Clustering

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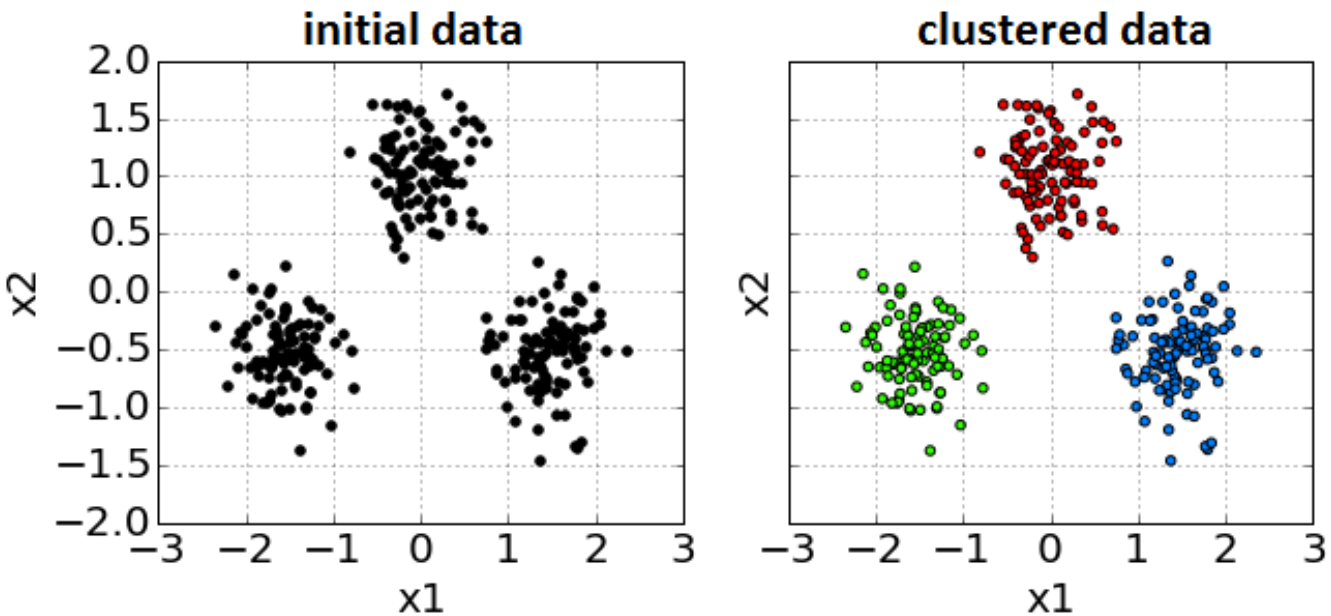
Aim of clustering

- Clustering is partitioning of objects into groups so that:
  - inside groups objects are very similar
  - objects from different groups are dissimilar
- Unsupervised learning
- No definition of "similar"
  - different algorithms use different formalizations of similarity

Clustering demo



Applications of clustering

- data summarization
  - feature vector is replaced by cluster number
- feature extraction
  - cluster number, distance to native cluster center / other clusters
- customer segmentation
  - e.g. for recommender service
- community detection in networks
  - nodes - people, similarity - number of connections
- outlier detection
  - outliers do not belong any cluster

Clustering algorithms comparison

We can compare clustering algorithms in terms of:

- computational complexity
- do they build flat or hierarchical clustering?
- can the shape of clustering be arbitrary?
  - if not is it symmetrical, can clusters be of different size?
- can clusters vary in density of contained objects?
- robustness to outliers

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Representative-based clustering

- Clustering is flat (not hierarchical)
- Number of clusters K is specified in advance
- Each object x_n is associated cluster z_n
- Each cluster C_k is defined by its prepresentative μ_k, $k = 1, 2, ...K$.[1]
- Criterion to find representatives $\mu_1, ...\mu_K$:

$$Q(z_1, ...z_K) = \sum_{n=1}^{N} \min_k \rho(x_n, \mu_k) \to \min_{\mu_1, ...\mu_K} \quad (1)$$

[1] Propose clustering algorithm that can extract a set of representatives for each cluster.

