Cluster analysis – advanced and special algorithms

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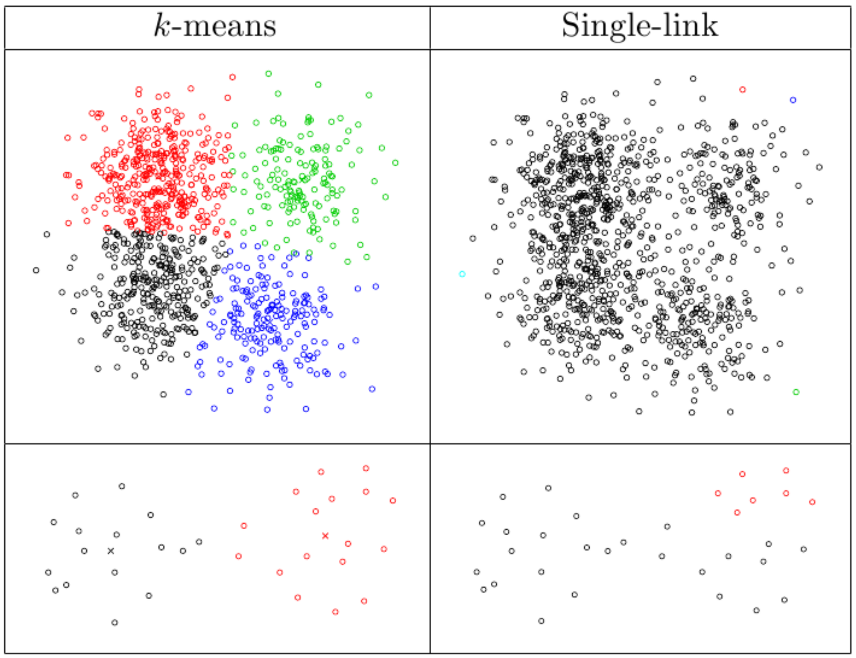
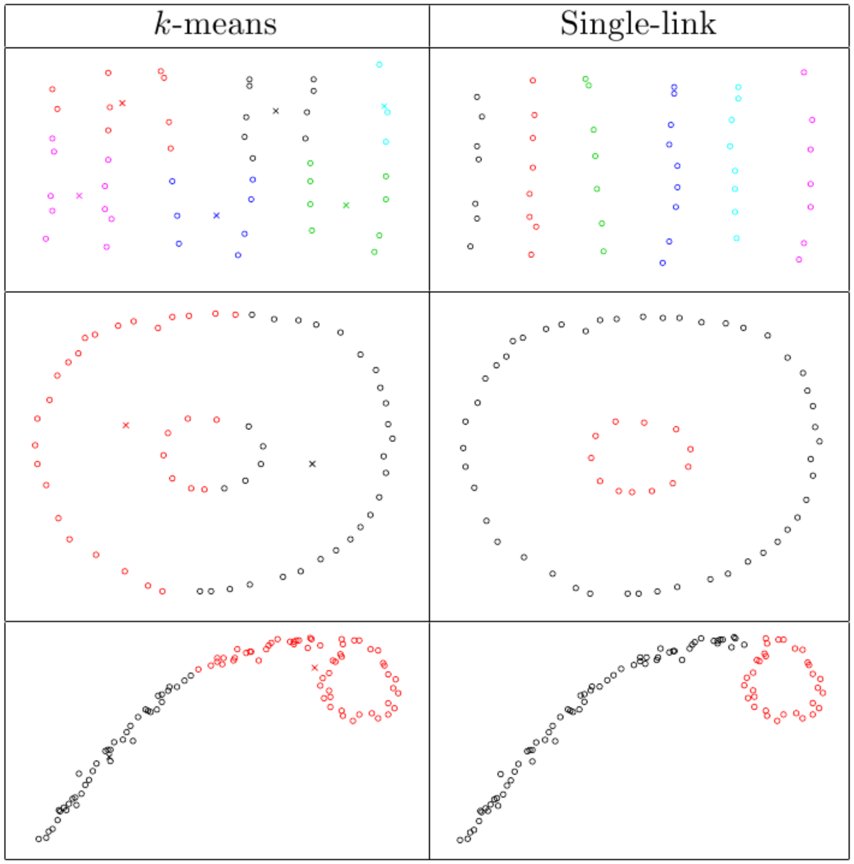
http://cw.felk.cvut.cz/wiki/courses/b4m36san/start

Comparison: k-means and hierarchical single-link

- single linkage tends to generate longer non-compact clusters,
- k-means makes compact clusters, complete linkage is outlier sensitive,



