Today's lecture

1. K-representatives clustering
   - Recap K-means (video)
   - other members of the family
2. Hierachical clustering
   - introduction (video)
   - more on linkage metrics, connections to graph theory, dendrograms

Book 6.3, 6.4

Main groups of clustering methods (Aggarwal)

- Representative-based
- Hierarchical
- Probabilistic model-based
- Density-based (including grid-based)
- Graph-based
- Matrix factorization based

Representative-based: K*-means*

Watch video "K-means clustering: how it works" (7.5 min) by Victor Lavrenko

`https://www.youtube.com/watch?v=_aWzGGNrcic`

Questions

- Why K-means is only for numerical data?
- Could we apply something similar to categorical data? or other data types?

K-means

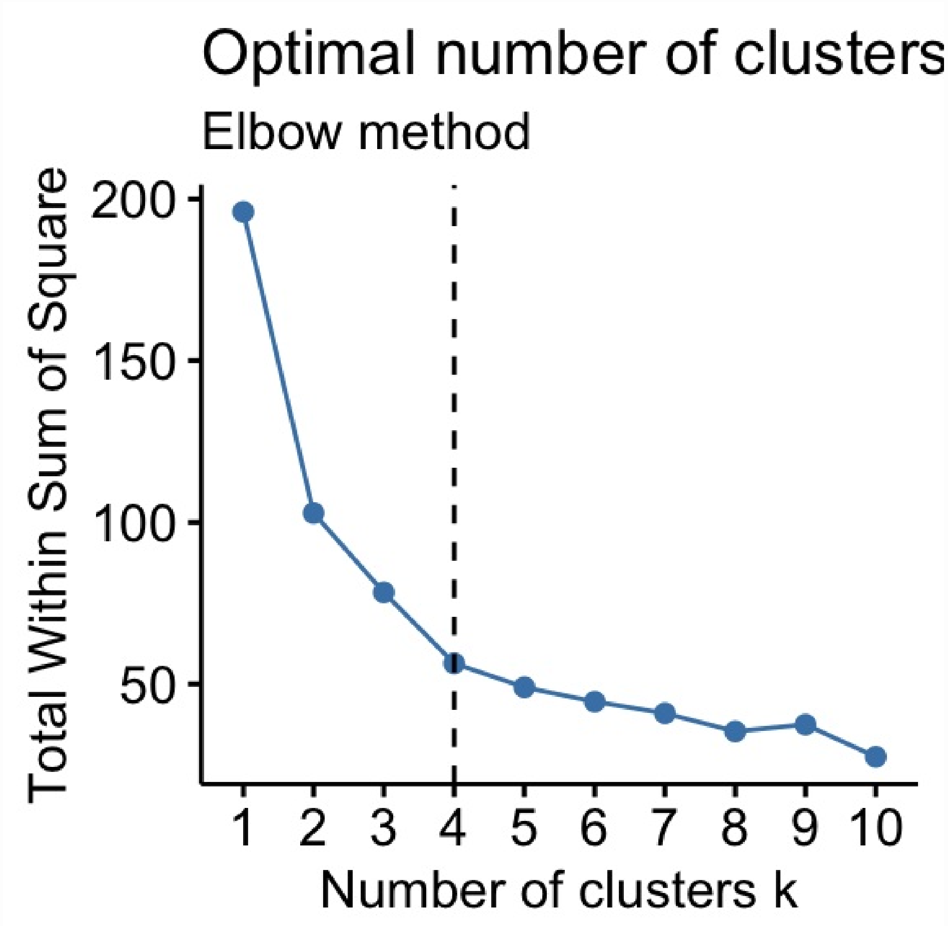
Notations: Data points $\mathbf{x}_i \in \mathcal{D}$, clusters $C_1, \ldots, C_K$, centroids $\mathbf{c}_1, \ldots, \mathbf{c}_k$, $\mathbf{m}$ mean of data.

