Cluster analysis – advanced and special algorithms

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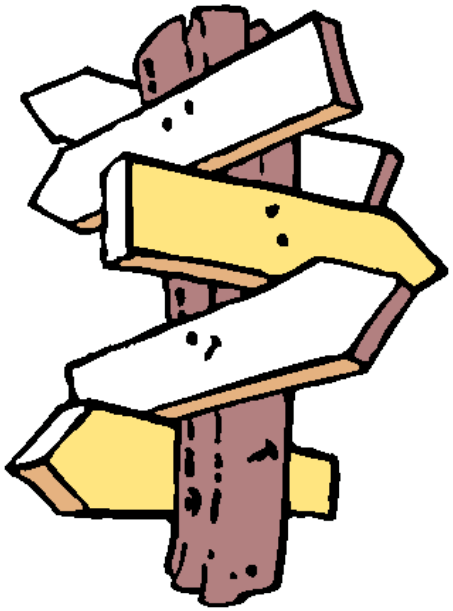
http://cw.felk.cvut.cz/wiki/courses/b4m36san/start

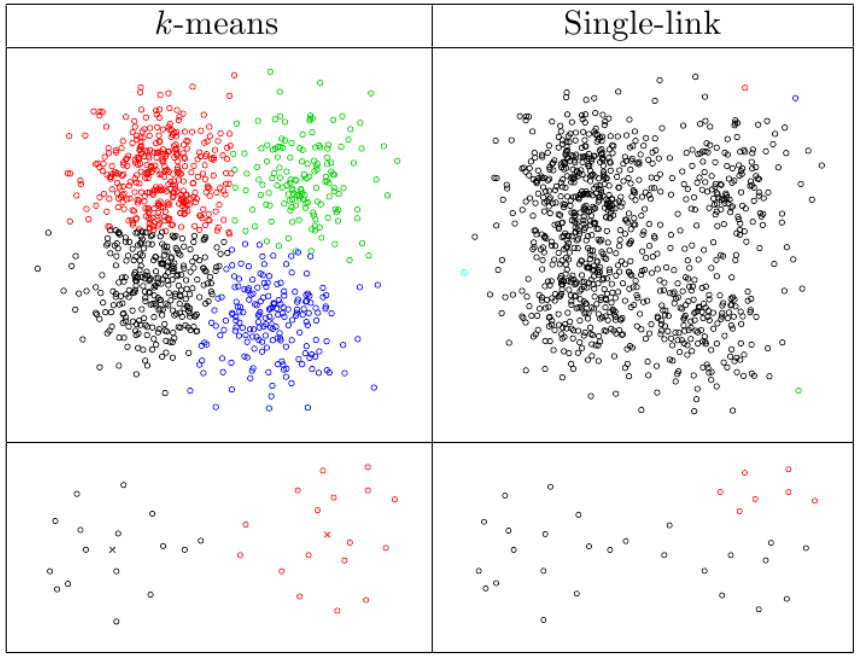
Outline

- robustness of the introduced methods – examples,
- k-means and hierarchical agglomerative clustering – complexity,
- clustering quality – evaluation
  - internal versus external partitioning evaluation,
- clustering definition?
- an advanced method
  - spectral clustering,