k-means intuitively correct

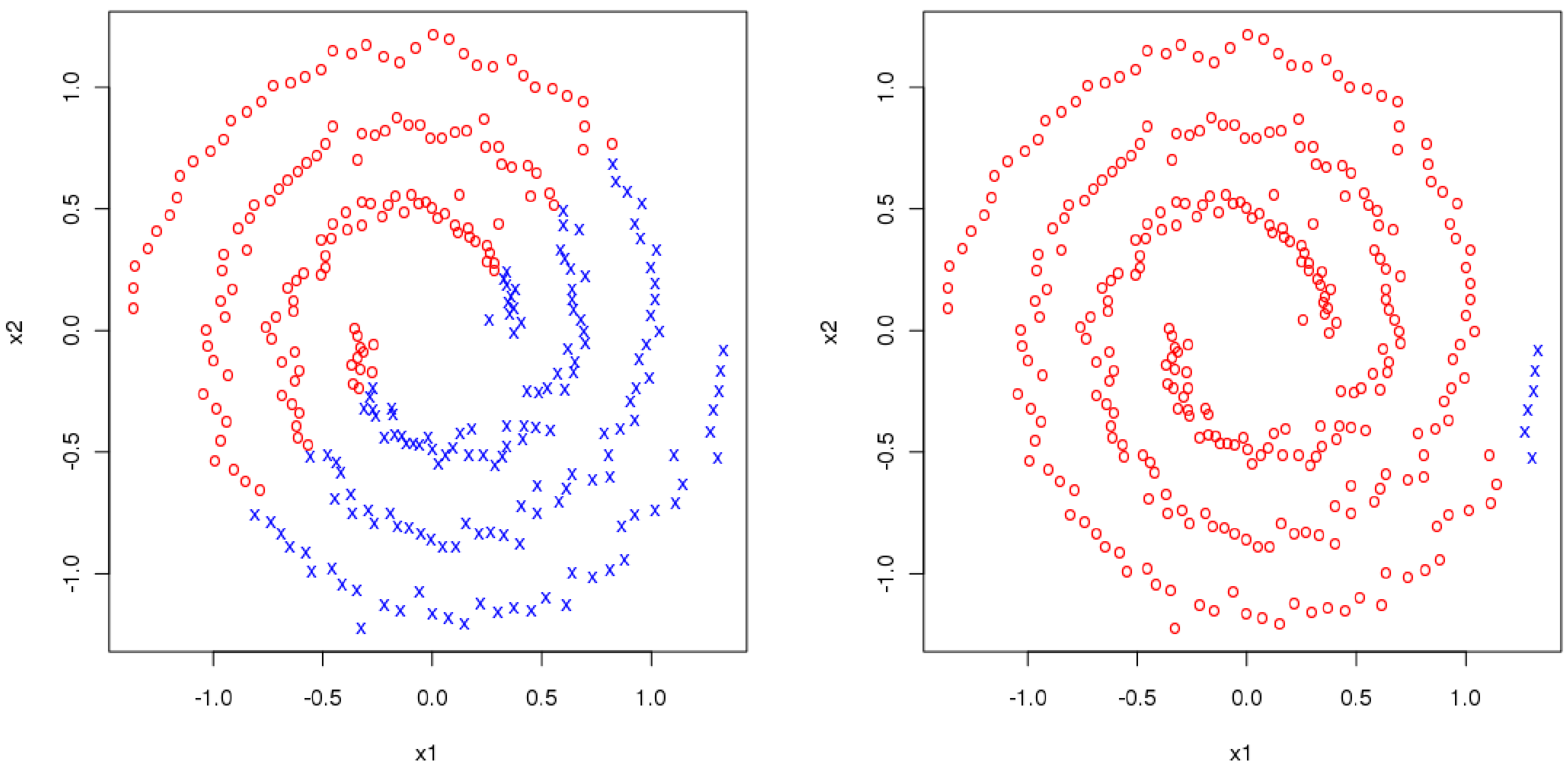


single linkage intuitively correct

Carnegie Mellon University, course: Statistics 36-350: Data Mining

Spectral clustering – motivation

- clustering algorithms assume certain cluster shapes
  - unexpected shapes cause difficulties (eg. linearly non-separable clusters),
  - “classical pairwise similarity” can be insufficient.



K-means application

Single linkage application

R, kernlab package, specc function demo

Spectral clustering – context

- frequent solution is a **feature space transformation**,
- a domain independent clustering algorithm, the transformation tuned for the domain
  - explicit transformation
    - get the object coordinates in the new feature space,
    - traditional clustering in the new space,
    - illustrative, but impractical,
  - implicit transformation
    - via similarity resp. kernel function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$,
    - purely a function of object pairs, no object coordinates in the new space,
    - very natural for clustering, similarity/distance its essential part anyway,
    - kernel trick analogy (SVM classification),
      - kernel k-means (see the next slide),
    - an implicit high-dimensional space, clusters (classes) potentially easily separable,
    - kernel PCA – kernel matrix → diagonalize → a low-dimensional feature space.

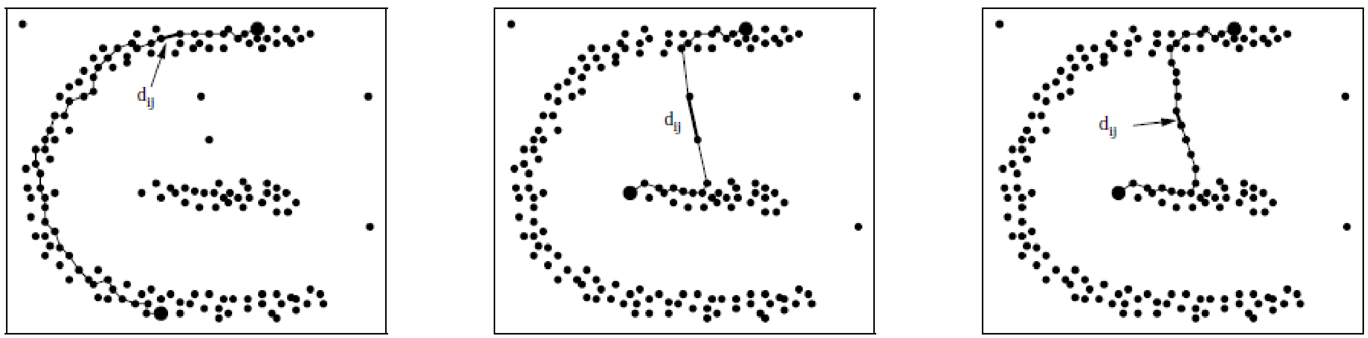
Kernel k-means

- apply k-means in the transformed feature space induced by a kernel function
  - the original objects: $x_1, x_2, \ldots, x_m$,
  - the transformed objects: $\Phi(x_1), \Phi(x_2), \ldots, \Phi(x_m)$ (not explicitly calculated),
  - the kernel function: $k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$,
  - cluster centers in the transformed space: $\mu_v = \frac{1}{|C_v|} \sum_{x_i \in C_v} \Phi(x_i)$ (not explicitly known),
  - only (squared) distances between objects and cluster centers need to be known:

