PA196: Pattern Recognition

10. Clustering

Dr. Vlad Popovici
popovici@iba.muni.cz

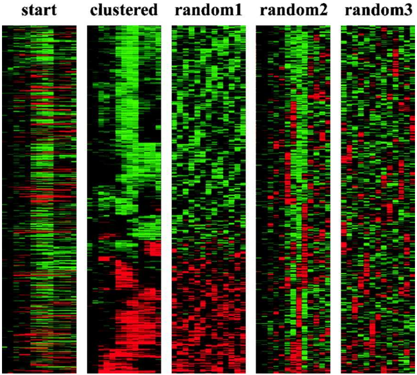
Institute of Biostatistics and Analyses
Masaryk University, Brno

Introduction

- clustering: a collection of methods for grouping data based on some measure of similarity
- technique for data exploration
- tries to identify some groupings of data: a partition of the given data set into some subsets that are (more or less) homogeneous in some sense
- different methods may lead to completely different partitions
- can be used as a starting point in a supervised analysis: the cluster labels may guide classifier design

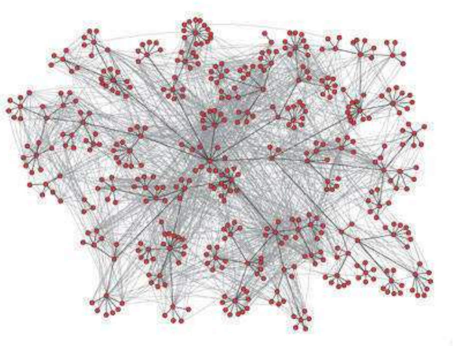
Why clustering?

Example: **Eisen et al, PNAS 1998**: "... statistical algorithms to arrange genes according to similarity in pattern of gene expression."



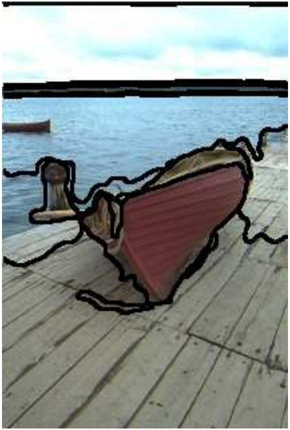
Why clustering?

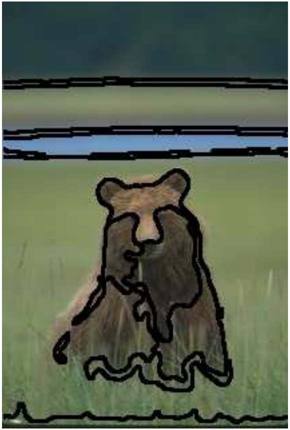
Example: **Adamic, Adar, 2005**: the social network - email communication within a corporation



Why clustering?

Example: **Mignotte , PRL 2011**: image segmentation





Why clustering?

Example: **Li et al., IEEE Trans Inf Theory, 2004**

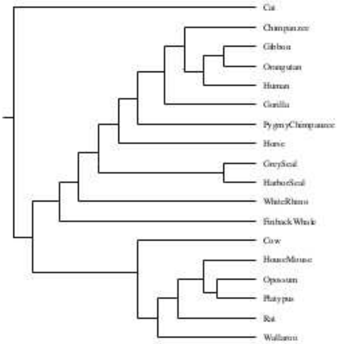


Fig. 1

The evolutionary tree built from complete mammalian mtDNA sequences using frequency of k-mers.

Two classes of algorithms

- flat clustering the data space is partitioned into a number of subsets (the most "meaningful"); requires the number of partitions to be specified
- hierarchical clustering: build a nested hierarchy of partitions

Outline

1. Flat clustering
   - Mixture densities
   - K–means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Assume a generative model:

- the observed data $\mathcal{D} = \{\mathbf{x}_i | i = 1, \dots, n\}$ originates from G groups
- each group has a prior $P(g_k)$, $k = 1, \dots, G$
- the class-conditional probabilities are of some known parametric form

$$p(\mathbf{x} | g_k, \boldsymbol{\theta}_k)$$

- the labels of the points $\mathbf{x}$ are unknown as are the parameters $\boldsymbol{\theta}_k$