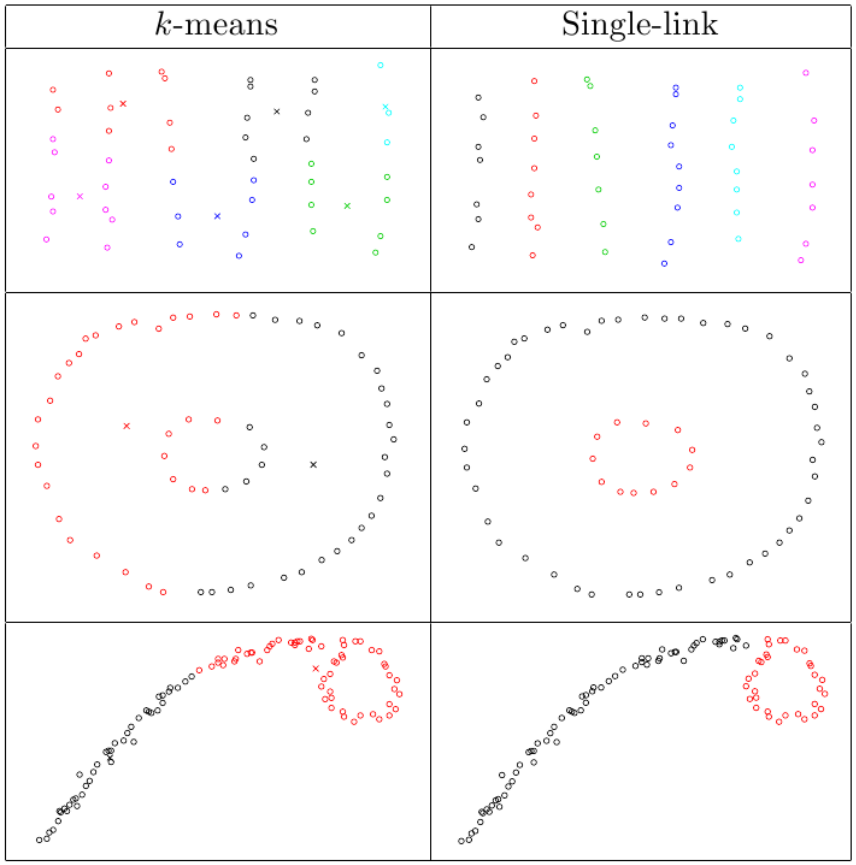


Comparison: k-means and hierarchical single-link

- 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

Complexity – comparison

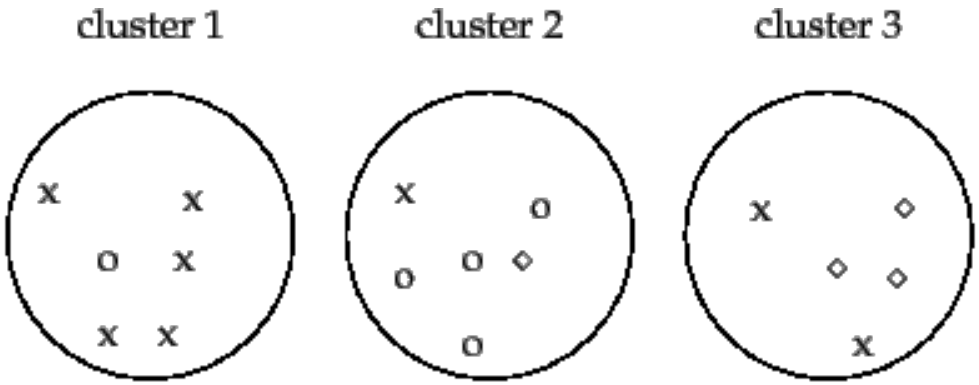
- assumed: $d(x_i, x_j) \in \mathcal{O}(n)$,
- k-means algorithm
  - assign instances into clusters: $\mathcal{O}(km)$ distance computations $\rightarrow f_E \in \mathcal{O}(knm)$,
  - modify centroids: $f_M \in \mathcal{O}(nm)$ (each instance used exactly once in one of the centroids),
  - unknown iteration number before stop: i (estimates vary from the constant with m up to $\mathcal{O}(m^{kn})$),
  - summary: $f = i(f_E + f_M) \in \mathcal{O}(iknm)$,
- hierarchical agglomerative clustering (single link)
  - initialize
    - compute distances among all instance pairs $f_I \in \mathcal{O}(m^2 n)$,
    - *next-best-merge* array – the nearest neighbor with its distance for each cluster (complexity hidden in the previous line),
  - $m - 1$ iterations to complete the dendrogram
    - find the smallest distance in the next-best-merge array $f_{E_0} \in \mathcal{O}(m)$,
    - adjust the distance matrix $f_{E_1} \in \mathcal{O}(m)$,
    - adjust the next-best-merge array $f_{E_2} \in \mathcal{O}(m)$,
  - summary: $f = f_I + (m-1)(f_{E_0} + f_{E_1} + f_{E_2}) \in \mathcal{O}(m^2 n)$.

Clustering quality – evaluation

- **internal:** quantifies three partitioning characteristics
  - homogeneity – are instances within clusters similar?
    $hom = \frac{1}{m} \sum_{i=1}^{k} \sum_{x_j \in C_i} d(x_j, \mu_i)$,
  - separability – are instances in different clusters dissimilar?
    $sep = \frac{1}{k(k-1)} \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{k} \exp\left(-\frac{d^2(\mu_i, \mu_j)}{2\sigma^2}\right)$,
  - stability – how many relations breaks up by adding noise or random instance sampling?
- internal evaluation criteria in the clustering algorithms
  - intra-cluster variability: (see homogeneity for k-means),
  - model likelihood: (for probabilistic models, see EM GMM),
  - the size of the balanced cut of similarity graph: (see spectral clustering later)
    $\frac{1}{2} \sum_{ij} s(x_i, x_j)(1 - \delta(C_i - C_j))(\frac{1}{|C_i|} + \frac{1}{|C_j|})$,
- clustering is subjective, the "objective" internal measure can be improper.

Clustering quality – evaluation

- **external:** match the partition Ω with a known annotation $G = \{G_1, \ldots, G_c\}$ (gold standard),
- basic external evaluation criteria
  - purity
    - the total major instance class ratio across clusters
      (each cluster has a major class, the higher its ratio in the cluster the better),
      $purity(\Omega, G) = \frac{1}{m} \sum_{i=1\ldots k} \max_{j=1\ldots c} |C_i \cap G_j|$
    - disadvantage: cannot compare partitions with different k,
    - example (figure): $purity = \frac{5+4+3}{17} = 0.71$