Generic algorithm

initialize $\mu_1, \ldots \mu_K$ from random training objects

while not converged:
  for $n = 1, 2, \ldots N$:
    $z_n = \arg\min_k \rho(x_n, \mu_k)$

  for $k = 1, 2, \ldots K$:
    $\mu_k = \arg\min_\mu \sum_{n:z_n=k} \rho(x_n, \mu)$

return $z_1, \ldots z_N$

- Comments:
  - different distance functions lead to different algorithms:
    - $\rho(x, x') = \|x - x'\|_2^2 \Rightarrow$ K-means
    - $\rho(x, x') = \|x - x'\|_1 \Rightarrow$ K-medians
  - μ_k may be arbitrary/constrained to be existing objects
  - converges in few iterations, complexity $O(NKD)$

Comments

- K - unknown parameter
  - if chosen small=>distinct clusters will get merged
  - better to take K larger and then merge similar clusters.
- Shape of clusters is defined by $\rho(\cdot,\cdot)$
- Close clusters will have similar size

2 Representative-based clustering
- K-means
- Kernel K-means
- Mahalanobis distance
- K-medoids

K-means algorithm

- Suppose we want to cluster our data into K clusters.
- Cluster i has a center μ_i, i=1,2,...K.
- Consider the task of minimizing

$$\sum_{n=1}^{N} \|x_n - \mu_{z_n}\|_2^2 \to \min_{z_1,...z_N,\mu_1,...\mu_K} \tag{2}$$

where $z_i \in \{1, 2, ...K\}$ is cluster assignment for x_i and $\mu_1, ...\mu_K$ are cluster centers.

- Direct optimization requires full search and is impractical.
- K-means is a suboptimal algorithm for optimizing (2).

K-means algorithm

Initialize μ_j, $j = 1, 2, ...K$.

repeat while stop condition not satisfied:
  for $i = 1, 2, ...N$:
    find cluster number of x_i:
    $z_i = \arg\min_{j \in \{1,2,...K\}} ||x_i - \mu_j||_2^2$
  for $j = 1, 2, ...K$:
    $\mu_j = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n = j]} \sum_{n=1}^{N} \mathbb{I}[z_n = j] x_i$

Dynamic K-means algorithm

Initialize μ_j, $j = 1, 2, ...K$, $z_i = 0, i = 1, 2, ...N$

repeat while stop condition not satisfied:
  for $i = 1, 2, ...N$:
    find cluster number of x_i:
    $z_i' = \arg\min_{j \in \{1,2,...K\}} ||x_i - \mu_j||_2^2$
    if $z_i' != z_i$:
      recalculate cluster means μ_{z_i} and $\mu_{z_i'}$:
      $\mu_{z_i} = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n' = z_i]} \sum_{n=1}^{N} \mathbb{I}[z_n' = z_i] x_i$
      $\mu_{z_i'} = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n' = z_i']} \sum_{n=1}^{N} \mathbb{I}[z_n' = z_i'] x_i$
      $z_i = z_i'$

Converges in less iterations, situation when no objects correspond to some cluster is impossible.

K-means properties

Possible stop conditions:

- cluster assignments $z_1, ...z_N$ stop to change (typical)
- maximum number of iterations reached
- cluster means $\{\mu_i\}_{i=1}^K$ stop changing significantly

Initialization:

- typically $\{\mu_i\}_{i=1}^K$ are initialized to randomly chosen training objects