- objective: minimize $SSE = \sum_{j=1}^{K} \sum_{\mathbf{x} \in C_j} L_2^2(\mathbf{x}, \mathbf{c}_j)$
  - minimizes wc, maximizes bc, since $\sum_{\mathbf{x} \in \mathcal{D}} L_2^2(\mathbf{x}, \mathbf{m}) = \sum_{j=1}^{K} \sum_{\mathbf{x} \in C_j} L_2^2(\mathbf{x}, \mathbf{c}_j) + \sum_{j=1}^{K} |C_j| L_2^2(\mathbf{c}_j, \mathbf{m})$
- tends to find **compact, hyperspherical** clusters
- **designed only for** L_2, but many K-representative variants for other distance measures
  - **warning**: if you use another distance in K-means, may not find even local optimum or converge. **Why?**
- very sensitive to the initialization of centroids! $\rightarrow$ **run multiple times**

K-means

- **+** can produce good results if clusters compact, well-separated, hyperspherical
- **+** easy to implement
- **+** quite efficient $O(nKq)$, q=number of iterations
- **–** basic form requires L_2 measure
- **–** sensitive to outliers
- **–** sensitive to initialization (some improved strategies)
- **–** converges to local optimum (not necessarily global)
- **–** sometimes convergation can be slow
- **–** needs parameter K

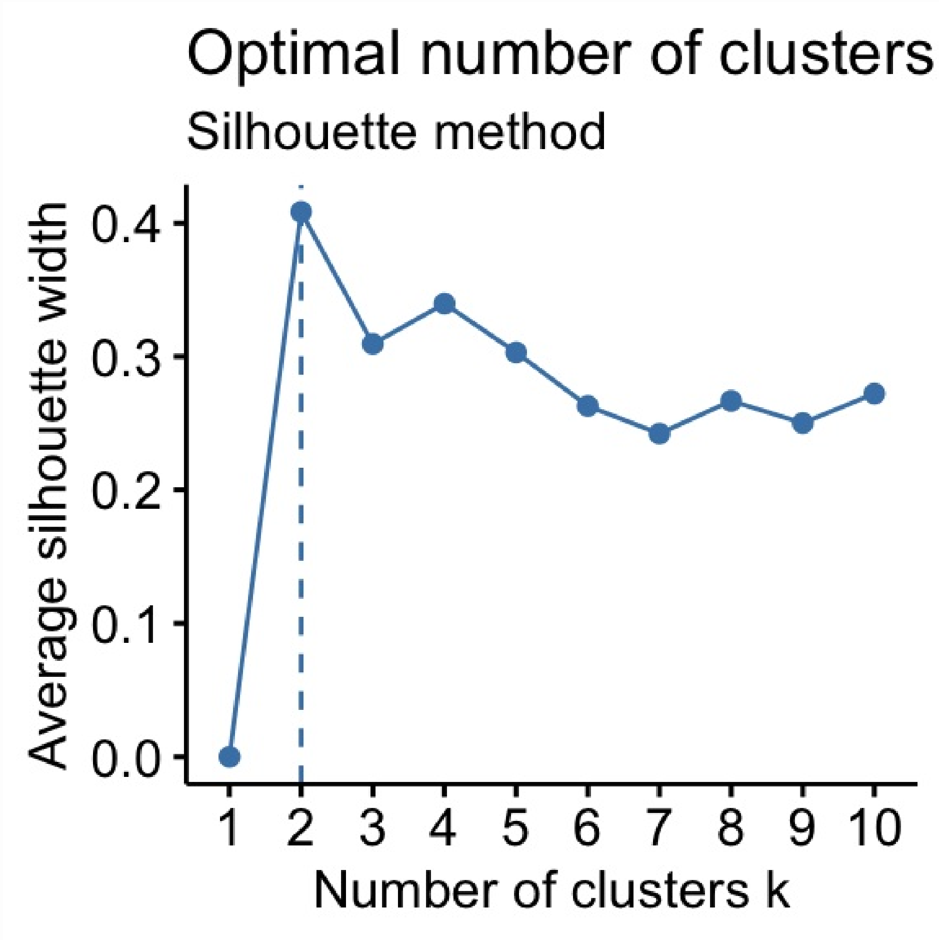
Choosing number of clusters: SSE elbow



- SSE decreases with K
- is there an elbow of the curve, where speed slows down?
- not always clear

source `https://www.datanovia.com/en/lessons/determining-the-optimal-number-of-clusters-3-must-know-methods/`

Choosing number of clusters: silhouette peak



- Silhouette tells how well an individual data point is clustered
- **Average silhouette** evaluates the entire clustering

source `https://www.datanovia.com/en/lessons/determining-the-optimal-number-of-clusters-3-must-know-methods/`