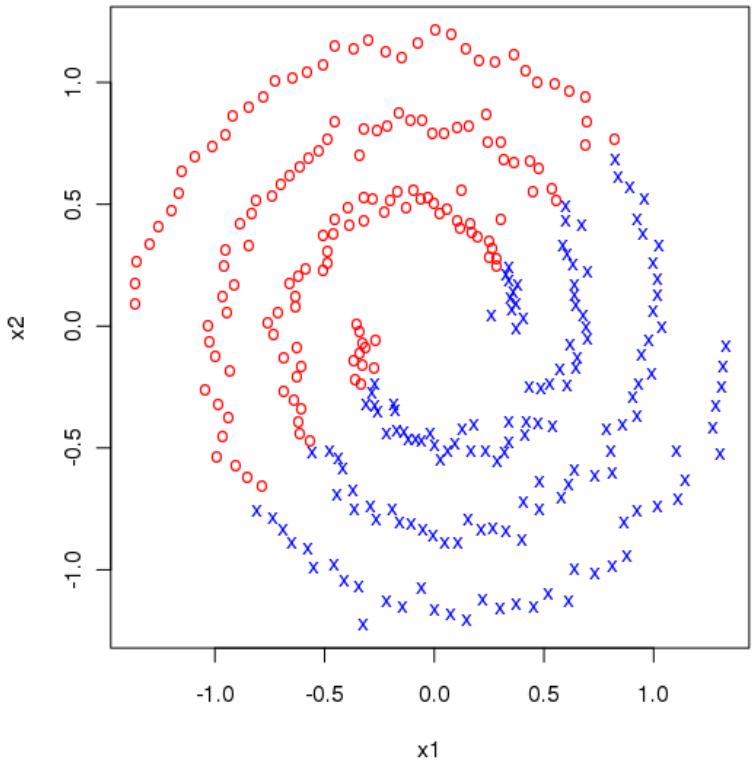
Manning et al.: Introduction to Information Retrieval.
http://nlp.stanford.edu/IR-book/html/htmledition/irbook.html

Clustering quality – evaluation

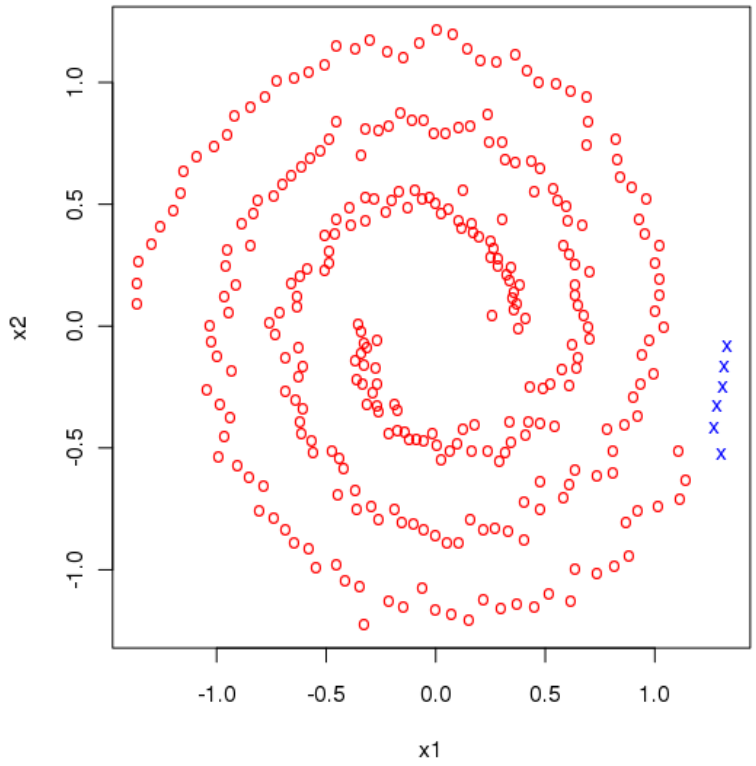
- basic external evaluation criteria (continuation)
  - normalized mutual information
    - based on information entropy,
      $NMI(\Omega, G) = \frac{2I(\Omega,G)}{H(\Omega)+H(G)}$
      $I(\Omega, G) = -\sum_{i=1\ldots k}\sum_{j=1\ldots c} P(C_i \cap G_j)\log_2\left(\frac{P(C_i \cap G_j)}{P(C_i)P(G_j)}\right)$
      $H(\Omega) = -\sum_{i=1\ldots k} P(C_i)\log_2(P(C_i))$, $H(G) = -\sum_{j=1\ldots c} P(G_j)\log_2(P(G_j))$
    - example (figure): $H(\Omega) = -2\frac{6}{17}log_2(\frac{6}{17}) - \frac{5}{17}log_2(\frac{5}{17}) = 1.58$, $H(G) = 1.52$
      $NMI = \frac{2\times 0.96}{1.58+1.52} = 0.62$
  - rand index
    - clustering is interpreted as a sequence of $\binom{m}{2} = \frac{m(m-1)}{2}$ decisions,
    - decision = the partitioning either puts a instance pair into the same cluster or not,
    - $TP\ldots$ an instance pair in the same cluster in Ω and the same class in G,
    - $TN\ldots$ an instance pair in different clusters in Ω and different classes in G,
    - $RI(\Omega, G) = \frac{TP+TN}{TP+TN+FP+FN} = \frac{2(TP+TN)}{m(m-1)}$
    - example (figure): $RI = \frac{2(\binom{5}{2}+\binom{4}{2}+\binom{3}{2}+\binom{2}{2}+5\times 8+1\times 7+4\times 5+1\times 2+1\times 3)}{17\times 16} = 0.68$

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 $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$,
    - 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 $\to$ diagonalize $\to$ a low-dimensional feature space.

