Cluster analysis – formalism, algorithms

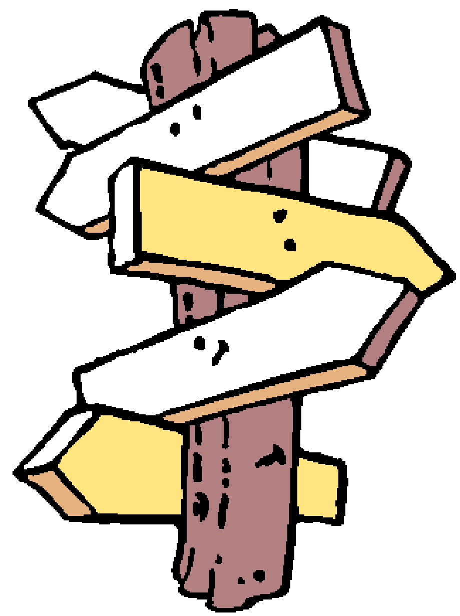
Jiří Kléma

Department of Cybernetics,
Czech Technical University in Prague

http://ida.felk.cvut.cz

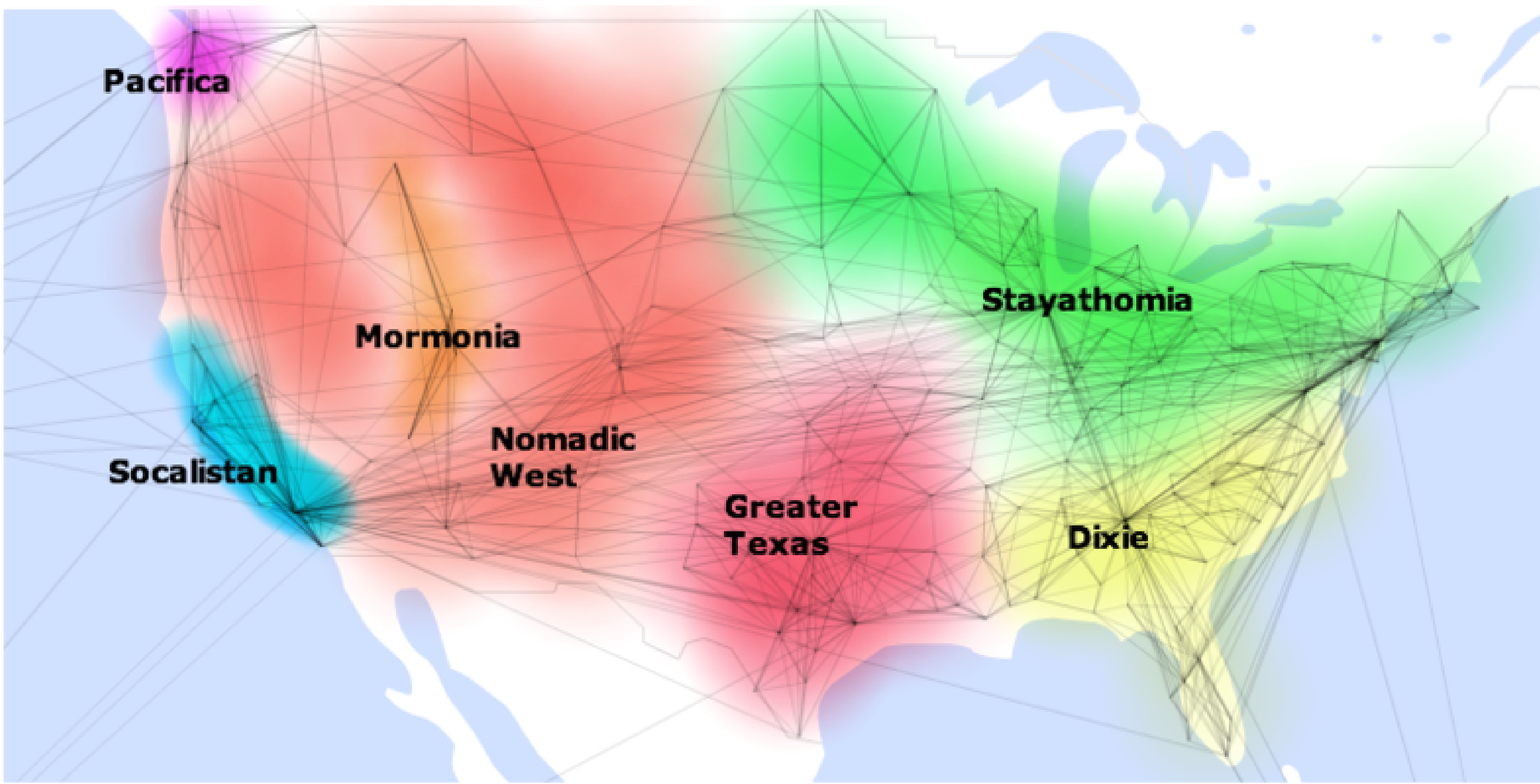
Outline

- motivation
  - why clustering? applications,
- clustering as an optimization task
  - complexity,
- k-means algorithm
  - direct greedy search,
  - (dis)advantages,
- generalization
  - k-means as an instance of EM algorithm,
  - soft clustering,
  - EM algorithm and Gaussian distribution mixture,
- hierarchical clustering
  - motivation – extras?
  - agglomerative and divisive approach,
- summary, method categorization.