$$
\begin{aligned}
||\Phi(x) - \mu_v||^2 &= ||\Phi(x) - \frac{1}{|C_v|} \sum_{x_i \in C_v} \Phi(x_i)||^2 = \\
&= \langle \Phi(x) - \frac{1}{|C_v|} \sum_{x_i \in C_v} \Phi(x_i), \Phi(x) - \frac{1}{|C_v|} \sum_{x_i \in C_v} \Phi(x_i) \rangle = \\
&= \langle \Phi(x), \Phi(x) \rangle - \frac{2}{|C_v|} \sum_{x_i \in C_v} \langle \Phi(x), \Phi(x_i) \rangle + \frac{1}{|C_v|^2} \sum_{x_i \in C_v, x_j \in C_v} \langle \Phi(x_i), \Phi(x_j) \rangle = \\
&= k(x, x) - \frac{2}{|C_v|} \sum_{x_i \in C_v} k(x, x_i) + \frac{1}{|C_v|^2} \sum_{x_i \in C_v, x_j \in C_v} k(x_i, x_j)
\end{aligned}
$$

Example: spirals – connectivity kernel, Gaussian kernel

- connectivity kernel
  - the object pair distance given by the max edge on the path connecting the objects,
  - if there are more paths, the one minimizing the criterion above is taken,
  - e.g., this kernel makes k-means behave similar to single linkage hierarchical clustering,

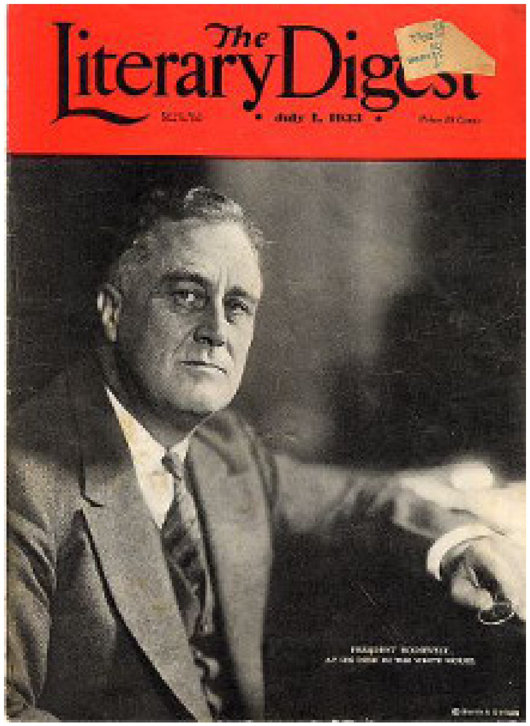


(a) (b) (c)

Fischer et al.: Clustering with the Connectivity Kernel

- Gaussian (RBF) kernel
  - $s(x_i, x_j) = \exp(-||x_i - x_j||/\sigma^2)$,
  - σ set to have a “tight” object neighborhood,
  - an implicit feature space (infinite dimension).

Famous statistical blunders . . .