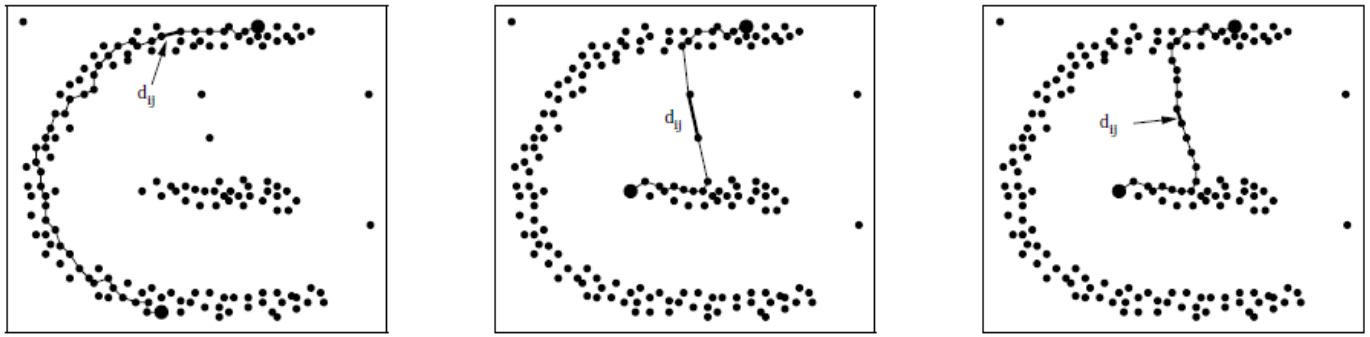
Kernel k-means

- 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,
  - more robust than single linkage,

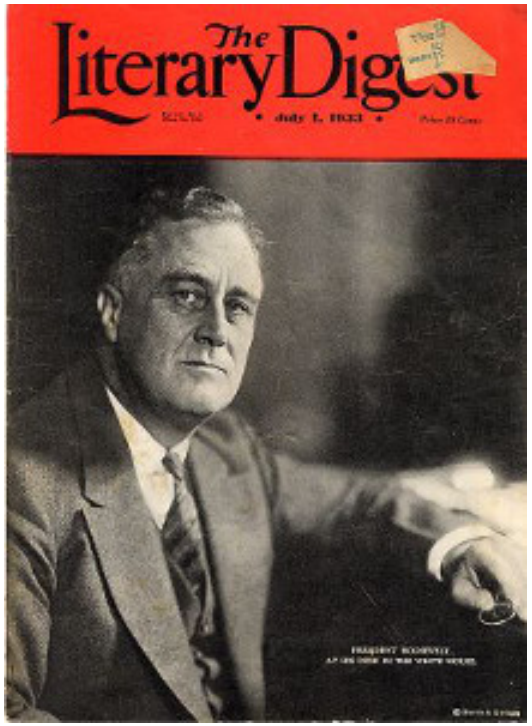


(a) (b) (c)

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

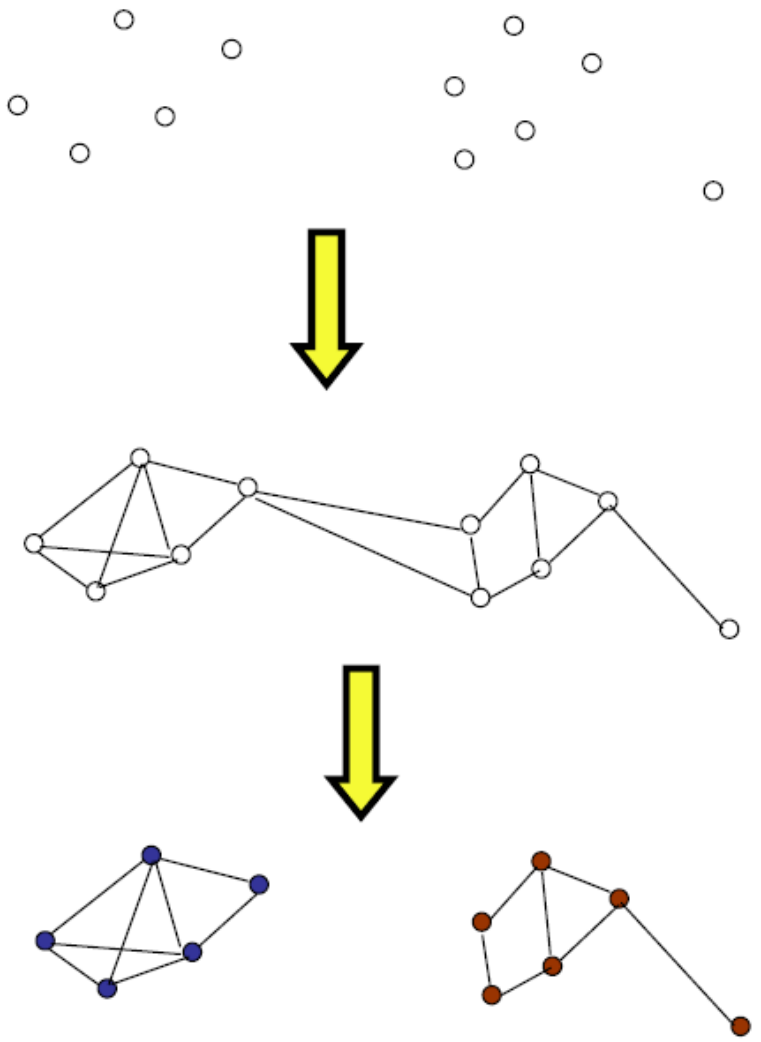
Vietnam war

Financial crisis, 2008

Gaussian copula function

Spectral clustering in a nutshell

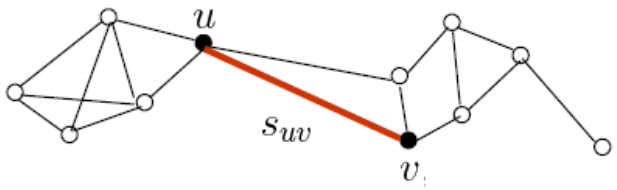
- input: a set of objects,
- described as a graph,
- edges encode similarity,
- graph decomposed into components = clusters,
- graph partitioned by its spectral properties.