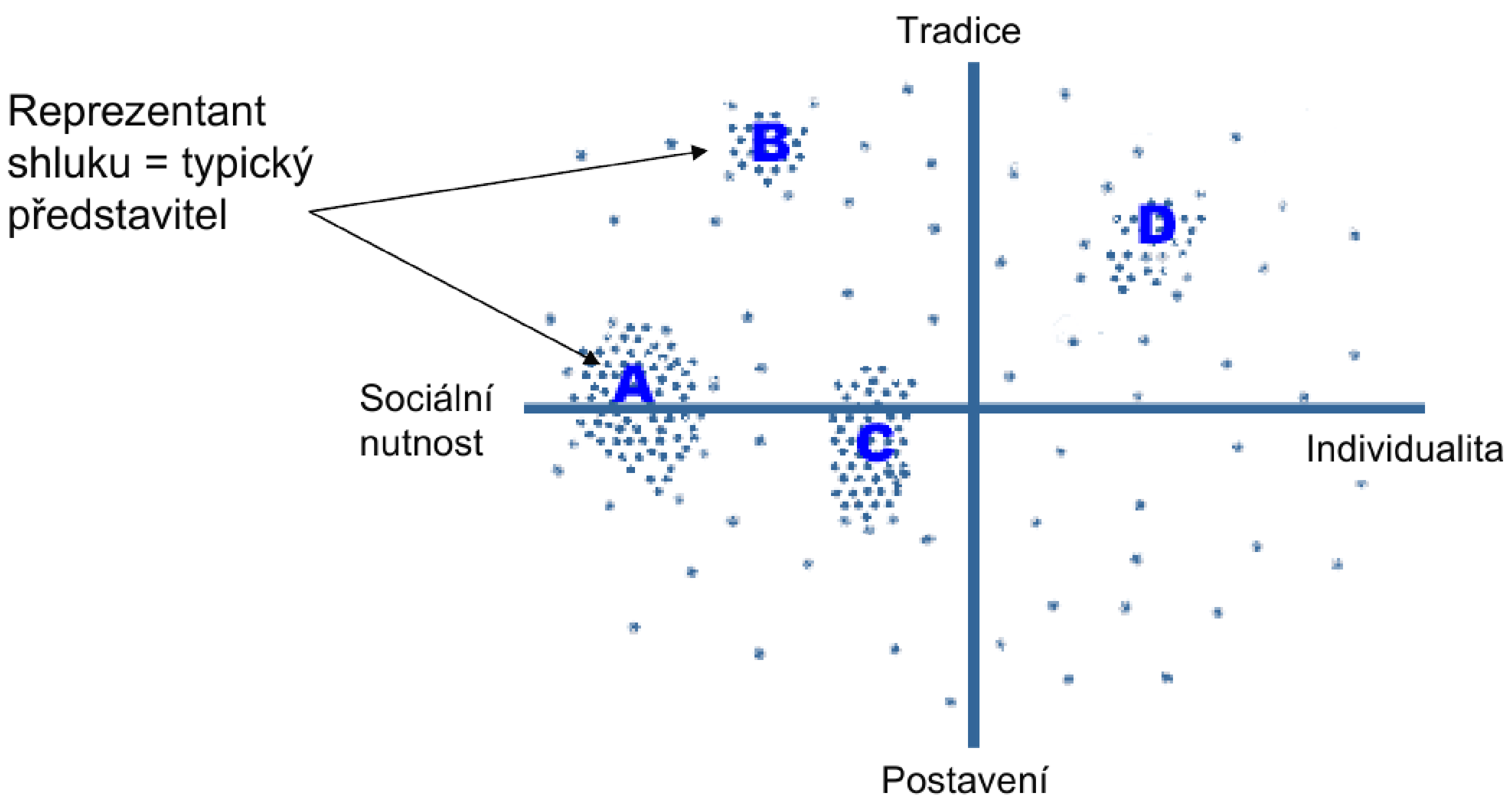
Clustering – example

- clusters and their prototypes bring new domain knowledge,
- interpretation e.g. in connection with geographic data and visualization,
- "clustering" 210 million Facebook profiles based on friendship connections,



Clustering – example

- clusters and their prototypes bring new domain knowledge,
- survey: why do people drink alcohol?
- goal: to find "sample drinkers" and represent condensed people's attitude to alcohol,



Kordík: Y336VD

Clustering – example

- application for image segmentation,
- features: (coordinates), (a) color components, (b) brightness for b&w image.

Xiao Zhang: Image Segmentation.

Clustering – utilization, applications

- clustering for learning
  - class discovery in (unannotated) data,
  - unsupervised learning,
- data understanding, their structured representation
  - taxonomies (biology – organisms, genes),
  - rapid access to pieces of information (web search engine output organization),
  - outlier detection,
- usage of prototypes
  - summarization (original objects completely forgotten),
  - compression (vector quantization),
  - efficient nearest neighbor search.

Clustering – formalization

- goal
  - split unclassified objects into mutually disjoint subsets, **clusters**,
  - we divide so that the objects
    1. are similar inside a cluster,
    2. are dissimilar when lying in different clusters,
  - disjoint **partition** of an object set defined in an input space (usually $\mathbb{R}^n$) into $k > 1$ classes
    $\mathcal{X} \ldots$ a set of m objects, $\Omega = \{C_1, \ldots, C_k\} \ldots$ partition of the set $\mathcal{X}$,
    $\forall i, j \leq k, i \neq j \; C_i \neq \emptyset, \; C_i \cap C_j = \emptyset, \; C_1 \cup C_2 \cup \cdots \cup C_k = \mathcal{X}$,
- we solve an **optimization problem**
  - inputs
    * training data,
    * distance function (dissimilarity function),
    * (optimization criterion).
  - unknown
    * the number of clusters,
    * cluster-object links – partition,
    * (prototypes – cluster ethalons, typical examples).

Clustering – complexity

- variant of a Bayesian decision-making task

  develop a strategy $Q : \mathcal{X} \to D$ (D stands for decisions) minimizing
  $\underset{q}{\operatorname{argmin}} \sum_{x \in \mathcal{X}} p(x) W(x, q(x))$ (W is a loss function),

- how large space to be searched?

  – the number of different disjoint partitions: **Stirling number** of the second kind