Silhouette coefficient

Silhouette of a point $\mathbf{x}$ is

$$S(\mathbf{x}) = \begin{cases} 0 & \text{if singleton} \\ \frac{b-a}{\max\{a,b\}} & \text{otherwise} \end{cases}$$

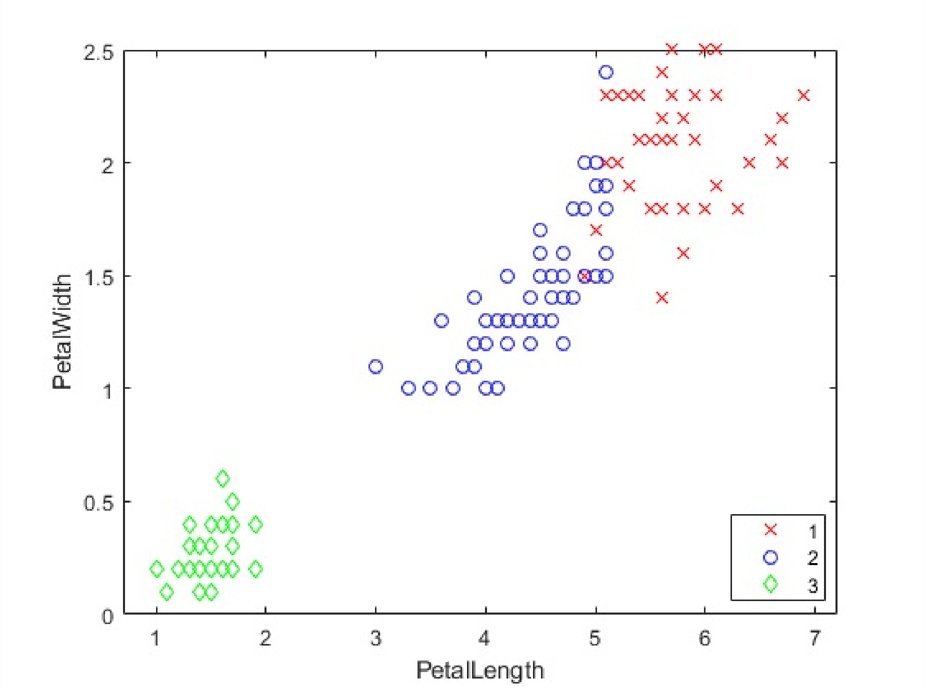
a=mean distance of $\mathbf{x}$ to points in the same cluster
b=mean distance of $\mathbf{x}$ to points in the closest neighbouring cluster

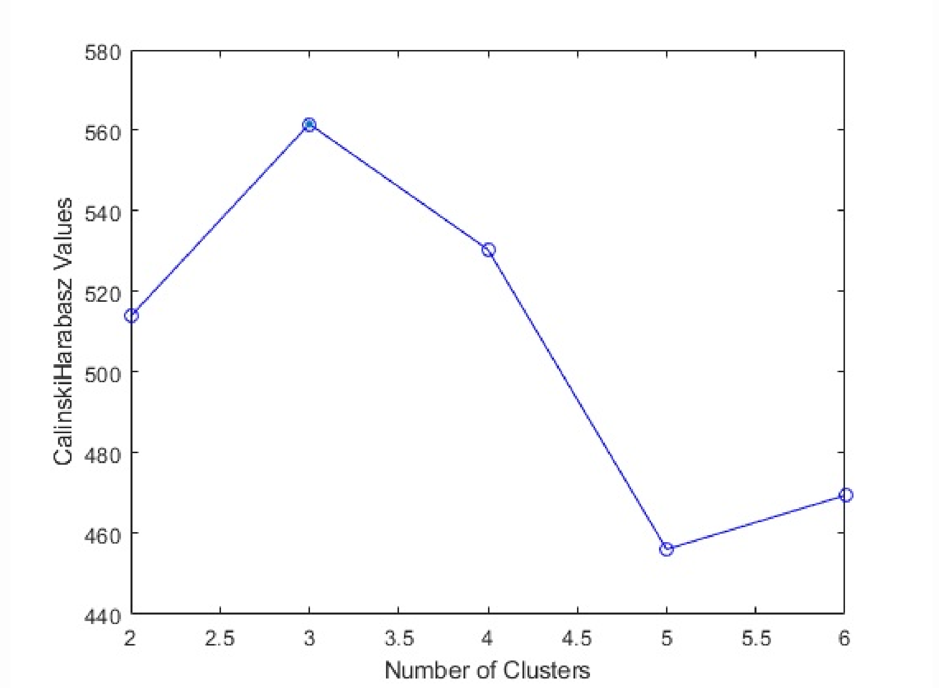
$\Rightarrow$ average Silhouette $S_{avg} = \frac{1}{n} \sum_{\mathbf{x}\in\mathcal{D}} S(\mathbf{x})$