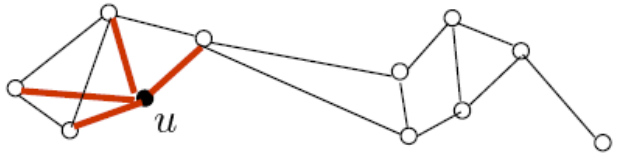
Azran: A Tutorial on Spectral Clustering

Graph theory – basic terms

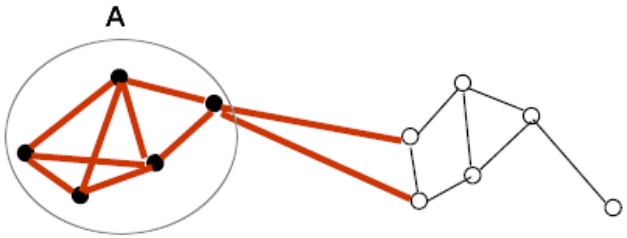
- vertex (object) similarity (affinity)
  - $s_{uv} = \langle u, v \rangle$,



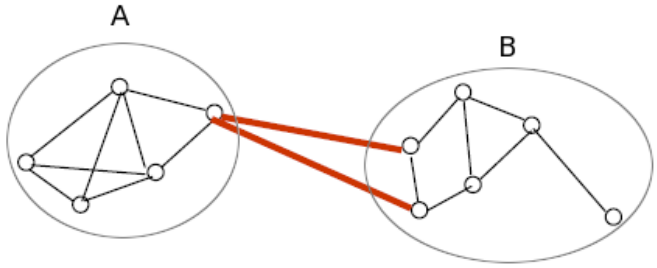
- vertex degree (volume), degree matrix
  - $d_u = \sum_{v=1}^{m} s_{uv}$,
  - $\mathcal{D} = diag(d_1, \ldots, d_m)$,



- size and degree of a vertex set (cluster)
  - $|A|$ ... the number of vertices in A,
  - $vol(A) = \sum_{u \in A} d_u$,



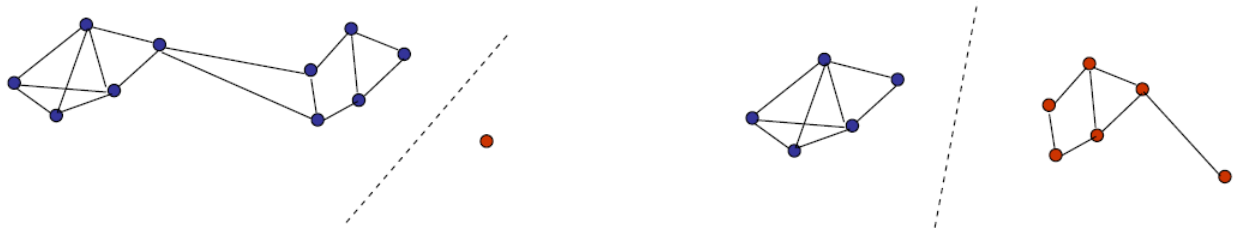
- an edge cut between two components
  - $cut(A, B) = \sum_{u \in A} \sum_{v \in B} s_{uv}$.



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
    - $\min_{A \subset S} cut(A, \bar{A})$,
    - 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.

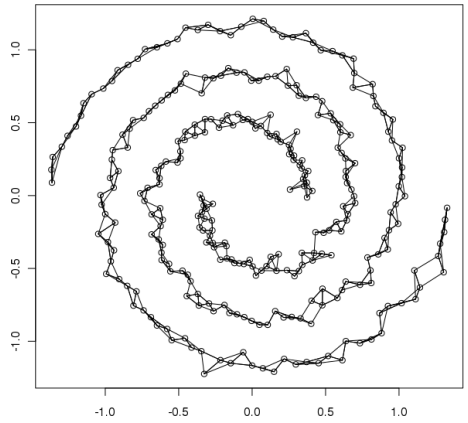
Spectral clustering – algorithm

- inputs: $\mathcal{X} = [x_{ij}]_{m \times n} = \{x_1, \ldots, x_m\} \subset \mathbb{R}^n$, k

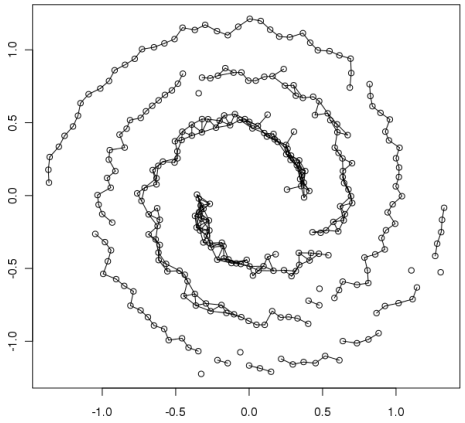
1. select the similarity function
   - linear, RBF, polynomial, etc.
   - a general rule assigning functions to problems does not exist,
2. compute the similarity (adjacency) matrix $\mathcal{S} = [s_{ij}]_{m \times m}$
   - (a new implicit feature space originates),
3. construct a "reasonable" similarity 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