US presidential elections, 1936

FD Roosevelt - Alf Landon

Draft lottery, 1970

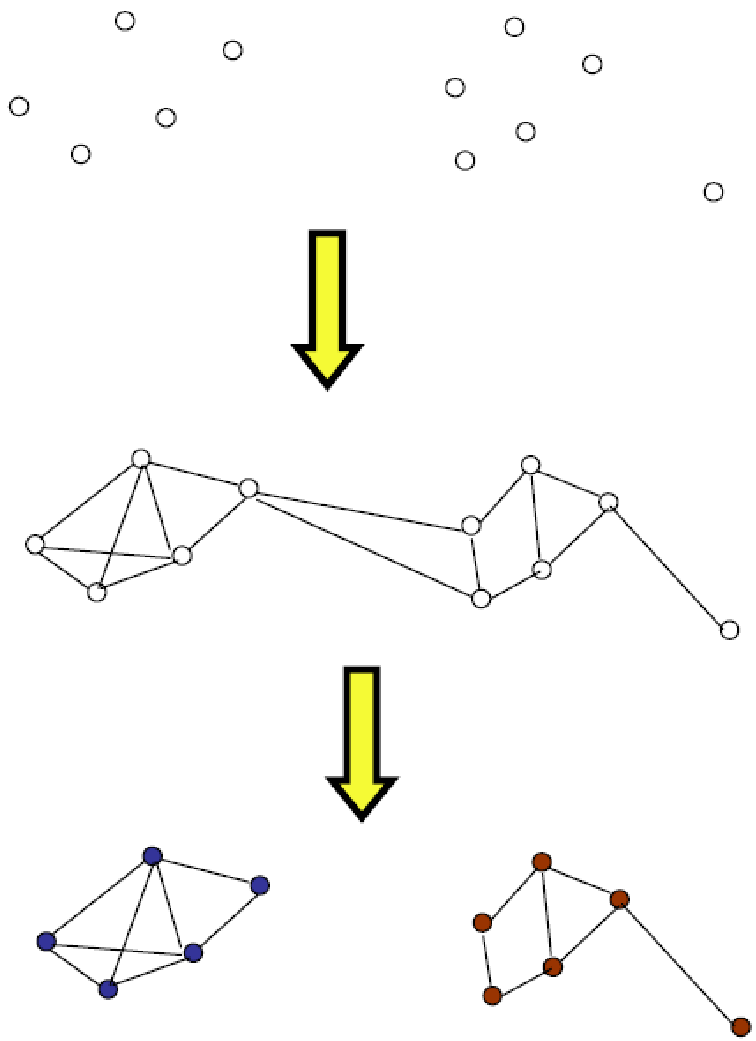
Vietnam war

Financial crisis, 2008

Gaussian copula function

Spectral clustering in a nutshell

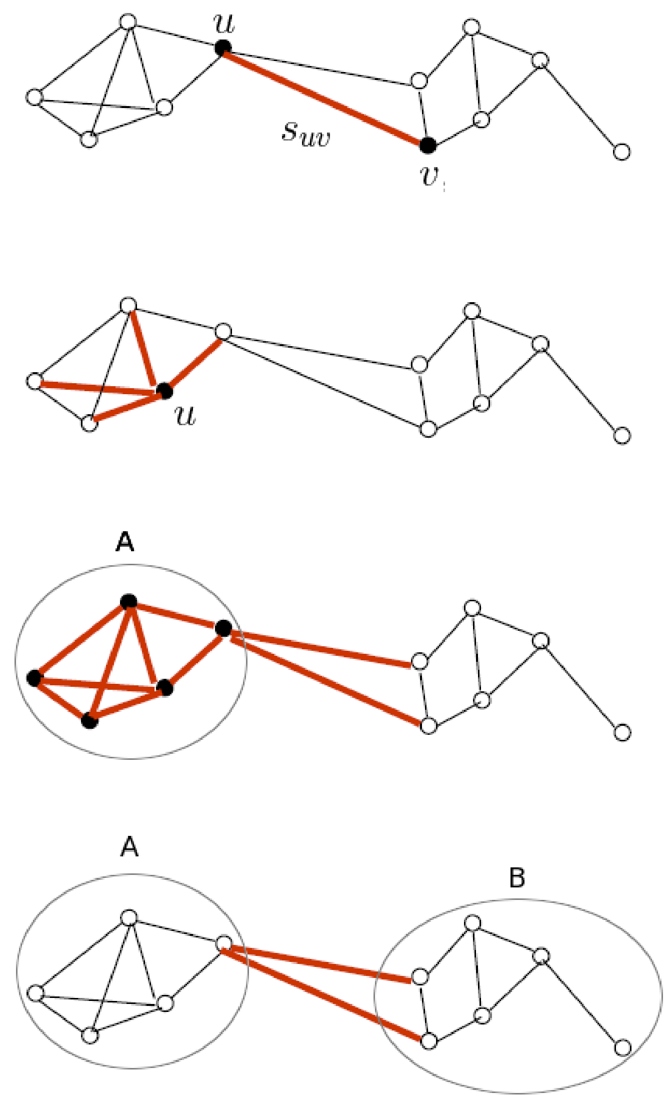
- input: a set of objects,
- described as a graph,
- edges encode similarity,
- graph decomposed into components = clusters,
- graph partitioned by its spectral properties.



Azran: A Tutorial on Spectral Clustering

Graph theory – basic terms

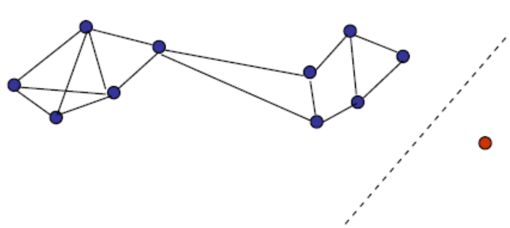
- vertex (object) similarity (affinity)
  - $s_{uv} = \langle u, v \rangle$,
- vertex degree (volume), degree matrix
  - $d_u = \sum_{v=1}^{m} s_{uv}$,
  - $\mathcal{D} = diag(d_1, \ldots, d_m)$,
- size and degree of a vertex set (cluster)
  - $|A|$ . . . the number of vertices in A,
  - $vol(A) = \sum_{u \in A} d_u$,
- an edge cut between two components
  - $cut(A, B) = \sum_{u \in A} \sum_{v \in B} s_{uv}$.



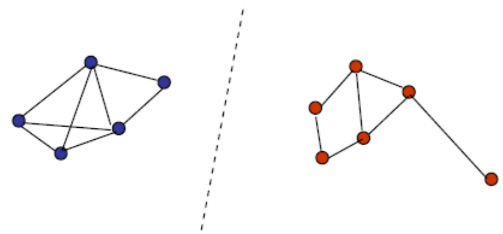
Azran: A Tutorial on Spectral Clustering

Spectral clustering as an approximated minimum graph cut

- clustering $\sim$ partition the similarity graph into components,
- can be solved as an optimization problem
  - search for a minimum edge cut in the similarity graph $\mathcal{S}$ to make it disconnected
    - $\min\limits_{A \subset S} cut(A, \bar{A})$,
    - a computationally feasible problem, but rather unsatisfactory partitions,



mincut, incorrect



RatioCut, Ncut, correct

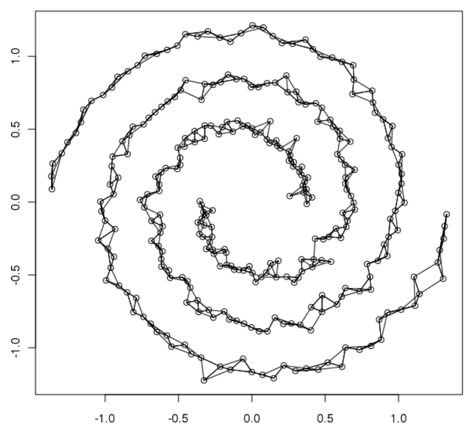
  - a "reasonable" size of the components needs to be required
    - minimize one of the balanced cut criteria,
    - $RatioCut(A, B) = cut(A, B)\left(\frac{1}{|A|} + \frac{1}{|B|}\right)$,
    - $Ncut(A, B) = cut(A, B)\left(\frac{1}{vol(A)} + \frac{1}{vol(B)}\right)$,
    - the dark side of the coin: NP-hard problems,
- spectral clustering provides a relaxed and feasible solution to the balanced cut problem.