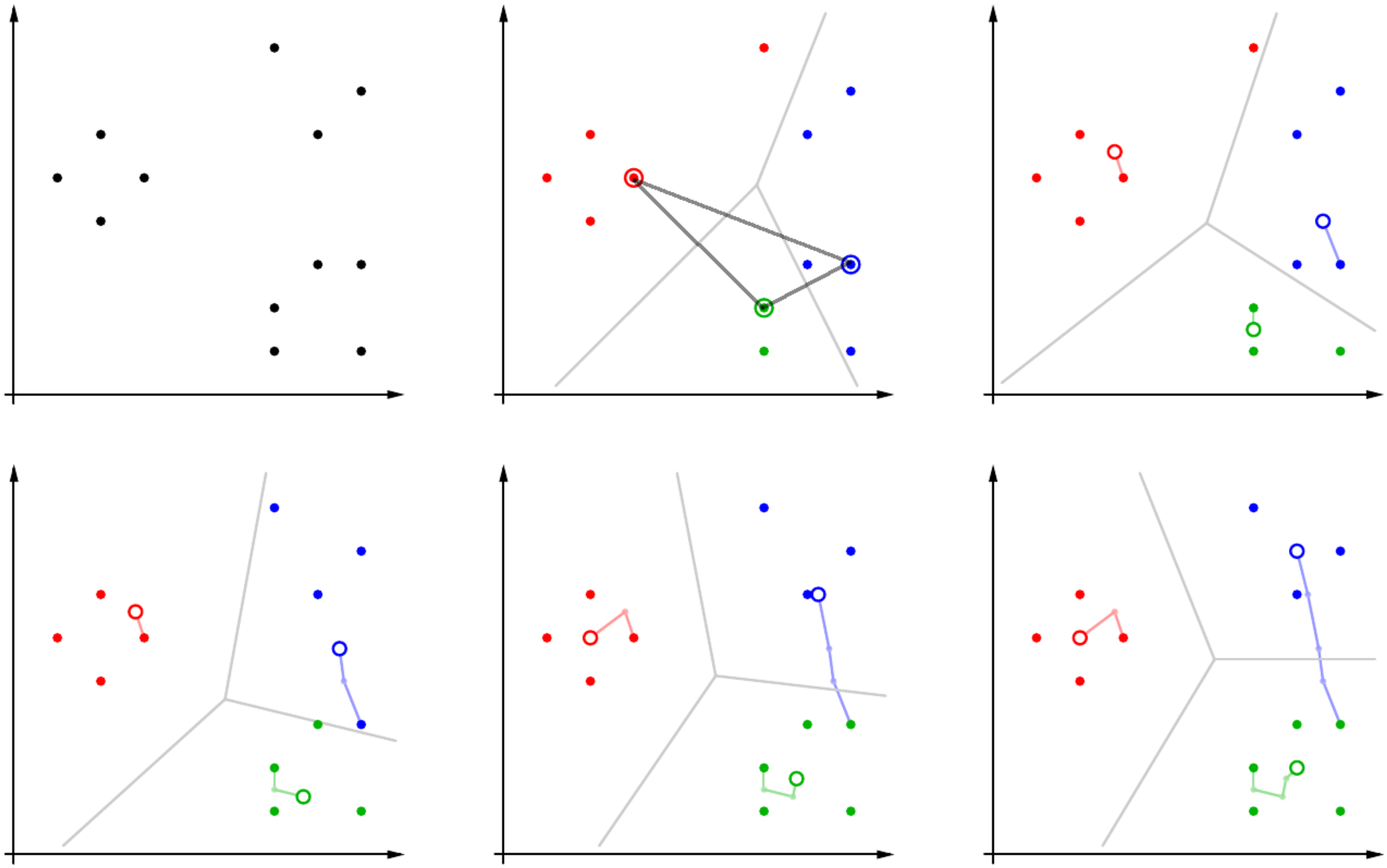
  $S(m,k) = \left\{ {m \atop k} \right\} = \frac{1}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} j^m$, among other $S(m,2) = \left\{ {m \atop 2} \right\} = 2^{m-1} - 1$

m\k	1	2	3	4	5	6	7	8
2	1	1						
3	1	3	1					
4	1	7	6	1				
5	1	15	25	10	1			
6	1	31	90	65	15	1		
7	1	63	301	350	140	21	1	
8	1	127	966	1701	1050	266	28	1

  – the optimization criterion cannot be applied in a naïve way (exhaustive search),

- NP-hard problem, heuristic solutions.

K-means – strategy, an ideal run (Borgelt: IDA slides)



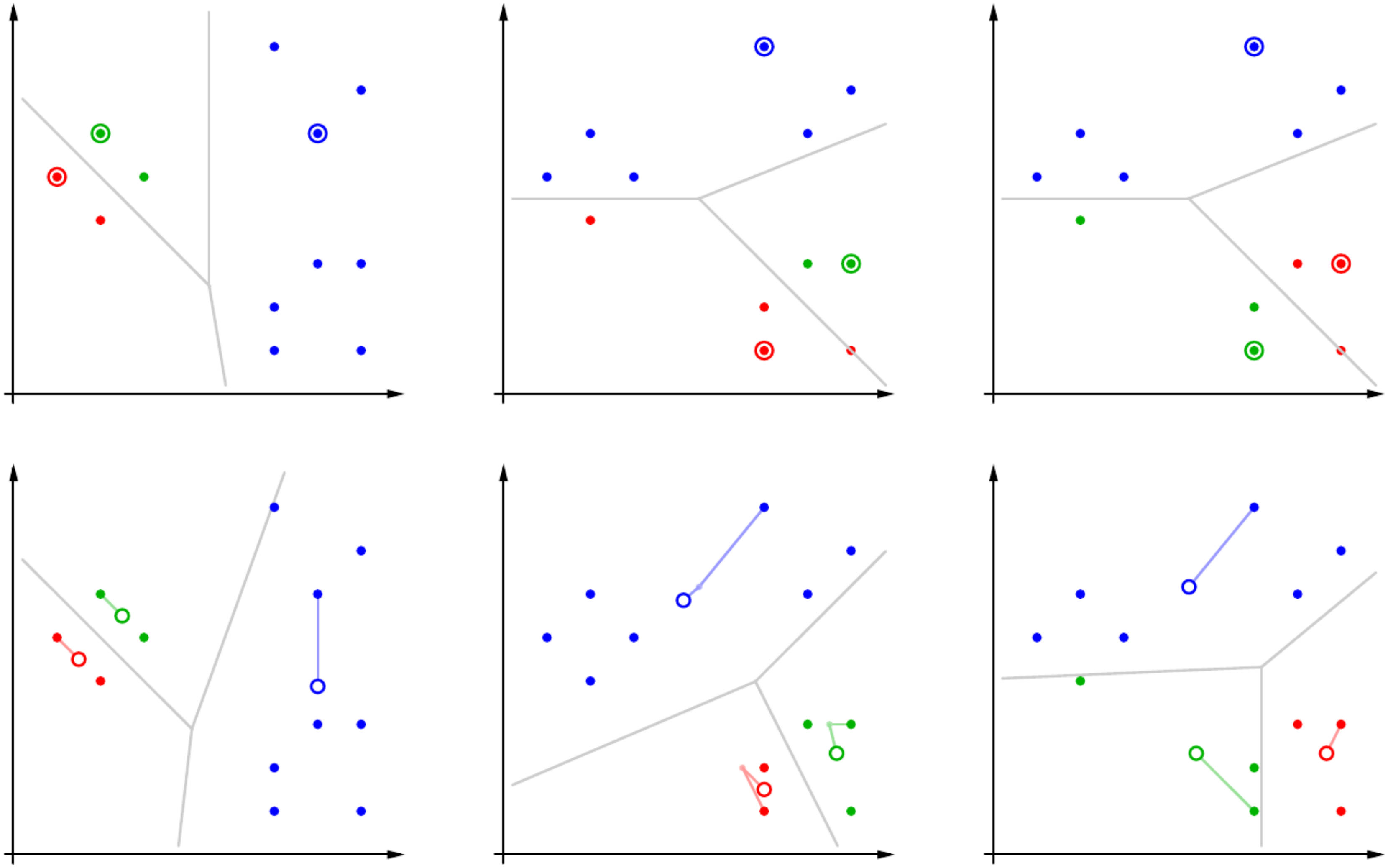
K-means algorithm

- global homogeneity criterion: $W(k) = \underset{\Omega}{\operatorname{argmin}} \sum_{i=1}^{k} \sum_{x_j \in C_i} d(x_j, \mu_i)$,
- inputs: $\mathcal{X} = \{x_1, \ldots, x_m\} \subset \mathbb{R}^n$, $k \in \mathbb{N}$, $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$,

1. randomly **initialize** cluster centroids μ_j (e.g. select k objects),
2. each object $x_i \in \mathcal{X}$ **assign** to the nearest centroid – $\forall i \underset{j=1 \ldots k}{\operatorname{argmin}} d(x_i, \mu_j)$,
3. **recompute** cluster centroids – centroid is a mean vector of objects assigned to the cluster,
4. repeat steps 2 and 3 until cluster centroids change.