$\rightarrow$ More on lecture 5

Choosing number of clusters: Calinski-Harabasz

based on inter-cluster and intra-cluster variances





source `https://www.mathworks.com/help/stats/clustering.evaluation.calinskiharabaszevaluation-class.html`

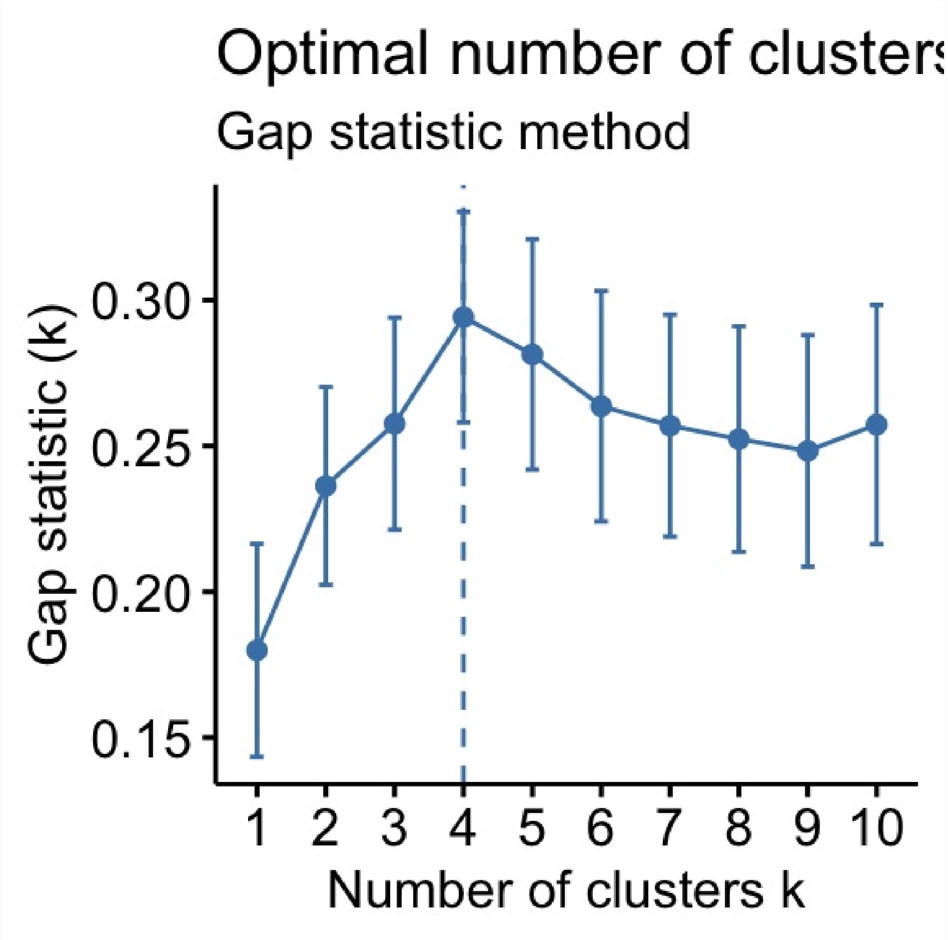
Choosing number of clusters: Calinski-Harabasz

$$S_{CH} = \frac{(n-K)B}{(K-1)W}$$

- between-cluster variance $B = \sum_{i=1}^{K} |C_i| L_2^2(\mathbf{c}_i, \mathbf{m})$ ($\mathbf{m}$ = mean of the whole data)
- within-cluster variance $W = \sum_{i=1}^{K} \sum_{\mathbf{x} \in C_i} L_2^2(\mathbf{x}, \mathbf{c}_i)$
- well suitable to K-means!