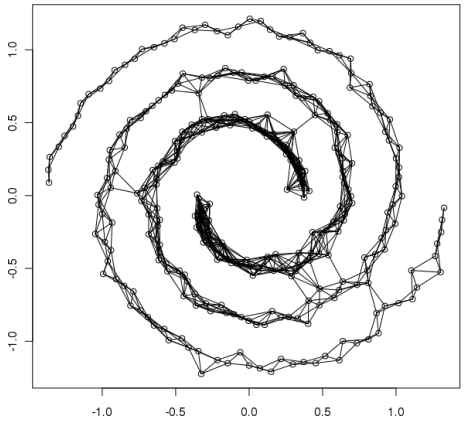
- reduce the complete graph to an undirected graph concerning local neighborhoods,
- vertices shall have a reasonable degree ($\ll m$),
- basic approaches
  - ϵ-neighborhood
    - $s_{ij} > \epsilon \rightarrow$ vertices i and j connected by an edge, otherwise $s_{ij} = 0$,
  - k-nearest neighbors
    - 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

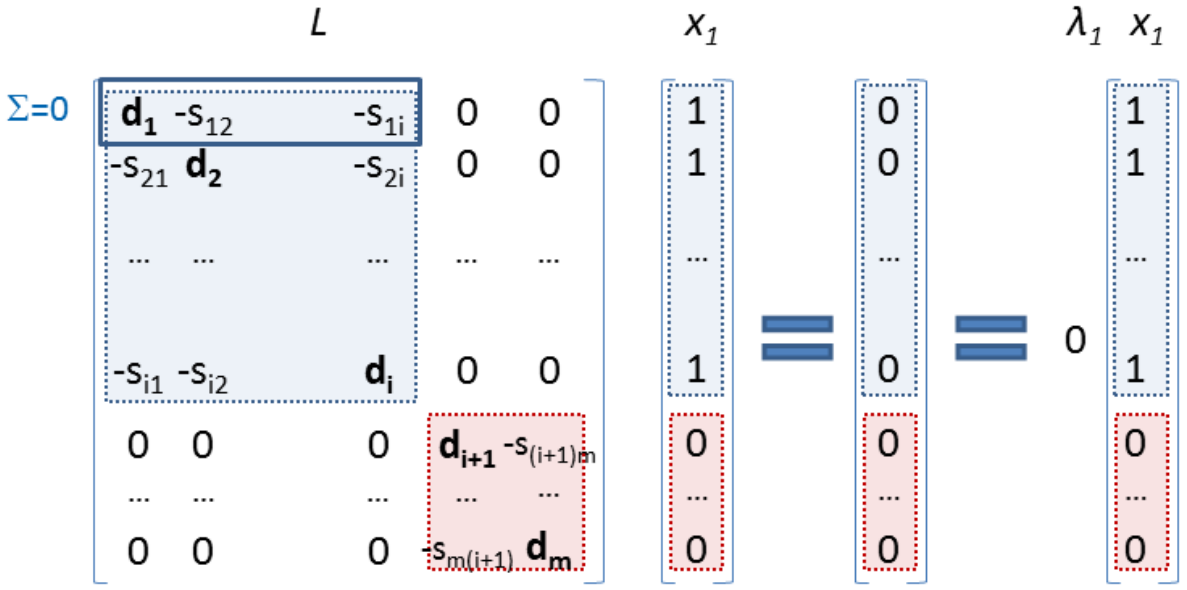
- concern the unnormalized option: $\mathcal{L} = \mathcal{D} - \mathcal{S}$
- then for $\forall f \in \mathbb{R}^m$

$$
\begin{aligned}
f'\mathcal{L}f &= f'\mathcal{D}f - f'\mathcal{S}f = \\
&= \sum_{i=1}^{m} d_i f_i^2 - \sum_{i,j=1}^{m} f_i f_j s_{ij} = \\
&= \frac{1}{2}\Big(\sum_{i=1}^{m}\big(\sum_{j=1}^{m} s_{ij}\big) f_i^2 - 2\sum_{i,j=1}^{m} f_i f_j s_{ij} + \sum_{j=1}^{m}\big(\sum_{i=1}^{m} s_{ij}\big) f_j^2\Big) = \\
&= \frac{1}{2}\sum_{i,j=1}^{m} s_{ij}(f_i - f_j)^2
\end{aligned}
$$

