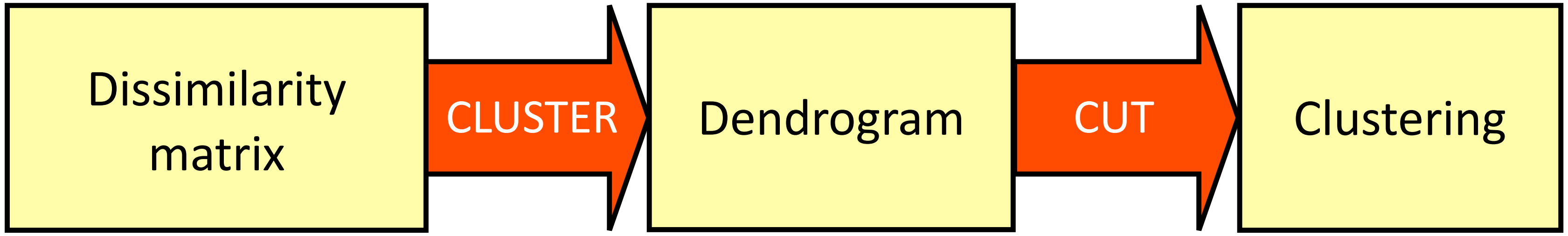
Agglomerative clustering

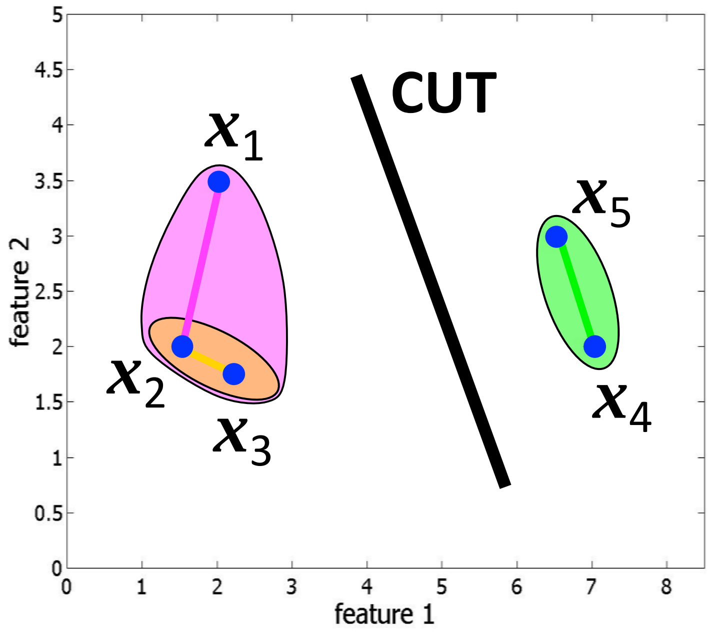
- Repeat steps 1-3 untill a single cluster remains