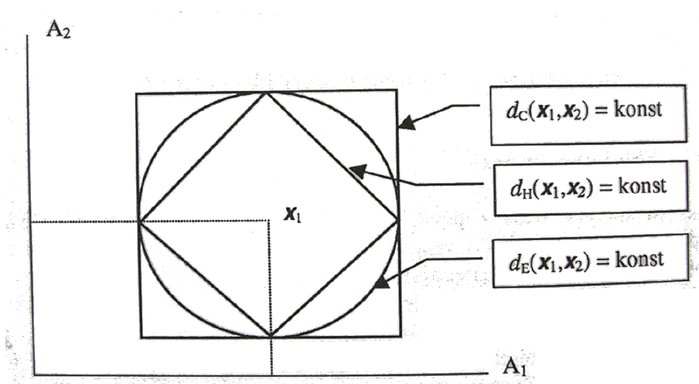
- greedy algorithm
  - guaranteed convergence, typically fast,
  - finds a locally optimal solution,
  - initialization sensitive,
- illustrative demo applet
  - http://www.kovan.ceng.metu.edu.tr/~maya/kmeans/index.html.

K-means – stucked in local optima (Borgelt: IDA slides)

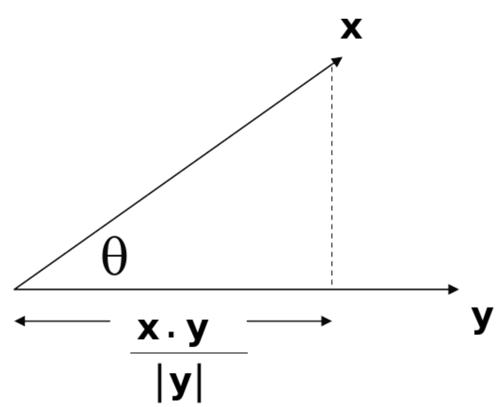


Distance function

- typically **metric** on $\mathcal{X}$, $\forall x, y, z \in \mathcal{X}$:
  - $d(x,y) \geq 0$, $d(x,y) = 0 \Leftrightarrow x = y$, $d(x,y) = d(y,x)$, $d(x,z) \leq d(x,y) + d(y,z)$
- common functions
  - Minkowski metric: $d(x,y) = \left(\sum_{i=1}^{n}(x_i - y_i)^k\right)^{\frac{1}{k}}$
    * selection of k: $d_H(k=1)$ (Manhattan, Hamming, taxi), $d_E(k=2)$ (Euclid), $d_C(k=\infty)$ (Chebyshev),
  - cosine dissimilarity (documents): $d(x,y) = 1 - cos(\theta) = 1 - \frac{x \cdot y}{|x||y|}$
  - edit (Levenshtein) distance (words, strings, sequences)
    * minimum number of edits (change, insert, delete) to transform one string into the other.