- 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 $\mathcal{L}$

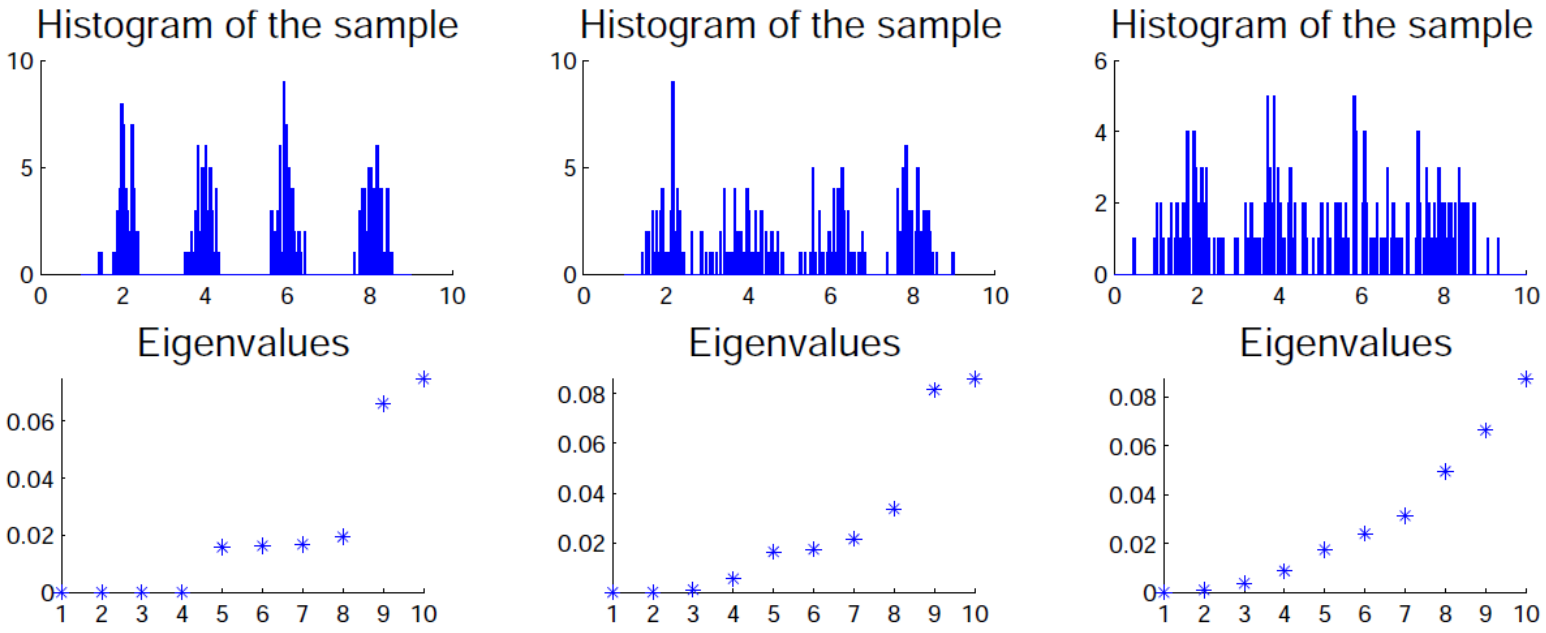
- eigenvectors x of $\mathcal{L}$ matix ($\mathcal{L}x = \lambda x$) provide a good graph partitioning indication,
- an ultimate (ideal) case: graph has exactly k components
  - k smallest eigenvectors ideally split k clusters,
  - $\lambda_1 = \cdots = \lambda_k = 0 < \lambda_{k+1} \leq \cdots \leq \lambda_m \rightarrow x_1, \ldots, x_k$,
- 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 $\mathcal{L}$

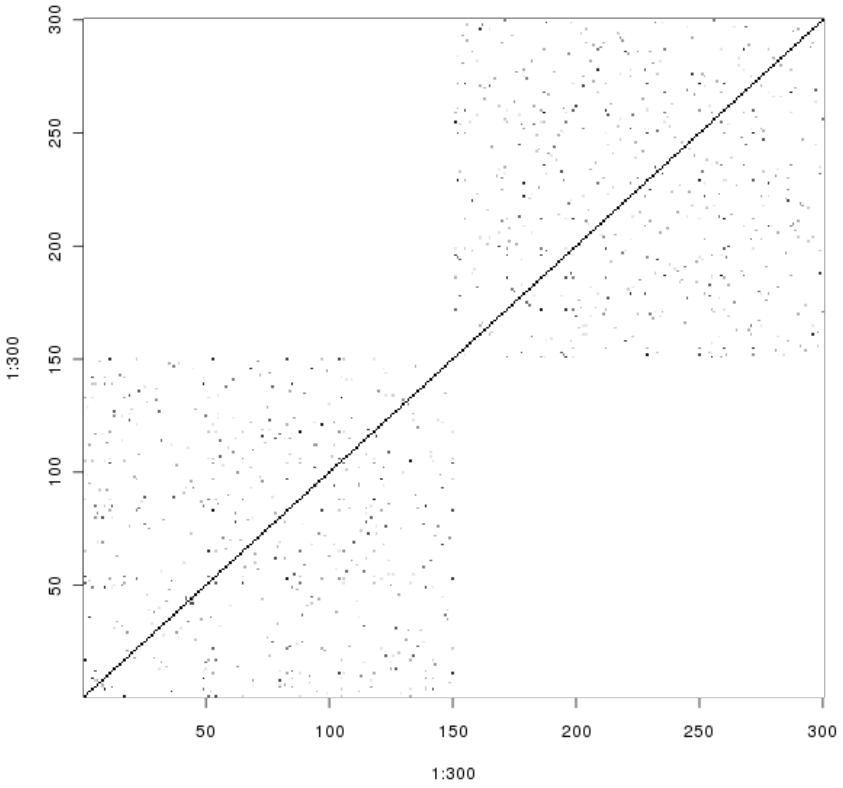
- provided k is unknown, **eigengap** statistic
  - a k-means gap heuristic analogy,
  - concern only small eigenvectors before the first jump in eigenvalues,
  - the number of clusters matches the number of selected eigenvectors.