PDF:

$$p(\mathbf{x}|\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_G\}) = \sum_{i=1}^{G} p(\mathbf{x}|g_i, \boldsymbol{\theta}_i)P(g_i)$$

- this is a mixture density
- $p(\cdot)$ are the *mixture components* and $P(\cdot)$ are the *mixing parameters*
- the goal is to estimate $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_G$

Maximum likelihood estimates

Let $\mathbf{T} = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_G\}$. The *likelihood* of the observed data is

$$p(\mathcal{D}|\mathbf{T}) = \prod_{i=1}^{n} p(\mathbf{x}_i|\mathbf{T})$$

The *maximum likelihood estimate* $\hat{\mathbf{T}}$ is

$$\hat{\mathbf{T}} = \arg\max_{\mathbf{T}} p(\mathcal{D}|\mathbf{T})$$

The maximum likelihood estimate is usually obtained through an iterative process: expectation maximization.

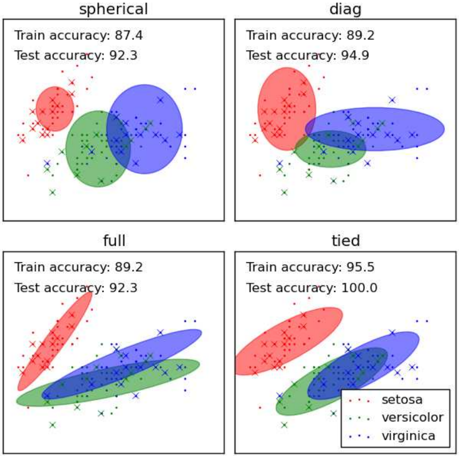
Repeat until convergence:

1. **Expectation step** (E-step) compute the expected log-likelihood under current estimates $\hat{\mathbf{T}}^{(t)}$
2. **Maximization step** (M-step) find $\hat{\mathbf{T}}^{(t+1)}$ that maximizes the expectation

Gaussian Mixture Models

- depending on how constraint is the model, different forms can be fitted
- usually, the constraints are on the form of the covariance matrices: spherical, diagonal, full

Example (from scikit-learn):



Outline

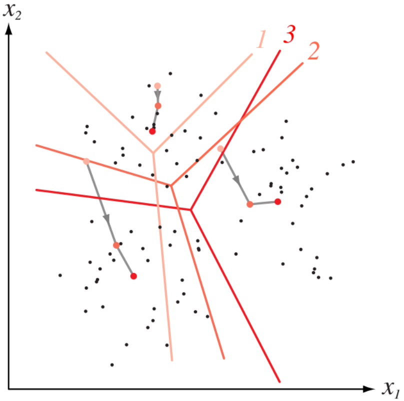
1. Flat clustering
   - Mixture densities
   - K−means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

- given are n data points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ and the number K of clusters
- in the Gaussian mixture model, assume the covariance matrices to be identity matrices → the Mahalanobis distance becomes Euclidean distance
- goal: find the K cluster centres (based on Euclidean distance)

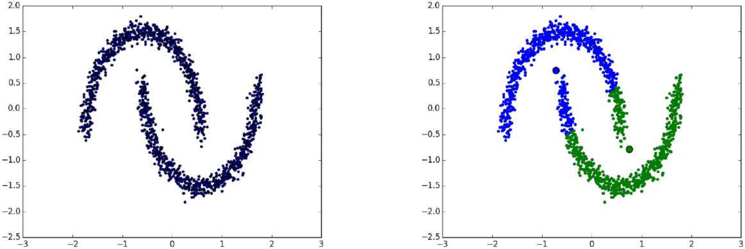
Overview of the algorithm:

1. choose randomly K cluster centres
2. assign all the points to the cluster defined by the closest centre
3. re-compute the cluster centres
4. repeat 2-3 until no more changes (or some other convergence criterion)

[DHS -Fig 10.3]

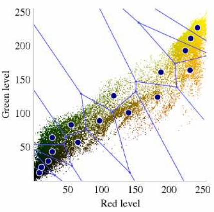


Example:



Application of $K-$means clustering: vector quantization

Goal: find a limited number of levels to represent a (possibly continuous) range of values.
Example: color quantization. Reduce the number of colors in an image in an adaptive way. (From Wikipedia:)



"Rosa Gold Glow 2 small noblue color space". Licensed under Public domain via Wikimedia Commons

Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Some definitions

- **Graph:** A *(simple, unoriented) graph* G is a pair of sets $G = (V, E)$, where V is a vertex set and E is an edge set.
- An *edge* $(i, j) \in E$ is an unordered pair of vertices $i, j \in V$.
- **Oriented graph**: A *oriented graph* G is a pair of sets $G = (V, E)$, where V is a vertex set and E is an arc set. An *arc* $(i, j) \in E$ is an ordered pair of vertices $i, j \in V$, with i called *tail* and j called *head.*

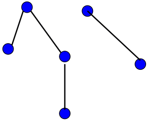


Figure : A simple graph.

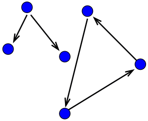


Figure : An oriented graph.

- A *path* of length r from i to j is a sequence of $r+1$ distinct and adjacent vertices starting with i and ending with j.
- A *connected* graph is a graph where any two vertices may be linked by a path.
- A *connected component* is an induced subgraph maximal that is connected.
- The *degree* d_i of a vertex i is the number of incident edges to i.
- The *in–degree* $d_i^{(i)}$ of a vertex i is the number of arcs ending with i. The *out–degree* $d_i^{(o)}$ of a vertex i is the number of arcs starting with i.

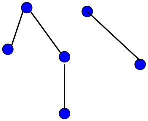
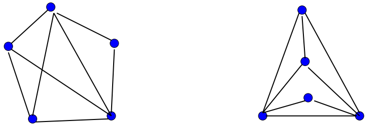


Figure : A graph with 2 connected components.

Graph isomorphism

Two graphs G_1 and G_2 are *isomorphic* if there exists a bijection $\varphi : V_{G_1} \to V_{G_2}$ such that $(i,j) \in E_{G_1}$ iff $(\varphi(i), \varphi(j)) \in E_{G_2}$.



Adjacency and incidence matrices

The *adjacency matrix* $A(G) = [a_{ij}]$ of a graph G is a $|V| \times |V|$ 01−matrix, with $a_{ij} = \mathbb{I}_{(i,j)\in E}$. The *incidence matrix* $B(G) = [b_{ij}]$ of a graph G is a $|V| \times |E|$ matrix with $b_{ik} = -1$ and $b_{jk} = 1$, where $k = (i,j) \in E$.

Properties:

- for a graph G: $BB^t = \text{diag}(d_1, ..., d_{|V|}) - A$
- let G_1 and G_2 be two isomorph graphs; then

$$\det(xI - A(G_1)) = \det(xI - A(G_2)),$$

so, they have the same spectrum.
- the number of paths of length r from i to j is given by $(A^r)_{ij}$.

Laplacian of a graph

The *Laplacian* of the graph G is the matrix $L(G) = BB^t$, where B is the incidence matrix of G.

Properties:

- $L_{ij} = \begin{cases} d_i & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$
- L is symmetric (by construction) positive semi–definite
- $L\mathbf{1}_{|V|} = 0$ so the smallest eigenvalue is $\lambda_1 = 0$ and the corresponding eigenvector is $\mathbf{1}_{|V|}$.
- the number of connected components of G equals the number of null eigenvalues.

Warning: there are various other variants of L's definition (e.g. admittance matrix, Kirchhoff matrix).

Generalizations:

- A is replaced by a *weight/similarity matrix* W (still symmetric)
- the *degree* of a vertex i becomes $d_i = \sum_{j=1}^{|V|} w_{ij}$
- the Laplacian becomes (see its properties): $L = D - W$, where $D = \mathrm{diag}(d_1, ..., d_{|V|})$
- the *normalized Laplacian* is defined as $D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}}$.