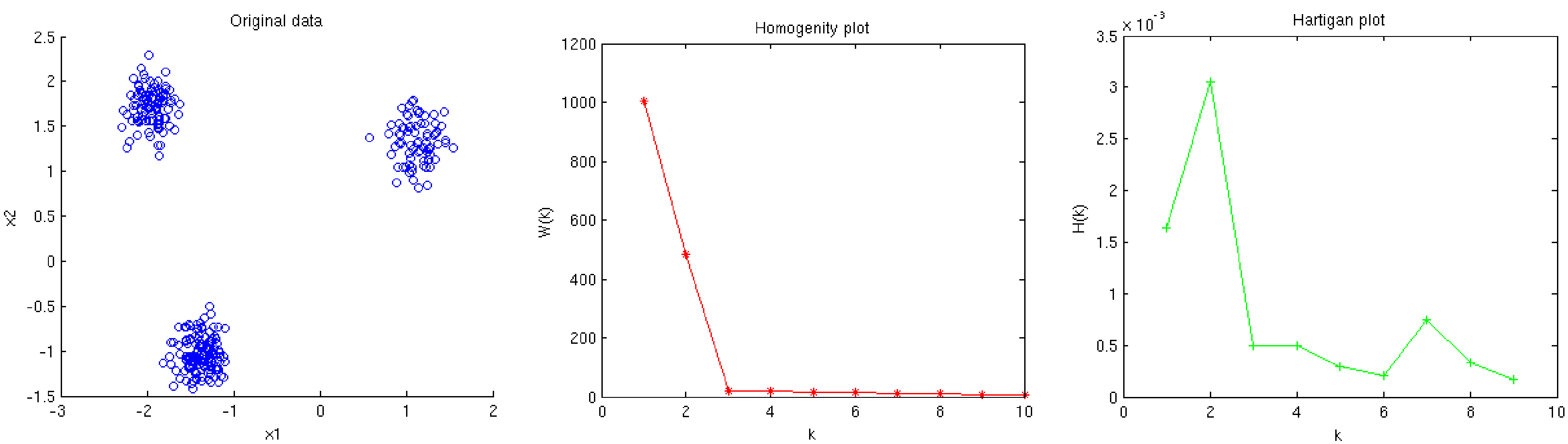
Minkowski distance, Berka: Dolování dat



cosine dissimilarity

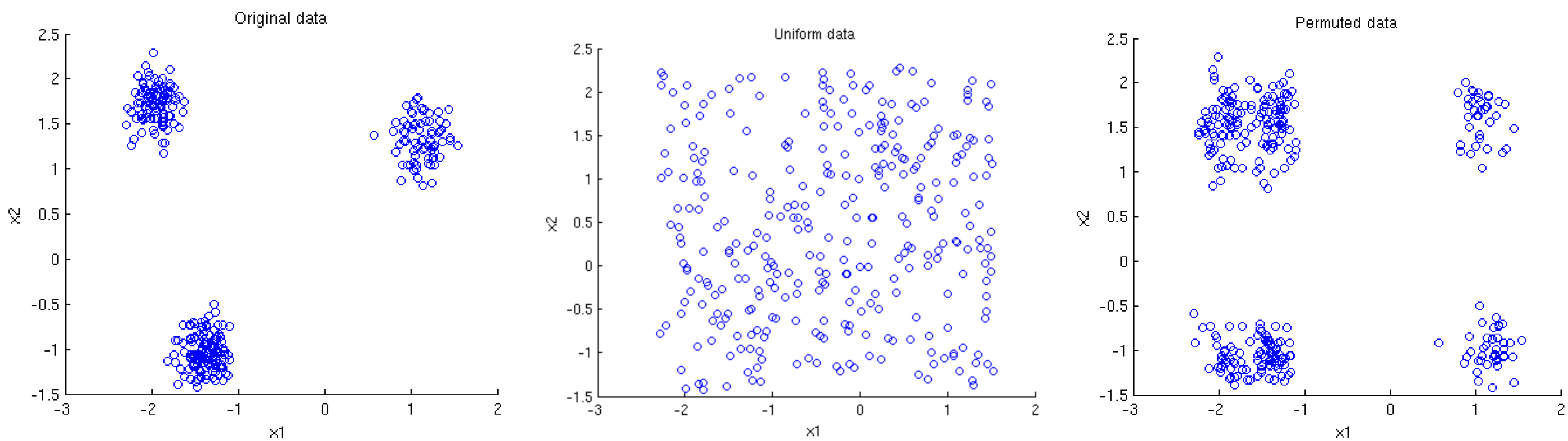
K-means: the number of clusters choice

- k known a priori,
- k based on the object number only: $k \sim \sqrt{\frac{m}{2}}$,
- homogeneity W necessarily monotonously increases with increasing k, a heuristic "elbow" method:
  - run k-means algorithm repeatedly with increasing k,
  - a proper k is in the point of sudden non-homogeneity decrease or in a curve elbow,
  - Hartigan criterion: $H(k) = \frac{W(k)-W(k+1)}{W(k+1)(m-k-1)}$
    choose the smallest $k \geq 1$ with $H(k)$ small enough.

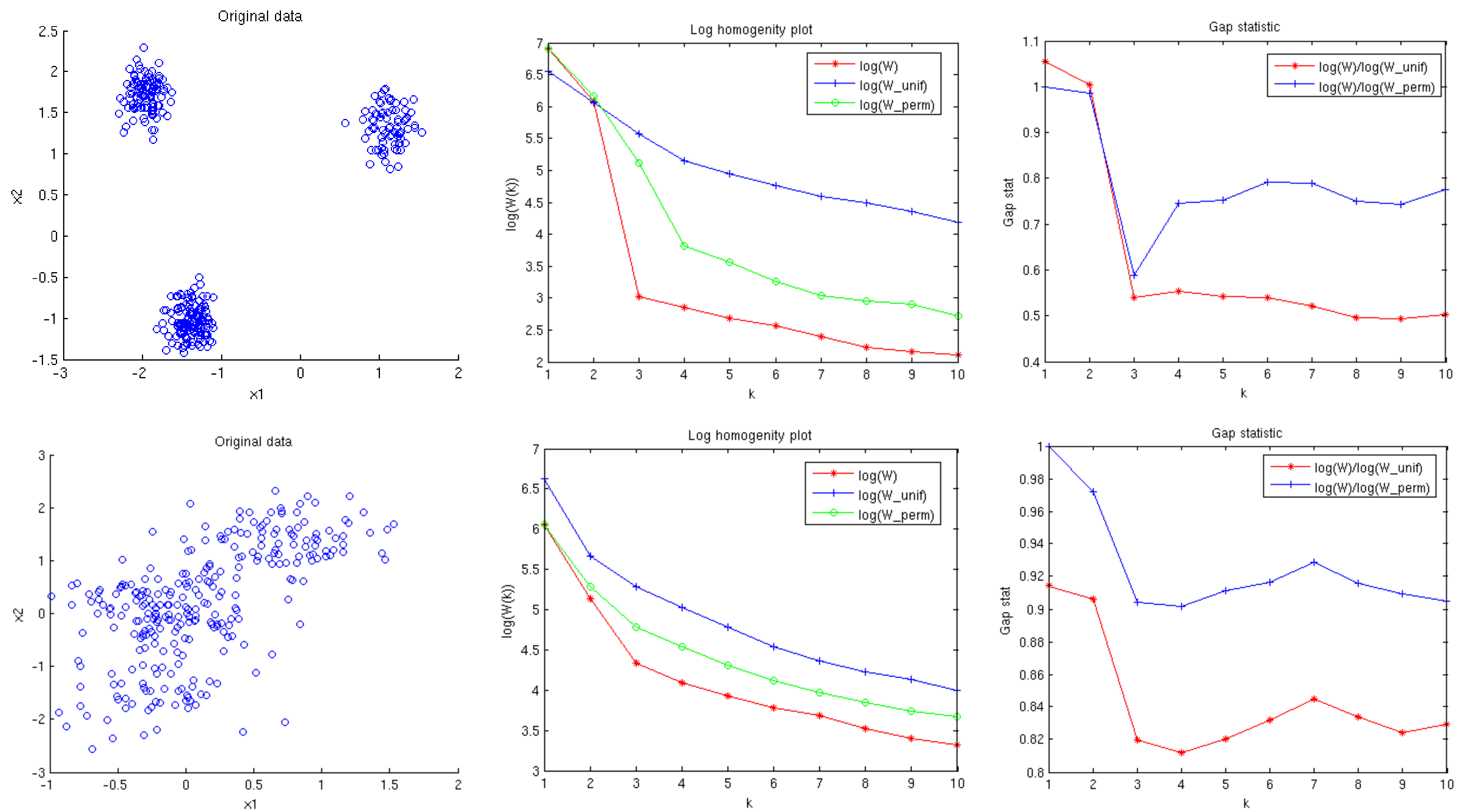


K-means: the number of clusters choice

- Tibshirani (2001): **gap statistic**
  - compares development of $W(k)$, resp $log(W(k))$, with the referential curve $W_{ref}(k)$,
  - instead of $log(W(k))$ searches minimum in $\frac{log(W(k))}{log(W_{ref}(k))}$,
  - $W_{ref}(k)$ can be obtained in two ways
    - ∗ uniform distribution homogeneity "without clusters" $(W_{unif}(k))$,
    - ∗ permuted distribution homogeneity – feature values randomly shuffled $(W_{perm}(k))$,
    - ∗ the domain is kept in both,
  - the method originated in statistics.