Spectral clustering – algorithm

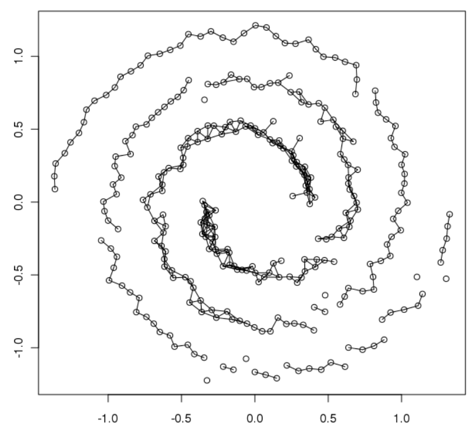
- inputs: $\mathcal{X} = [x_{ij}]_{m\times n} = \{x_1, \ldots, x_m\} \subset \mathbb{R}^n$, k
  1. select the similarity function
     - linear, RBF, polynomial, etc.
     - a general rule assigning functions to problems does not exist,
  2. compute the similarity (adjacency) matrix $\mathcal{S} = [s_{ij}]_{m\times m}$
     - (a new implicit feature space originates),
  3. construct a "reasonable" similarity graph by editing $\mathcal{S}$
     - $\mathcal{S}$ is a complete graph, vertices $\sim$ objects, similarities $\sim$ edges,
     - remove long (improper) edges,
  4. derive the Laplace matrix $\mathcal{L}$ out of the similarity matrix $\mathcal{S}$
     - unnormalized: $\mathcal{L} = \mathcal{D} - \mathcal{S}$,
     - normalized: $\mathcal{L}_{rw} = \mathcal{D}^{-1}\mathcal{L} = \mathcal{I} - \mathcal{D}^{-1}\mathcal{S}$,
  5. project into an explicit space of k first eigenvectors of $\mathcal{L}$,
     - $\mathcal{V} = [v_{ij}]_{m\times k}$, eigenvectors of $\mathcal{L}$ as columns,
  6. k-means clustering in $\mathcal{V}$ matrix
     - $\mathcal{V}$ rows interpreted as new object positions in k-dimensional space.

Spectral clustering – similarity graph

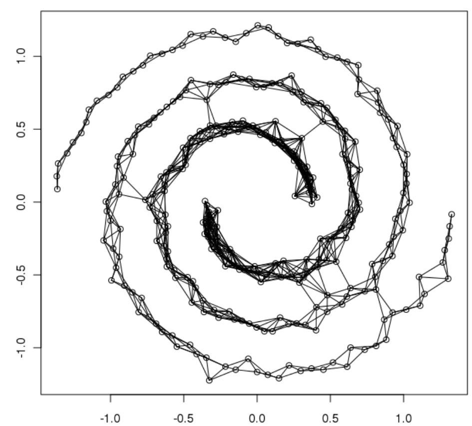
- reduce the complete graph to an undirected graph concerning local neighborhoods,
- vertices shall have a reasonable degree ($\ll m$),
- basic approaches
  - ϵ-neighborhood
    - $s_{ij} > \epsilon \rightarrow$ vertices i and j connected by an edge, otherwise $s_{ij} = 0$,
  - k-nearest neighbors
    - symmetric: connect i and j if i belongs to k nearest neighbors of j **or** vice versa,
    - mutual: connect i and j if i belongs to k nearest neighbors of j **and** vice versa,
  - keep the complete graph
    - usually with the RBF or other strictly local kernel.



Euclidean similarity, 3 nearest neighbors (var sym)



RBF kernel, too small ϵ



RBF kernel, a suitable ϵ

Spectral clustering – graph Laplacian

- concern the unnormalized option: $\mathcal{L} = \mathcal{D} - \mathcal{S}$
- then for $\forall f \in \mathbb{R}^m$