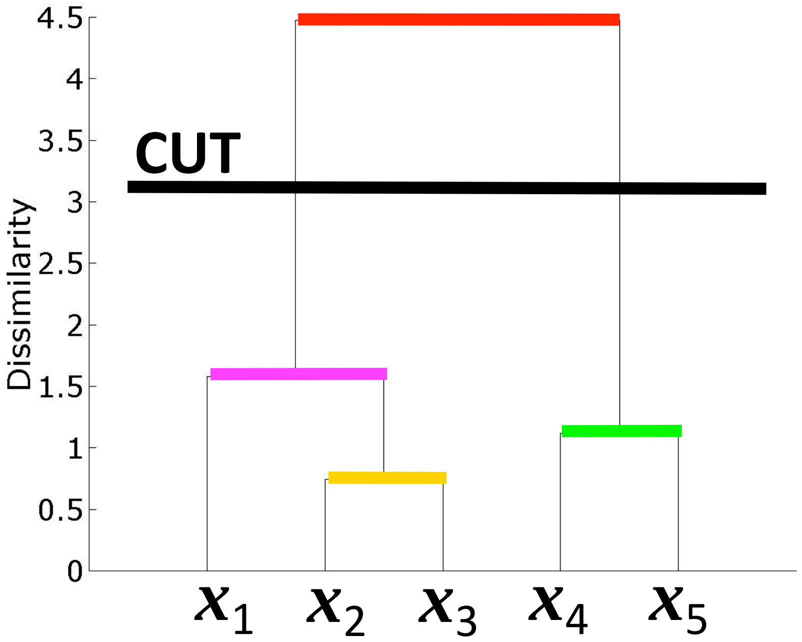




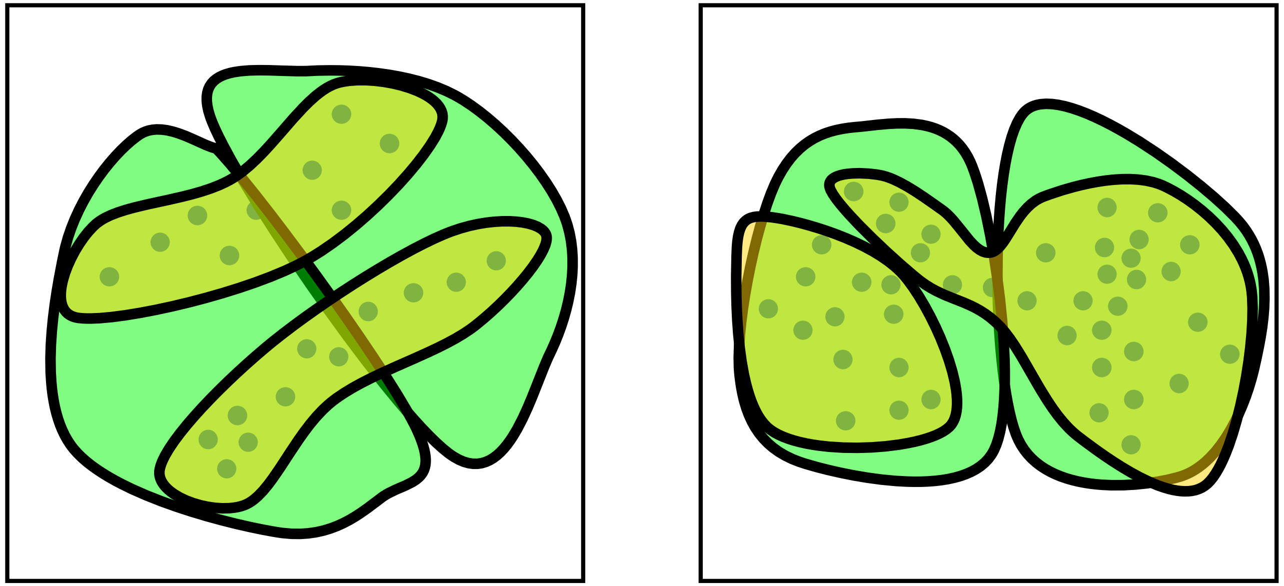
Agglomerative clustering







Linkage and cluster shape



Complete linkage

Single linkage

Question: hierarchical clustering

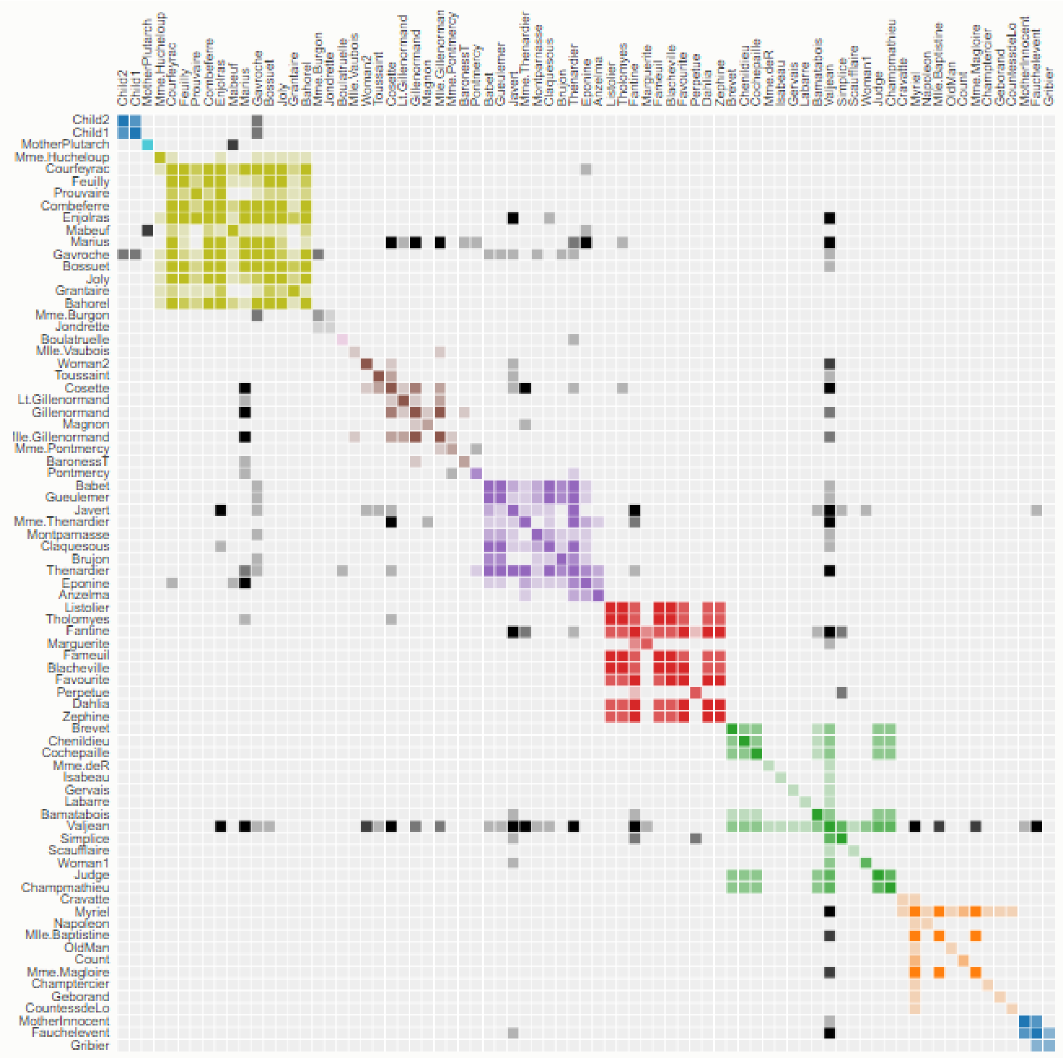
- Given is a dataset: (4, 10), (7,10), (4, 8), (10, 5), (11, 4), (3, 4), (9, 3), (5, 2)
- Cluster the points using agglomerative clustering
- Use single link method with Euclidean distance
- Stopping criterion: 3 clusters
- Detail your methodology, show steps and dendrogram