K-means: the number of clusters choice



- EM with theoretically well-founded AIC or BIC criteria.

Expectation Maximization (EM) algorithm

- k-means is an EM algorithm specialization,
- maximizes **likelihood** $Pr(\mathcal{X}|\theta)$

$$\theta^* = \underset{\theta}{\operatorname{argmax}} Pr(\mathcal{X}|\theta) = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} Pr(x_i|\theta)$$

- introduces a latent variable Q, which simplifies maximization of $Pr(\mathcal{X}|\theta)$
  - **E-step**:
    - estimate latent variable (distribution) for the given data and current param values θ,
  - **M-step**:
    - modify parameters θ so that likelihood is maximized wrt given Q,
- k-means specification
  - Q gives binary cluster membership,
  - E-step: assign objects and centroids,
  - M-step: recalculate cluster centroids.

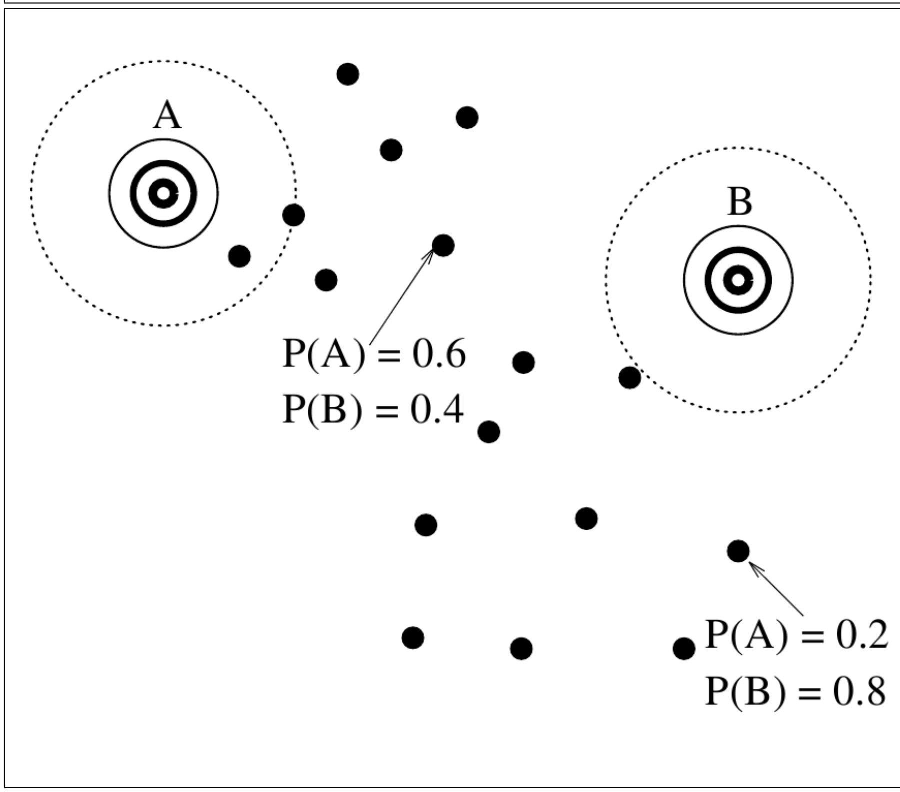
Soft (probabilistic) clustering

- "hard" object membership in a single cluster not needed,
- membership function $Pr(C_j|x_i)$ is understood as probability
  - it must hold: $\forall i = 1, \ldots, m : \sum_{j=1,\ldots,k} Pr(C_j|x_i) = 1$
- a soft clustering algorithm – "soft" k-means
  - EM principle,
  - a model with parameters θ used to calculate $Pr(C_j|x_i)$,
  - θ most often defines a Gaussian Mixture Model (GMM),
    - $Pr(x_i|\theta) = \sum_{j=1}^{k} \alpha_j \frac{1}{(2\pi)^{n/2}|\Sigma_j|^{1/2}} e^{-\frac{1}{2}(x_i-\mu_j)^t \Sigma_j^{-1}(x_i-\mu_j)}$
    - $\theta = \{\alpha_1, \ldots, \alpha_k, \mu_1, \ldots, \mu_k, \Sigma_1, \ldots, \Sigma_k\}$, $\sum_{j=1}^{k} \alpha_j = 1$
    - $\alpha_i \ldots$ a mixture element weight, $\mu_i \ldots$ centroid vector, $\Sigma_i \ldots$ covariance matrix,
  - θ can also define a naïve bayes model etc.,
- EM GMM clustering
  - Q determines probability that an object was generated by a particular gaussian distribution,
- soft clustering is a special case of fuzzy clustering
  - membership $Pr(C_j|x_i)$ without constraints needed for probability.

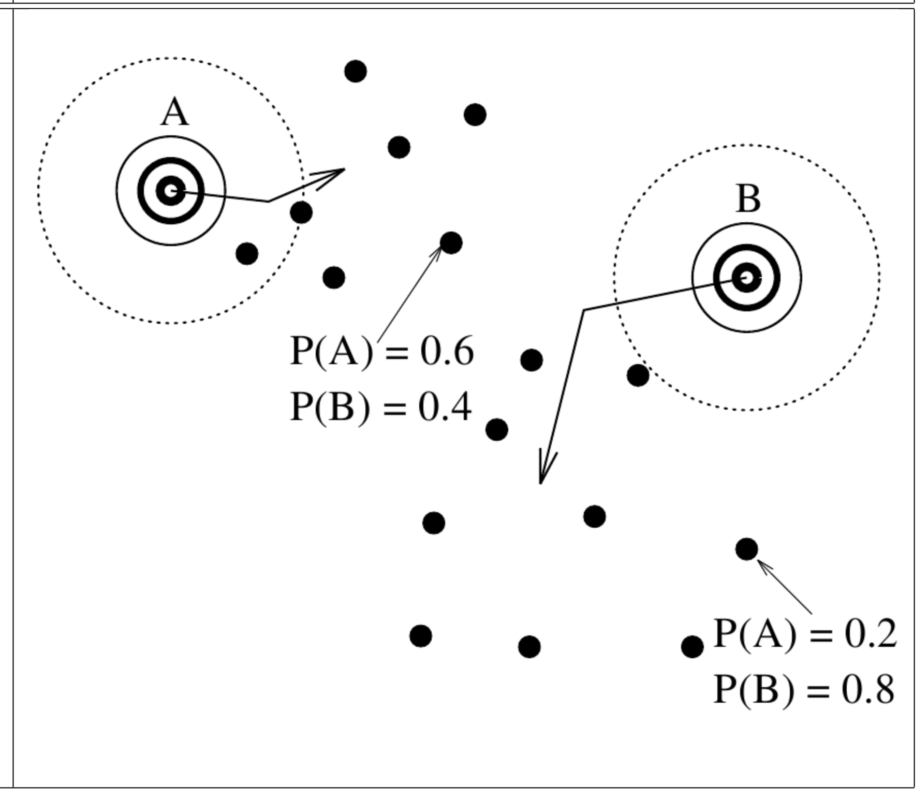
EM for GMM clustering

- EM is an iterative algorithm,
- illustration of one step after random initialization.