$\rightarrow$ More on lecture 5

Choosing number of clusters: Gap statistic



- Cluster data and evaluate $W_K = \sum_{r=1}^{K} \frac{1}{2|C_r|} \sum_{\mathbf{x},\mathbf{y} \in C_r} d(\mathbf{x}, \mathbf{y})$
- Evaluate W_K in B random data sets $\rightarrow W_{K1}, \ldots, W_{KB}$
- $Gap(K) = \frac{1}{B} \sum_{b=1}^{B} \log(W_{Kb}) - \log(W_K)$
- Choose $\min K$: $Gap(K) \geq Gap(K+1) - \sigma_{K+1}$

source `https://www.datanovia.com/en/lessons/determining-the-optimal-number-of-clusters-3-must-know-methods/`

Gap statistic

- σ_K= standard deviation of $W_{K1}, \ldots, W_{KB}$
- if $d = L_2^2$, W_K estimates SSE

+ suits to **any clustering method and distance** d

− computationally heavy (B random simulations for all tested K)

Further reading: Tibshirani et al.: Estimating the number of clusters in a data set via the gap statistic. Journal of the Royal Statistical Society, 2001.

K-means extensions

- K-**medians**
  - uses L_1 measure and medians
  - determine median values along each dimension separately
  - \+ more robust to outliers
  - – computationally more costly
- K-**medoids**
  - medoid = the center-most **data point** in a cluster
  - \+ more efficient (but slower than k-means)
  - \+ allows any distance function
  - \+ suits to any data type! (given distance function)

K-means vs. K-medoids

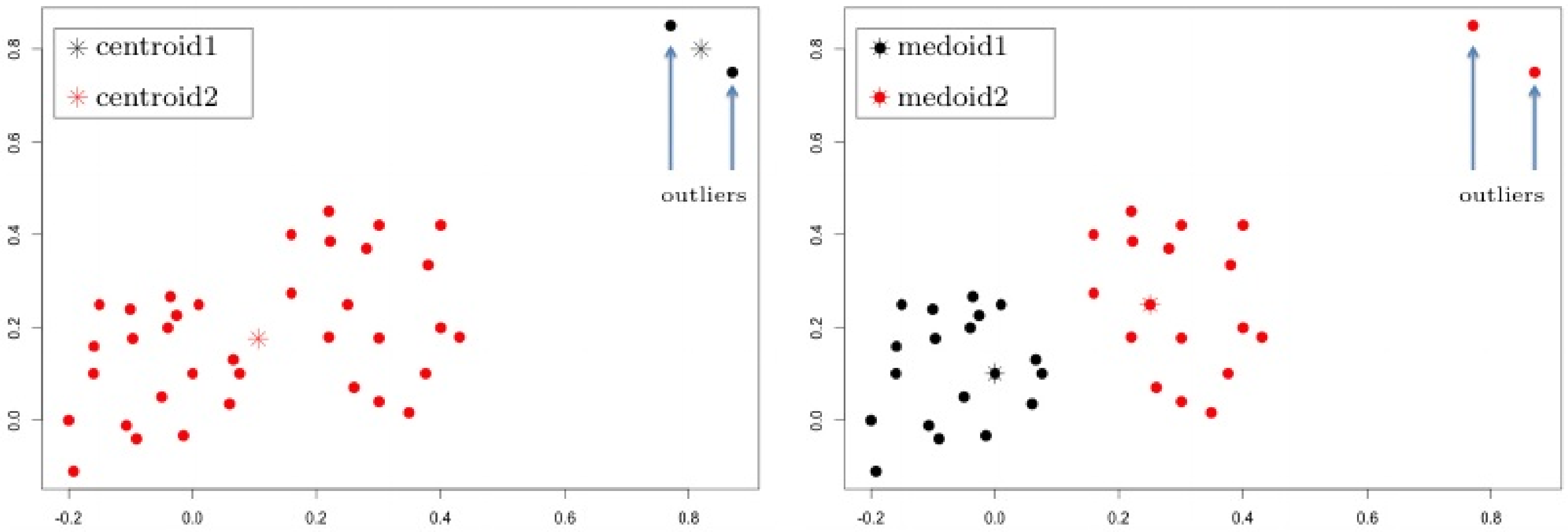


Figure 3.3: Outliers effect: k-means clustering (left) vs. k-medoids clustering (right)