Hierarchical clustering summary

- Pros
  - Dendrogram gives overview of all possible clusterings
  - Linkage type allows to find clusters of varying shapes
  - Different dissimilarity measures can be used

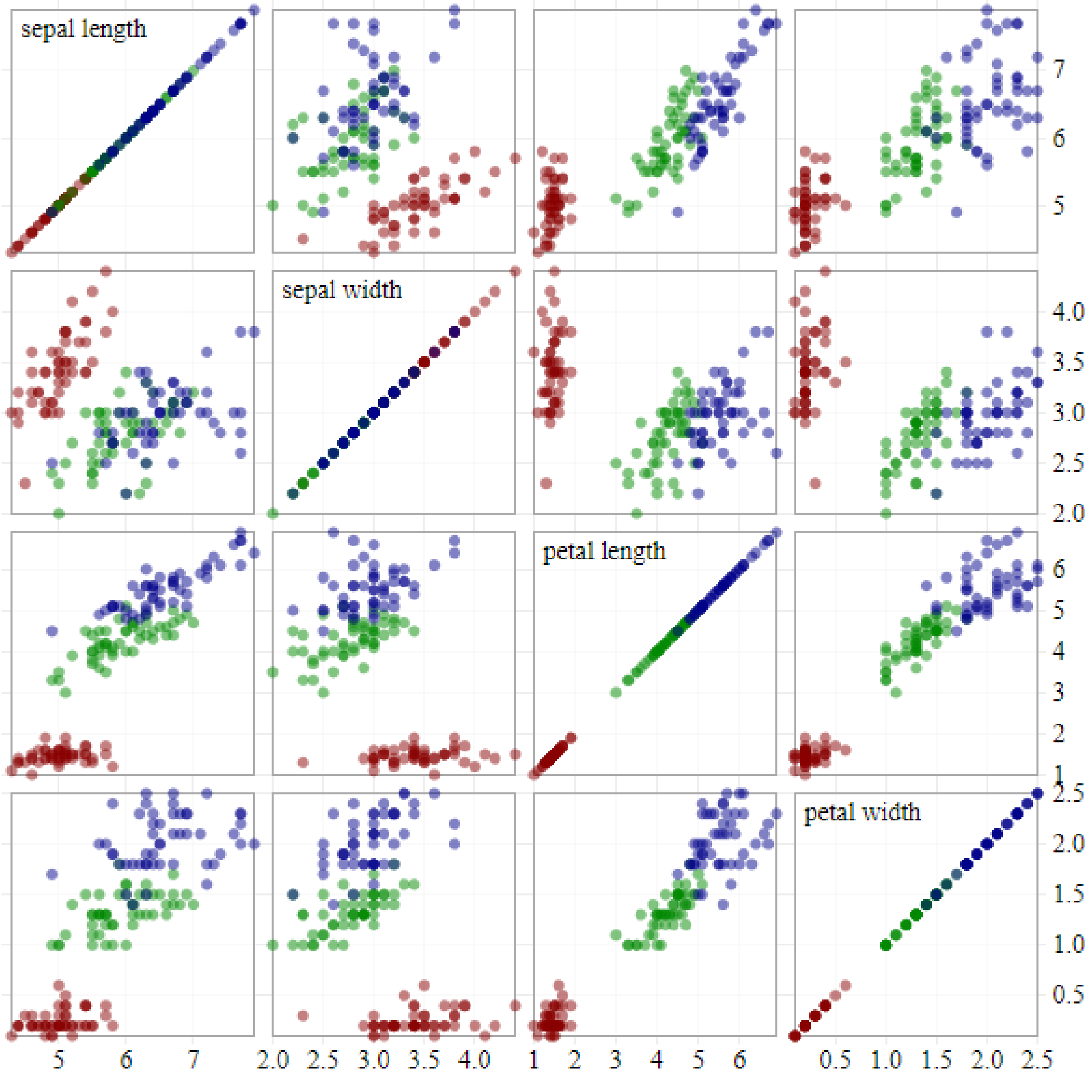
- Cons
  - Computationally intensive
  - Clustering limited to “hierarchical nestings”