E-step

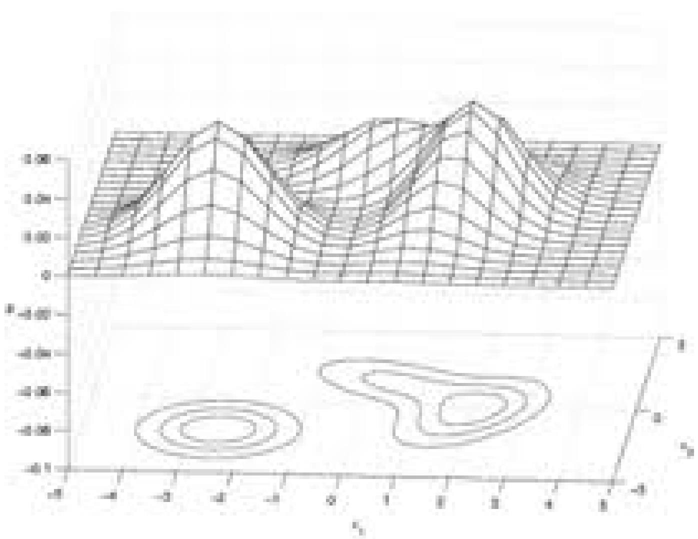


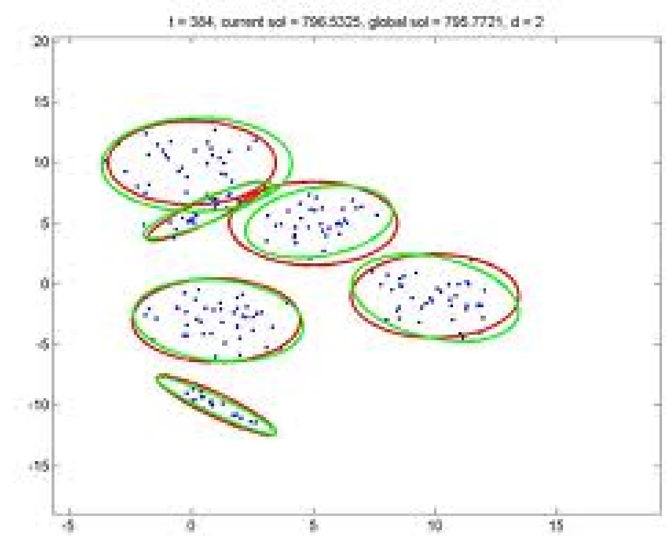
M-step



EM clustering – k-means comparison

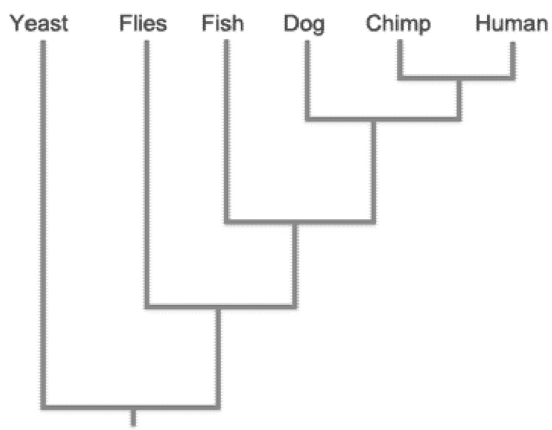
- clustering defined as GM optimization in n dimensions,
- the number of elements (distributions) k (can be a part of likelihood maximization resp. AIC),
- partition: object belongs to the distribution with the highest a posteriori prob $Pr(C_j|x_i)$,
- assumes a normal object distribution within a cluster,
- more robust, but slower than k-means,
- demo: http://staff.aist.go.jp/s.akaho/MixtureEM.html.





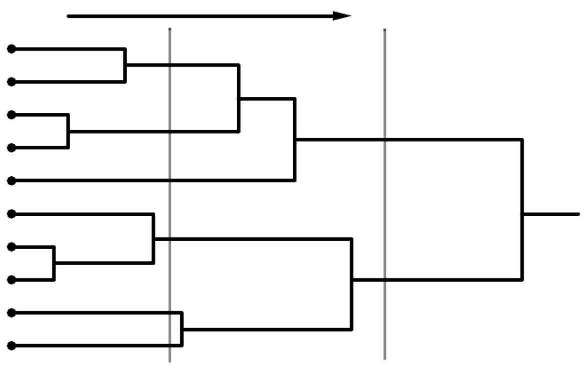
Hierarchical clustering – motivation

- **taxonomy** is more informative than partition
  - analyzes on various granularity levels,
  - binary tree = **dendrogram**,
- a reasonable decomposition of the clustering problem to subproblems
  - a straightforward and computationally efficient solution.



Hierarchical clustering – algorithm

- recursive application of the standard clustering step,
- agglomerative approach (bottom-up)
  - at the beginning each object makes a cluster,
  - iterate with merging the most similar clusters, typically pairs,
- divisive approach (top-down)
  - split the object set into clusters, typically two of them,
  - iterate with splitting the clusters,
  - more difficult to implement – needs an internal clustering algorithm,
  - more efficient than agglomerative, namely when the complete dendrogram not needed,
- needs no prior k, constructs a hierarchy.
- a partition results from a dendrogram cut.