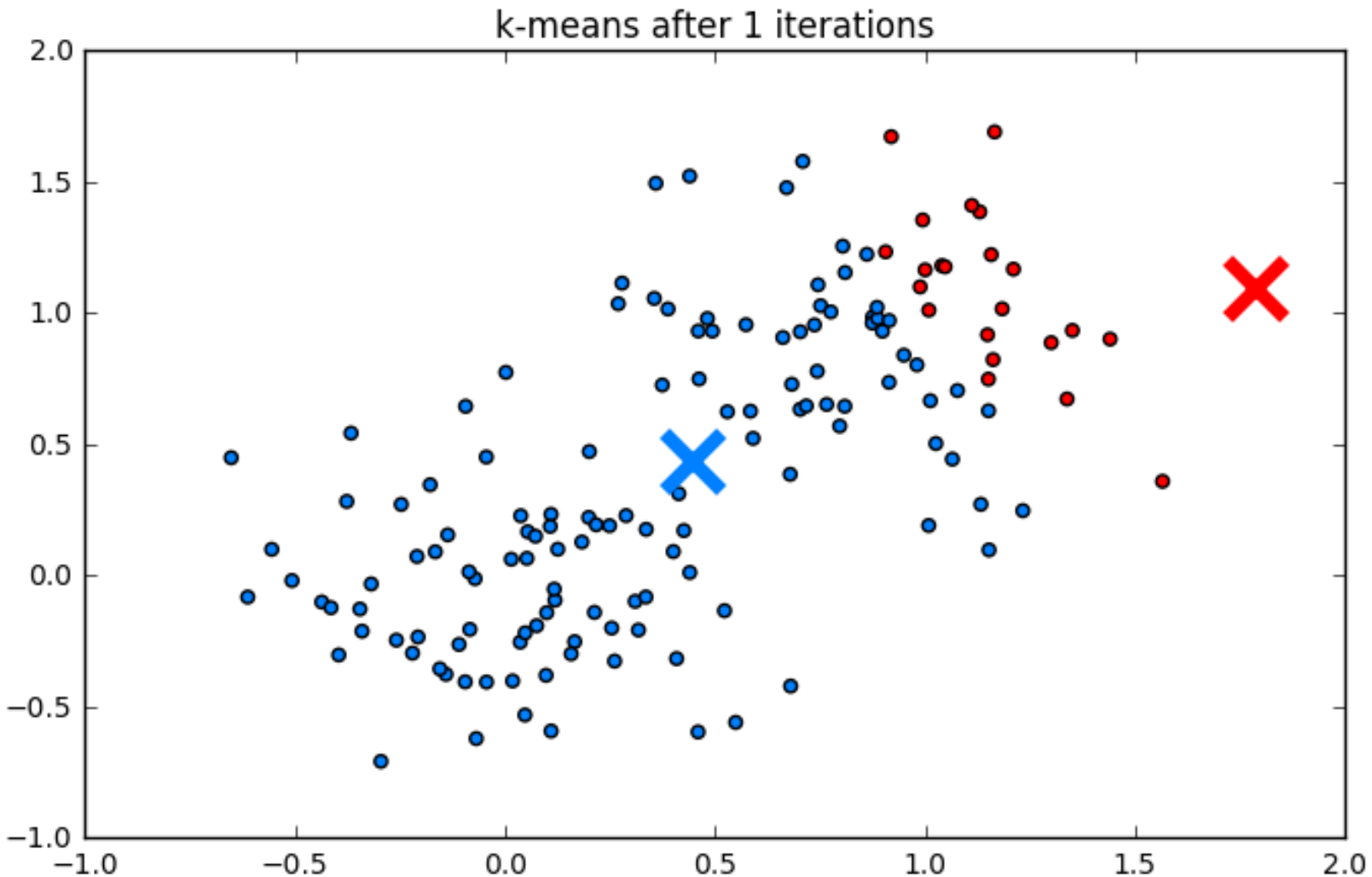
Optimality:

- criteria is non-convex
- solution depends on starting conditions
- we may restart several times from diff. random starting points and select solution giving minimal value of (2).