Overview of spectral clustering

Spectral clustering: partitioning the similarity graph under some constraints:

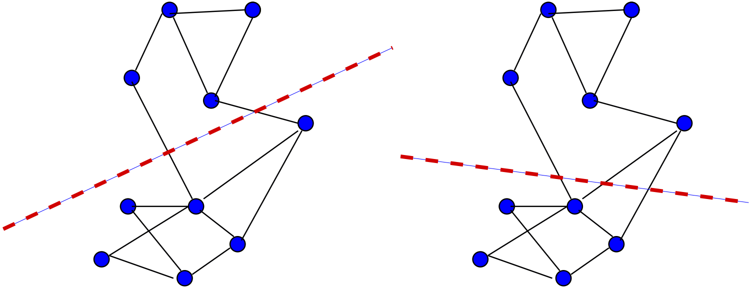


Figure : Where to cut??

- balance the size of the clusters?
- minimize the number of edges removed?

Let A, B be the two clusters/subgraphs and let $s(A, B) = \sum_{i \in A} \sum_{j \in B} w_{ij}$. Objective functions:

- *ratio cut*: $J(A, B) = \frac{s(A,B)}{|A|} + \frac{s(A,B)}{|B|}$, i.e. minimize similarity between A and B
- *normalized cut*: $J(A, B) = \frac{s(A,B)}{\sum_{i \in A} d_i} + \frac{s(A,B)}{\sum_{i \in B} d_i}$
- *min–max–cut*: $J(A, B) = \frac{s(A,B)}{s(A,A)} + \frac{s(A,B)}{s(B,B)}$, i.e. minimize the similarity between A and B and maximize the similarity within A and B.

All these lead to finding the smallest eigenvectors/eigenvalues of $L = D - W$.

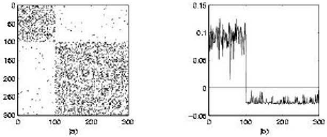
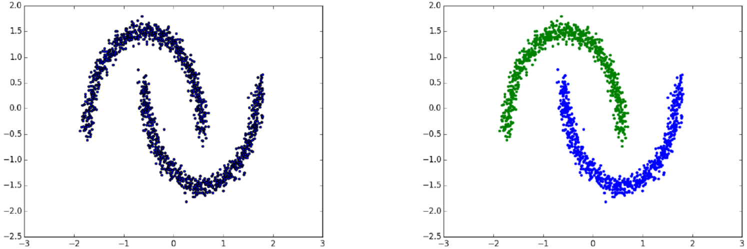


Figure : Adjacency matrix and the 2nd eigenvector

Spectral clustering - main algorithm

- input: a similarity matrix $\mathbf{S}$ and the number of clusters k
- compute the Laplacian L
- compute the eigenvectors $\mathbf{v}_i$ of L end order them in increasing order of the corresponding eigenvalues
- build $\mathbf{V} \in \mathbb{R}^{n \times k}$ with eigenvectors as columns
- the rows of $\mathbf{V}$ are the new data points $\mathbf{z}_i \in \mathbb{R}^k$ to be clustered
- use $k-$means to cluster $\mathbf{z}_i$

Example:

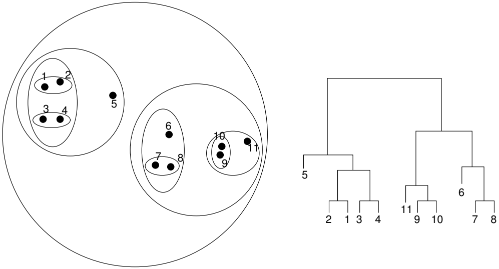


Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Hierarchical clustering

A nested set of partitions and the corresponding *dendrogram*:



- the height of the descendent segments is proportional with the distance/similarity between the partitions
- the ordering is irrelevant (i.e. you can swap left and right sub-trees without altering the meaning)
- it can be seen as a density estimation method

There are two main approaches to construct a hierarchical clustering:

- *agglomerative*: initially, each point is alone in a cluster; the *closest* two clusters/groups are merged to form a new cluster
- *divisive* starts with all points in a single cluster, which is iteratively split