Hierarchical clustering – cluster distance

- the key point is a generalized cluster distance function
  - makes a step from the object distance towards the object set distance,
  - originally: $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$,
  - now: $\delta : 2^{\mathcal{X}} \times 2^{\mathcal{X}} \rightarrow \mathbb{R}$,
- elemental δ definitions based on d
  - concern two most similar objects (single linkage)

    $$\delta(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y),$$

  - concern two most distant objects (complete linkage)

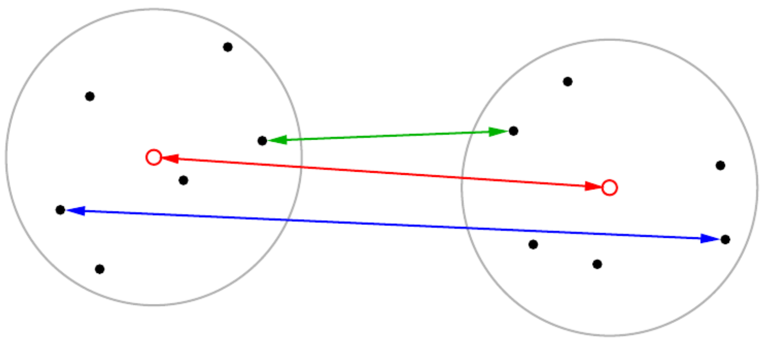
    $$\delta(C_i, C_j) = \max_{x \in C_i, y \in C_j} d(x, y),$$

  - average pair distance (average linkage)

    $$\delta(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i} \sum_{y \in C_j} d(x, y),$$

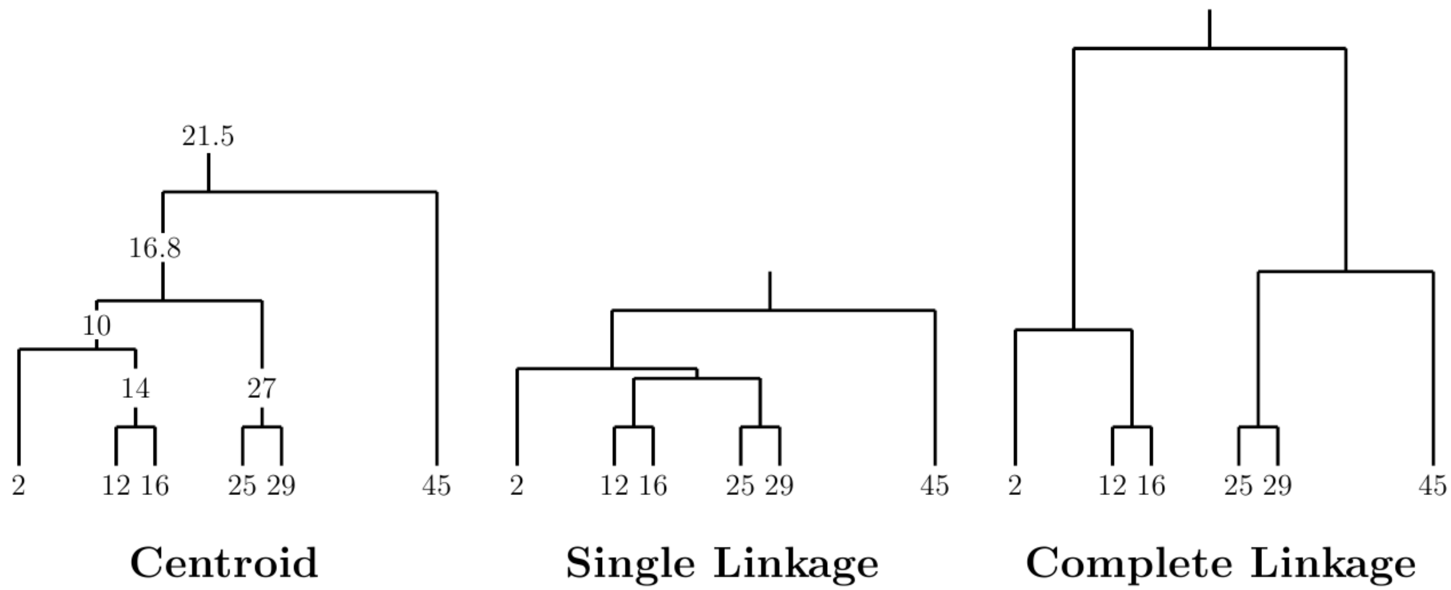
  - distance between cluster centroids (centroid)

    $$\delta(C_i, C_j) = d(\mu_i, \mu_j),$$



Example: relation between distance function and clustering outcome

- Ex.: 1 dimensional object set 2, 12, 16, 25, 29, 45.
  - the objects can be proportionally positioned on x dendrogram axis,
- different generalized distance functions lead to different dendrograms.



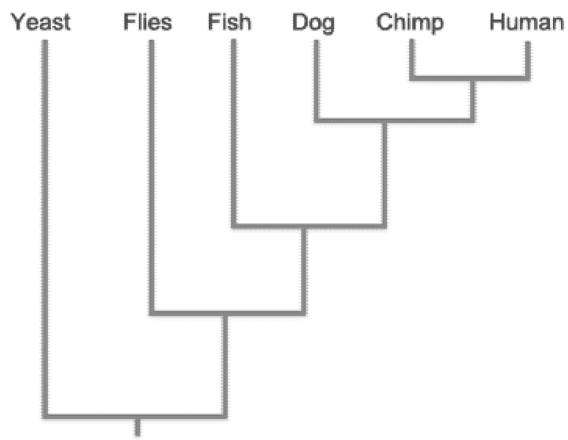
Borgelt: IDA slides

Clustering – summary

- Intuitively comprehensible principle, in many contexts, in many domains
  - in general identification of any frequent event co-occurrence in data,
- combinatorially difficult optimization problem
  - heuristic solutions, local optimality,
- basic steps
  - representation definition,
  - distance function selection,
  - clustering itself,
  - abstract representation of partition,
  - evaluation, iteration.
- clustering algorithm quality
  - scalability – no of objects, dimensions,
  - robustness – noise, outliers, feature types, distance function,
  - ability to deal with various cluster shapes.

Clustering – method categorization

- nonhierarchical methods
  - aim to deliver the partition that minimizes an optimization criterion,
  - apply a global homogeneity criterion,
  - cluster membership can be hard (crisp) as well as probabilistic,
  - examples: k-means, EM
- hierarchical methods
  - generate a cluster hierarchy
    - binary tree = dendrogram,
  - apply a local cluster similarity criterion,
  - agglomerative – bottom-up,
  - divisive – top-down, divide and conquer,
  - examples: AHC (a general principle).



Recommended reading, lecture resources

:: Reading

- Hastie et al.: **The Elements of Statistical Learning: DM, Inference and Prediction.**
  – Springer book.
- Jain et al.: **Data Clustering: A Review.**
  – ACM Computing Surveys,
  – http://www.prip.tuwien.ac.at/teaching/ss/einfuhrung-in-die-mustererkennung/download-area-and-links/p264-jain.pdf.
- Borgelt: **Intelligent Data Analysis.**
  – slides, a detailed intelligent data analysis course, clustering near the end,
  – http://www.borgelt.net/courses.html#ida,