$$f'\mathcal{L}f = f'\mathcal{D}f - f'\mathcal{S}f =$$

$$= \sum_{i=1}^{m} d_i f_i^2 - \sum_{i,j=1}^{m} f_i f_j s_{ij} =$$

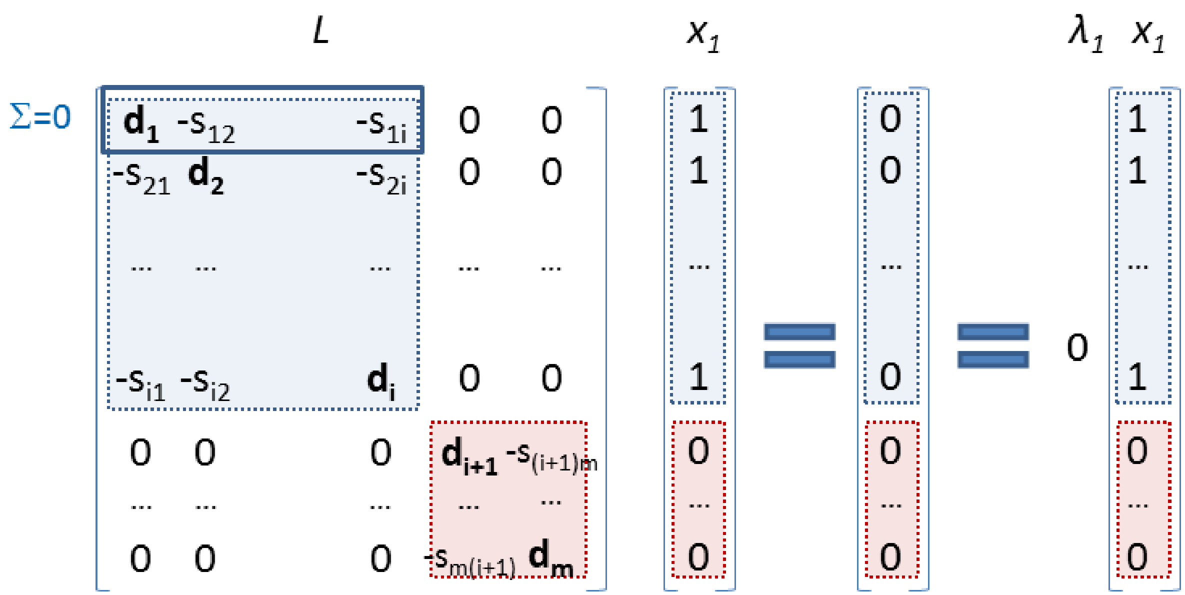
$$= \frac{1}{2}\left(\sum_{i=1}^{m}\left(\sum_{j=1}^{m} s_{ij}\right) f_i^2 - 2\sum_{i,j=1}^{m} f_i f_j s_{ij} + \sum_{j=1}^{m}\left(\sum_{i=1}^{m} s_{ij}\right) f_j^2\right) =$$

$$= \frac{1}{2}\sum_{i,j=1}^{m} s_{ij}(f_i - f_j)^2$$

- measures the variation of function f along the graph
  - the value $f'\mathcal{L}f$ is low when close vertices agree in their f_i,
  - assumes that near objects shall have close function values (f),
- the discrete Laplace operator encodes the same property,
- an interesting case: $f = \mathbb{1}_A$ ($f_i = 1$ if $v_i \in A$ otherwise $f_i = 0$), A is a graph component.

Spectral clustering – eigenvectors of $\mathcal{L}$

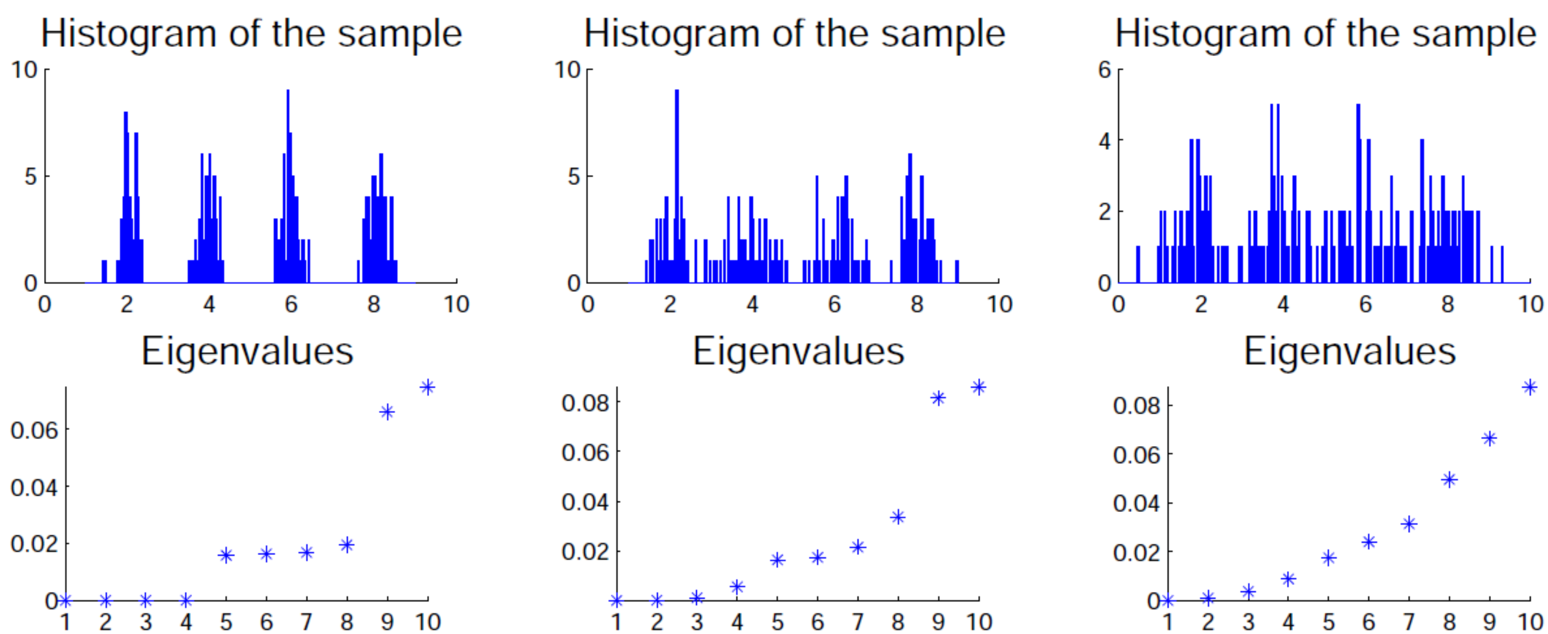
- eigenvectors x of $\mathcal{L}$ matix ($\mathcal{L}x = \lambda x$) provide a good graph partitioning indication,
- an ultimate (ideal) case: graph has exactly k components
  - k smallest eigenvectors ideally split k clusters,
  - $\lambda_1 = \cdots = \lambda_k = 0 < \lambda_{k+1} \leq \cdots \leq \lambda_m \rightarrow x_1, \ldots, x_k$,
- other (usual) cases: a connected graph, k component candidates exist
  - the space of k smallest eigenvectors (with nonzero λ) allows to form k clusters.