Outline

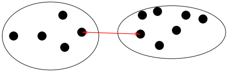
1. Flat clustering
   - Mixture densities
   - K−means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Linkage algorithms

- bottom-up/agglomerative strategy
- start with each point in its own cluster
- merge the two closest clusters
- continue until there is only one cluster
- Johnson: Hierarchical clustering schemes. Psychometrika, 2:241-254, 1967
- many applications, including phylogenetic trees
- the key is to define a distance over clusters space

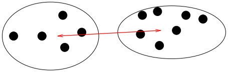
- single linkage:

$$\delta(C_1, C_2) = \min_{\mathbf{x}\in C_1, \mathbf{z}\in C_2} d(\mathbf{x}, bz)$$



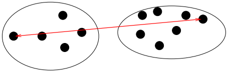
- average linkage:

$$\delta(C_1, C_2) = \frac{1}{|C_1||C_2|} \sum_{\mathbf{x}\in C_1, \mathbf{z}\in C_2} d(\mathbf{x}, \mathbf{z})$$



- complete linkage:

$$\delta(C_1, C_2) = \max_{\mathbf{x}\in C_1, \mathbf{z}\in C_2} d(\mathbf{x}, bz)$$



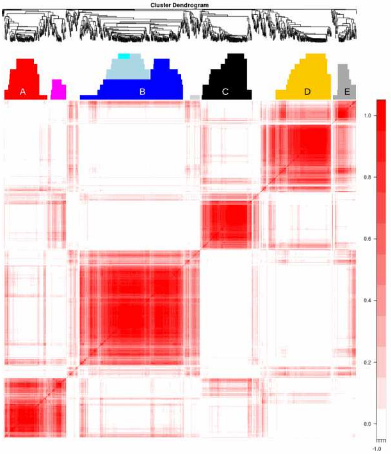
- other variations...

Comments:

- single linkage tends to produce non-balanced trees, with long "chains"
- complete linkage leads to more compact clusters
- single linkage: minimum spanning tree (cut the longest branch in MST and get the first two clusters)
- sensitive to outliers
- does not need a pre-specified number of clusters - but often you have to cut the dendrogram and to decide how many clusters are in data
- the clustering tree is not unique

Example: discovery of molecular subtypes in CRC

See Budinska et al, J Path. 2012



Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Other methods: information-theoretic methods

- idea: construct a clustering the preserves most of the "information" in data
- hence, you need a cost function (distortion function)
- density estimates based on frequencies (counts)
- no notion of similarity
- example: Information Bottleneck

Other methods: iterative refinement

- Karypis, Kumar: multilevel partitioning of graphs, SIAM J Sci Comp 1999
- start with a large graph
- merge nodes in "super-nodes" (coarsen the graph)
- cluster the coarse graph
- uncoarsen again: refine the clustering

Other methods: ensemble methods

- produce a series of clusterings based on perturbed versions of the original data (resampling, different parameters, etc)
- use the ensemble of clusters to decide for the final clustering
- see Strehl, Ghosh: cluster ensembles, JMLR 2002

Other methods

- support vector clustering
- subspace clustering
- co-clustering (bi-clustering): obtain a clustering of rows and columns of the data matrix
- etc. etc.

Outline

1. Flat clustering
   - Mixture densities
   - $K-$means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Cluster quality

- some cluster methods (e.g. k-means) define an objective function as the goal of the clustering
- there are quality functions that are algorithm independent (many!)
- two quantities are usually accounted for:
    - *within-cluster similarity* (cluster homogeneity): should be high
    - *between-cluster similarity*: should be low
- while mathematically attractive, they usually lead to an NP-hard problem
- the choice of quality function is rather ad-hoc

Cluster stability and optimal k

General idea:

- start with a data set $\mathcal{D} = \{\mathbf{x}_i\}$ and some clustering algorithm $\mathcal{A}$
- for various number of clusters (e.g. $k = 2, 3, \ldots, K$:
    - draw subsamples from $\mathcal{D}$
    - use $\mathcal{A}$ to cluster them into k clusters
- compare the resulting clusters by using a distance between clusterings and compute a *stability index* describing how variable/stable the clustering distances are
- choose k that gives the best stability

Distances between clusterings of the same data: let $f^{(1)}$ and $f^{(2)}$ be two clusterings and define N_{ij} as the number of pairs $(\mathbf{x}, \mathbf{z})$ for which $f^{(1)}(\mathbf{x}, \mathbf{z}) = i$ and $f^{(2)}(\mathbf{x}, \mathbf{z}) = j$, for $i, j \in \{0, 1\}$.