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image source: Soheily-Khah (2016): Generalized k-means based clustering for temporal data under time warp

K-modes

- for categorical data
- minimize $\sum_{\mathbf{x}\in C} \sum_{i=1}^{k} d_s(x_i, c_i)$, where

$$d_s(x_i, y_i) = \begin{cases} 1 & \text{if } x_i \neq y_i \\ 0 & \text{otherwise} \end{cases}$$

- “simple matching distance” = overlap distance without weights
- cluster centers $\mathbf{c}$ are “modes” (choose most frequent values of each feature)

K-modes: example

K=3. Original centers ("modes") individuals 1, 5, 10

Individual	Q1	Q2	Q3	Q4	Q5	C1	C2	C3
1	A	B	A	B	C	0	4	2
2	A	A	A	B	B	2	4	4
3	C	A	B	B	A	4	2	4
4	A	B	B	A	C	2	5	0
5	C	C	C	B	A	4	0	5
6	A	A	A	A	B	3	5	4
7	A	C	A	C	C	2	4	3
8	C	A	B	B	C	3	3	3
9	A	A	B	C	A	4	4	3
10	A	B	B	A	C	2	5	0

Note: Many ways to choose initial “modes”.

K-modes: example

Calculate new modes:

Cluster	Q1	Q2	Q3	Q4	Q5
1 (1), (2), (6), (7), (8)	A	A	A	B	C
2 (3), (5)	C	A	B	B	A
3 (4), (9), (10)	A	B	B	A	C

Example from "K-Modes intuition and example" by Aysan Fernandes
https://www.youtube.com/watch?v=b39_vipRkUo

K-prototypes

- for mixed data
- minimize

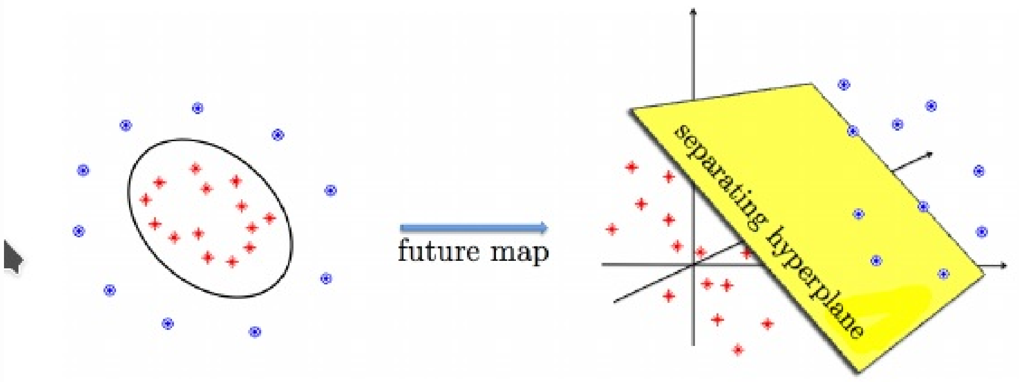
  $\sum_{\mathbf{x}\in C}\left(\sum_{i=1}^{q}(x_i - c_i)^2 + \gamma \sum_{i=q+1}^{k} d_s(x_i, c_i)\right)$, where

  $x_1 \ldots, x_q$ numerical values

  $x_{q+1}, \ldots, x_k$ categorical values
  γ=balancing weight
- cluster centroids $\mathbf{c}$ are “prototypes”

K-means extensions: Kernel-K-means

Idea: map data implicitely to a higher dimensional space and perform K-means there



The kernel trick - complex in low dimension (left), simple in higher dimension (right)

- \+ robust
- \+ can detect arbitrary shapes
- – expensive

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image source Soheily-Khah (2016): Generalized k-means based clustering for temporal data under time warp

Summary

- Basic idea of K-representatives method
  - K-means, K-medians, K-medoids, K-modes, K-prototypes
- Techniques to choose K
  - SSE elbow, Silhouette peak, Calinski-Harabasz, Gap statistic

Further reading:

- Gan, Ma, Wu: Data clustering – theory, algorithms, and applications. SIAM 2007.
- Jain and Dubes: Algorithms for clustering data. Prentice-Hall 1988.