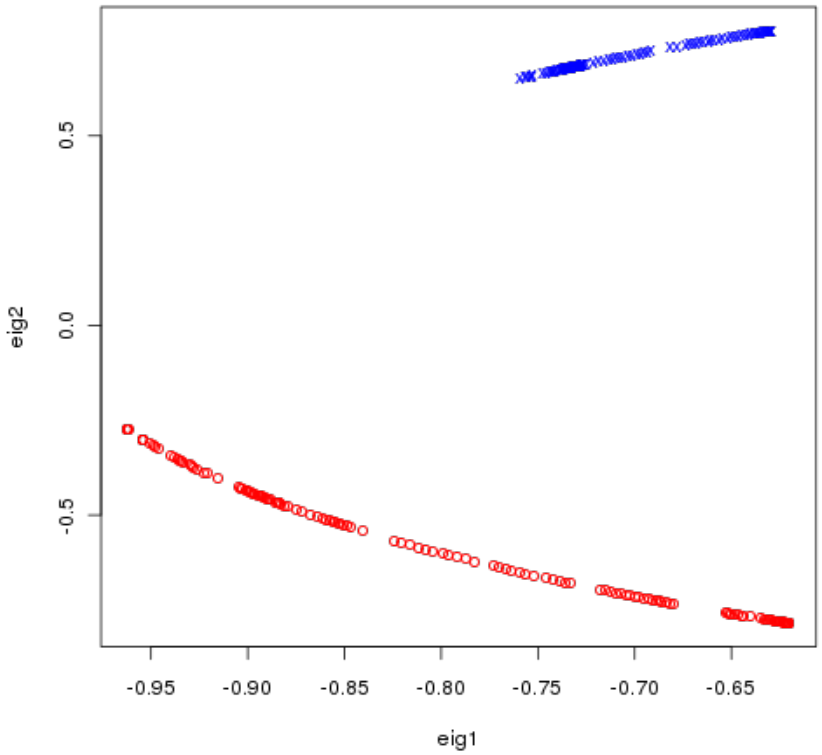
Luxburg: Clustering.

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



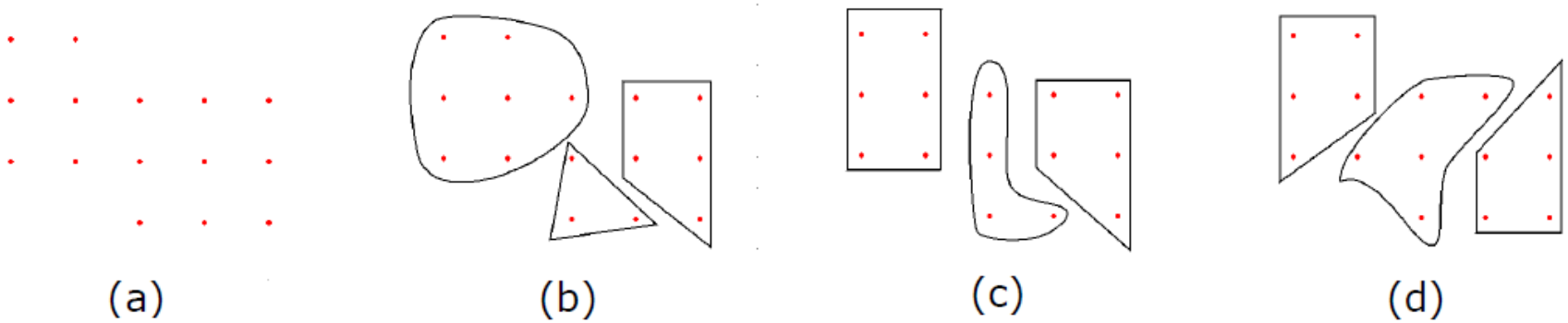
Projection – the first and second eigenvector space $\mathcal{S}$
colors give the real spiral membership, k-means clustering is trivial

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,

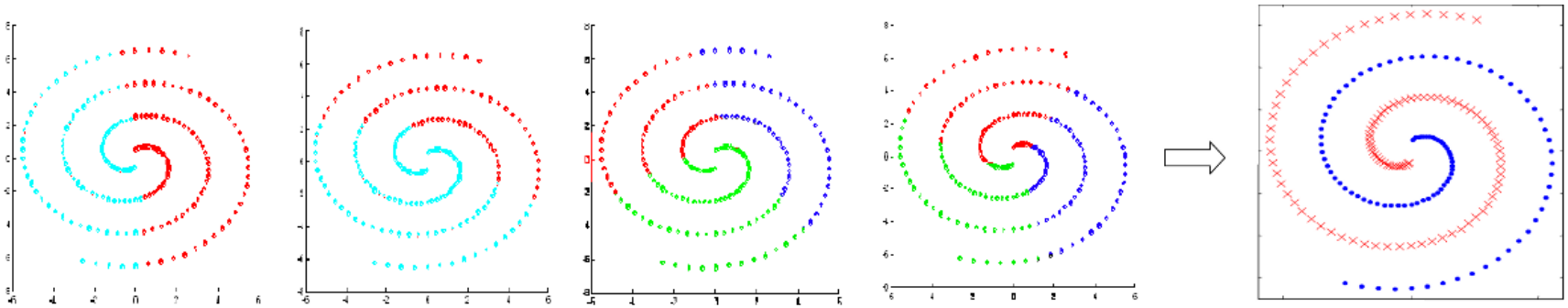


Jain: Data Clustering: 50 Years Beyond K-Means, modified

- 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/,