Similarity/distance functions (some of many):

- *Rand index*: $(N_{00} + N_{11})/[n(n-1)]$
- *Jaccard index*: $N_{11}/(N_{11} + N_{01} + N_{10})$
- *Hamming distance*: $(N_{01} + N_{10})/[n(n-1)]$
- information theoretic distance: Entropy($f^{(1)}$) + Entropy($f^{(2)}$) - Mutual information($f^{(1)}, f^{(2)}$)

What if the clusterings are not defined on the same data?

- far from being trivial
- idea "extend" clustering $f^{(1)}$ to $\mathcal{D}_2$ and $f^{(2)}$ to $\mathcal{D}_1$
- some clustering algorithms are easily extended: $k-$means just requires assignment of new data to the defined clusters, etc.
- other clustering algorithms are not so flexible (e.g. spectral clustering)
- use some classifiers for extension... what about classification errors?
- what if the 2 datasets are not exactly "aligned"?

How many clusters?

- most flat clustering algorithms require *k*
- the hierarchical clustering usually is cut at some height to yield the final number of clusters
- e.g. image segmentation $k = ?$
- one way, use cluster quality to choose best *k*
- or use the stability approach
- or use "gap statistic" - see Tibshirani et al, J Royal Statist Soc 2001

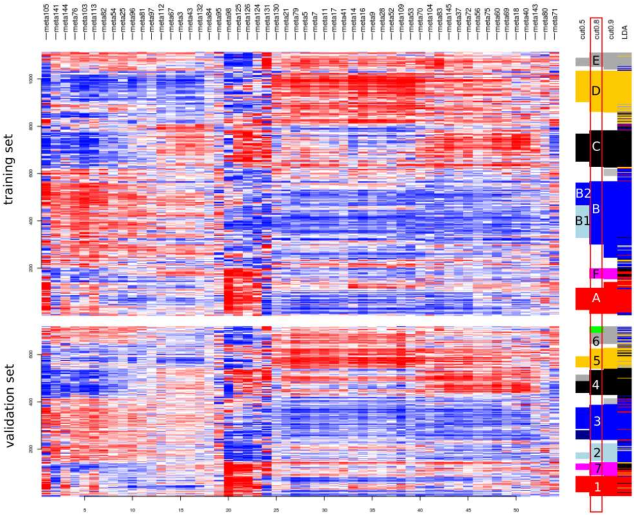
Outline

1. Flat clustering
   - Mixture densities
   - K–means clustering
   - Spectral clustering
2. Hierarchical clustering
   - Linkage algorithms
3. Further topics
   - Other methods
   - Cluster quality
   - Cluster validation

Cluster validation

- given a clustering, how confident are we that it represents "real" groups of points
- if a new data set is available, would we obtain the same clusters? and as many as before?
- complication: in real applications, data may not always come from the same conditions (e.g. change of measurement device, etc)
- maybe the original data set does not capture all the clusters that could arise in data
- no clear method for validation, but the ideas are the same as for cluster stability and quality

Example (Budinska et al, J Path 2012):


meta105
meta141
meta144
meta76
meta103
meta113
meta82
meta54
meta25
meta96
meta81
meta97
meta112
meta67
meta3
meta43
meta132
meta84
meta95
meta98
meta125
meta126
meta124
meta131
meta130
meta21
meta79
meta5
meta7
meta11
meta17
meta41
meta14
meta16
meta9
meta28
meta52
meta109
meta53
meta70
meta104
meta83
meta145
meta37
meta72
meta56
meta75
meta60
meta69
meta18
meta40
meta143
meta80
meta71
cut0.5
cut0.8
cut0.9
LDA
training set
validation set
E
D
C
B2
B
B1
F
A