Clusters visualized: Co-occurrence heatmap



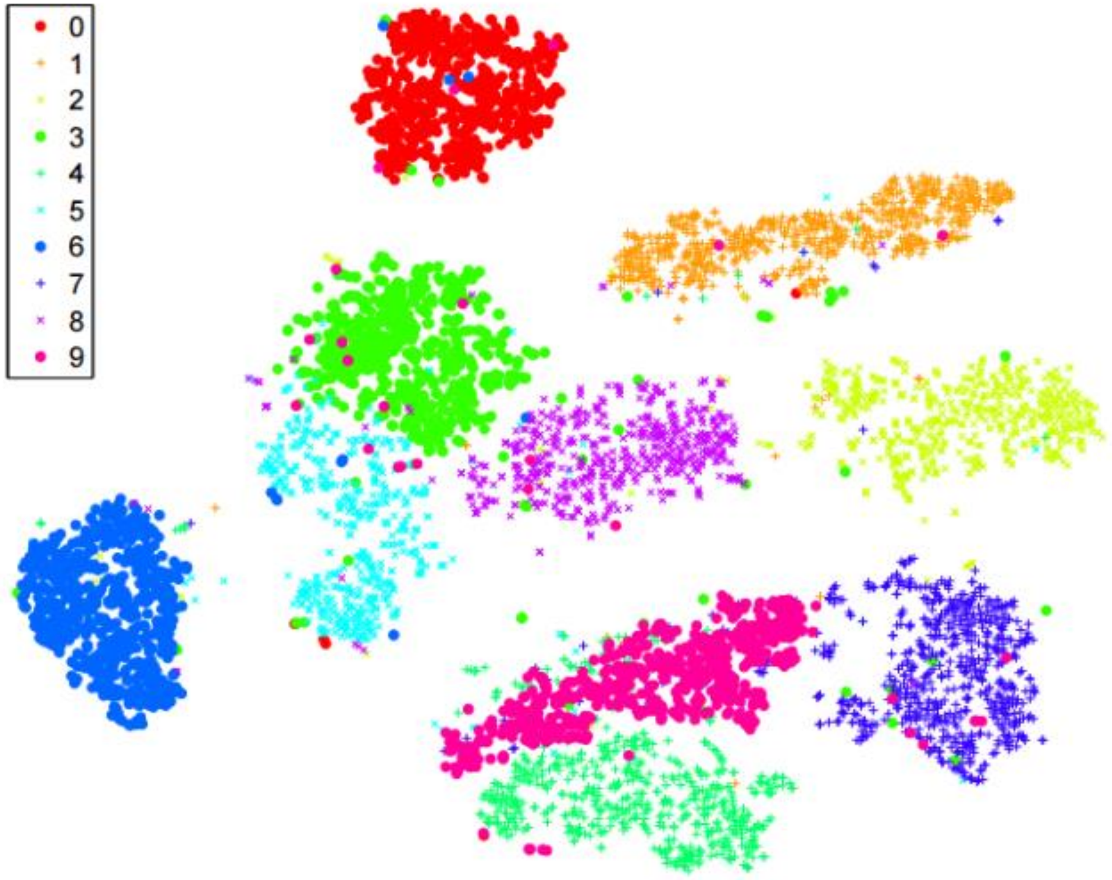
https://bost.ocks.org/mike/miserables/

Clusters visualized: scatterplot matrix



http://benjiec.github.io/scatter-matrix/demo/demo.html#

Clusters visualized: 2d embedding with t-SNE



https://lvdmaaten.github.io/tsne/

Clustering summary

- We can “classify” when we don’t have (training) labels: clustering
- Definition of clusters is vague and evaluation hard
- For clustering we need to :
  - define distance measure
  - define method to evaluate a clustering
  - select clustering algorithm
- Discussed clustering algorithms
  - Hierarchical clustering
  - k-means clustering