The ideal case for $k = 2$.

Spectral clustering – eigenvalues of $\mathcal{L}$

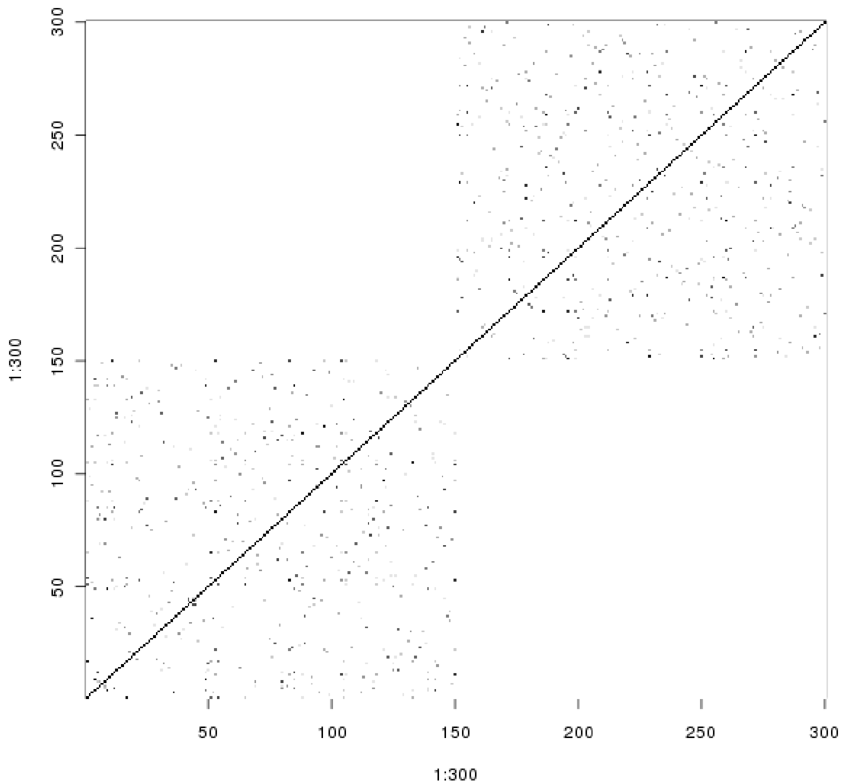
- provided k is unknown, **eigengap** statistic
  - a k-means gap heuristic analogy,
  - concern only small eigenvectors before the first jump in eigenvalues,
  - the number of clusters matches the number of selected eigenvectors.



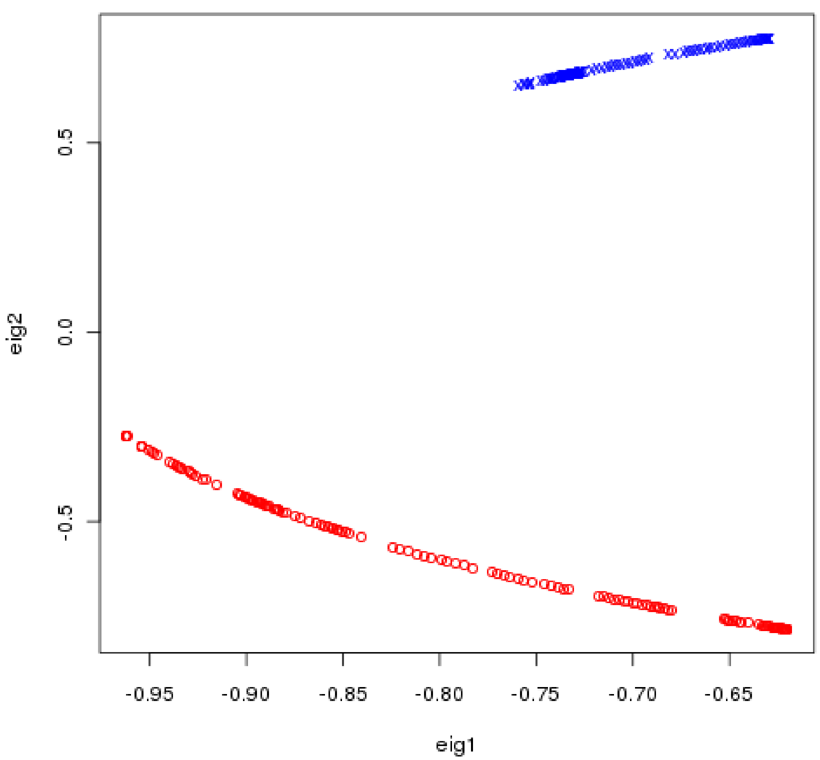
Luxburg: Clustering.

Example: spirals – eigenvectors

- similarity matrix splits the graph into components nearly ideally,
- the second eigenvector of $\mathcal{L}$ is a perfect component indicator.



Similarity matrix for RBF kernel with a suitable σ
the instance order is illustrative and keeps the real spiral membership



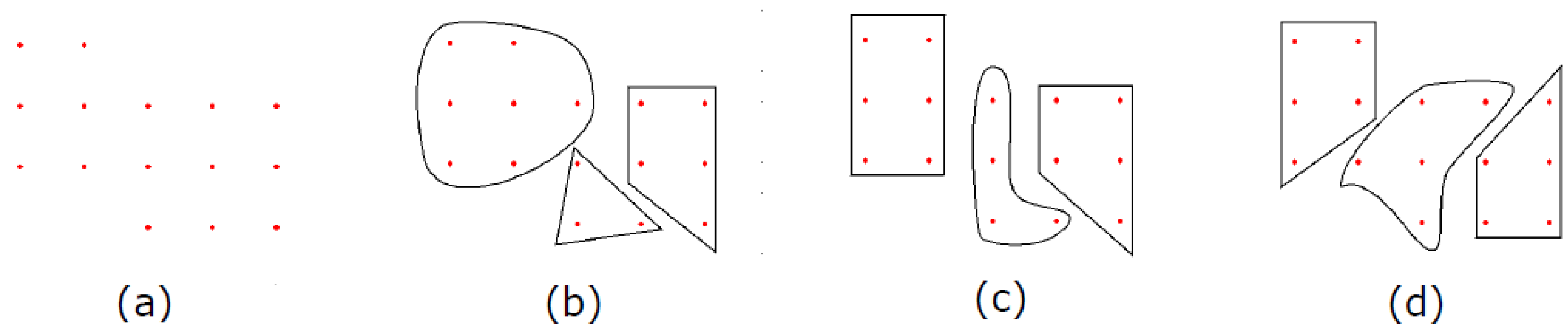
Projection – the first and second eigenvector space $\mathcal{S}$
colors give the real spiral membership, k-means clustering is trivial

Spectral clustering – summary

- advantages
  - does not make strong assumptions on cluster shape,
  - simple to implement – uses existing algorithms,
  - does not have a local optima, cannot stuck,
  - a modular approach applicable in a range of problems
    - modify the kernel or similarity graph to adapt to a new problem,
  - eigengap heuristic to find an optimal cluster number,
  - successful in a range of real problems,
- disadvantages
  - can be sensitive to choice of parameters, unclear how to set them,
    - kernels (eg. σ for RBF), graph similarity (ϵ or k),
  - computationally expensive on large non-sparse graphs,
    - use only after simpler algorithms fail,
  - not really clear what it does on non-regular graphs (e.g. power law graphs),
- demo
  - http://www.ml.uni-saarland.de/GraphDemo/GraphDemo.html.

Advanced clustering – summary

- Clustering covers a wide range of methods
  - not merely an instance set partitioning in $\mathbb{R}^n$ dealing with disjoint clusters,
  - in general, it discovers arbitrary frequent co-occurrence of events in data,
- unsupervised = subjective approach
  - "gold true" does not exist (compare with classification),
  - the outcome is influenced by the employed implicit and explicit knowledge,

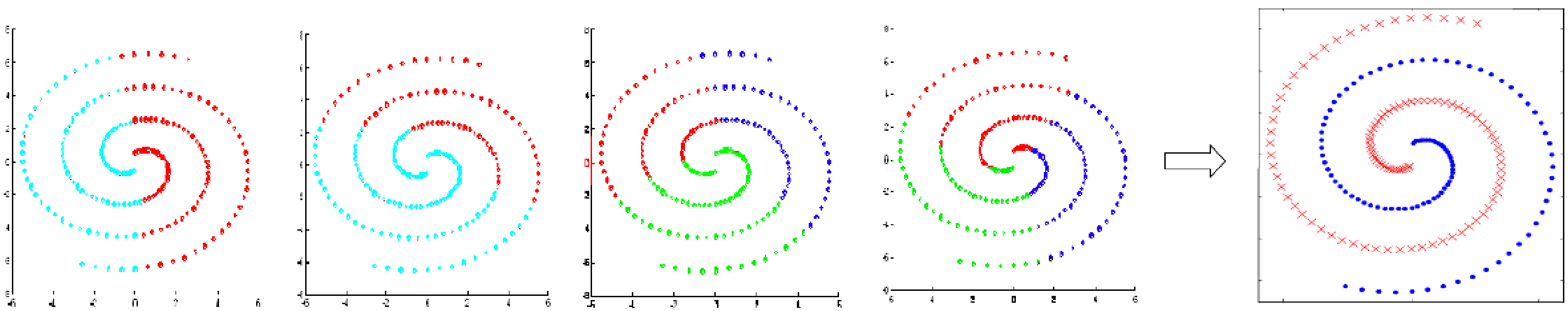


Jain: Data Clustering: 50 Years Beyond K-Means, modified

- tightly related to learning
  - conceptual clustering – knowledge-based with cluster/concept descriptions,
  - semi-supervised clustering – both annotated and unannotated instances,

Advanced clustering – summary

- exists in many modifications
  - bi-clustering
    - ∗ rather the local (context-sensitive) than global similarity.
- topics not covered
  - heterogenous data
    - ∗ that cannot be represented as a constant-size feature vector,
  - large scale clustering
    - ∗ efficient NN, incremental clustering, sampling, distributed computing, prior data summarization,
  - clustering ensembles
    - ∗ the result obtained by combining multiple partitions.



Jain: Data Clustering: 50 Years Beyond K-Means, modified

Recommended reading, lecture resources

:: Reading

- von Luxburg: **Lectures on Clustering.**
  - PASCAL Bootcamp in Machine Learning, Vilanova (Barcelona), 2007,
  - http://videolectures.net/bootcamp07_luxburg_clu/,