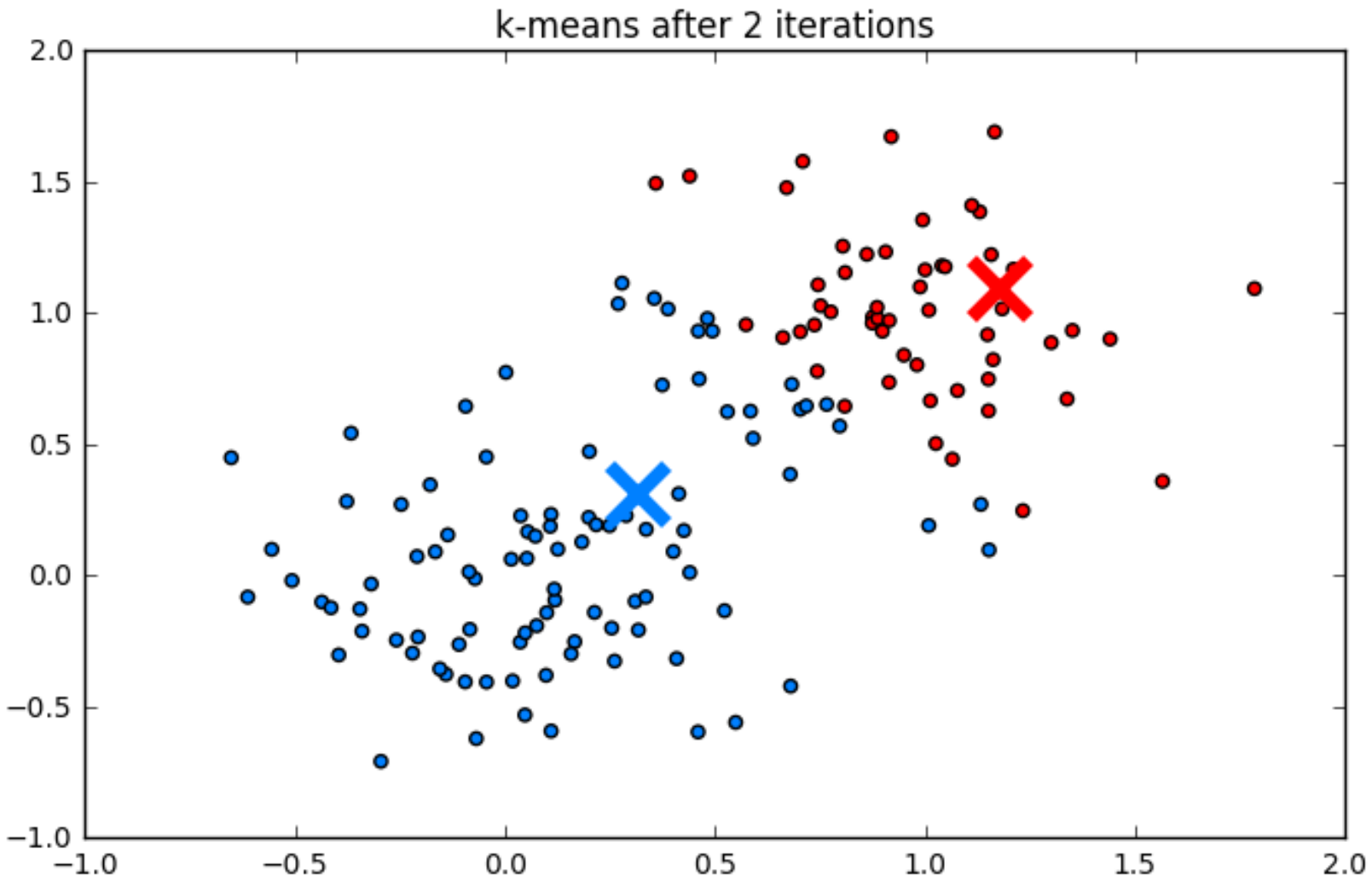
Complexity: $O(NDKI)$, where K is the number of clusters and I is the number of iterations.

- Usually algorithm converges in small number of iterations I.

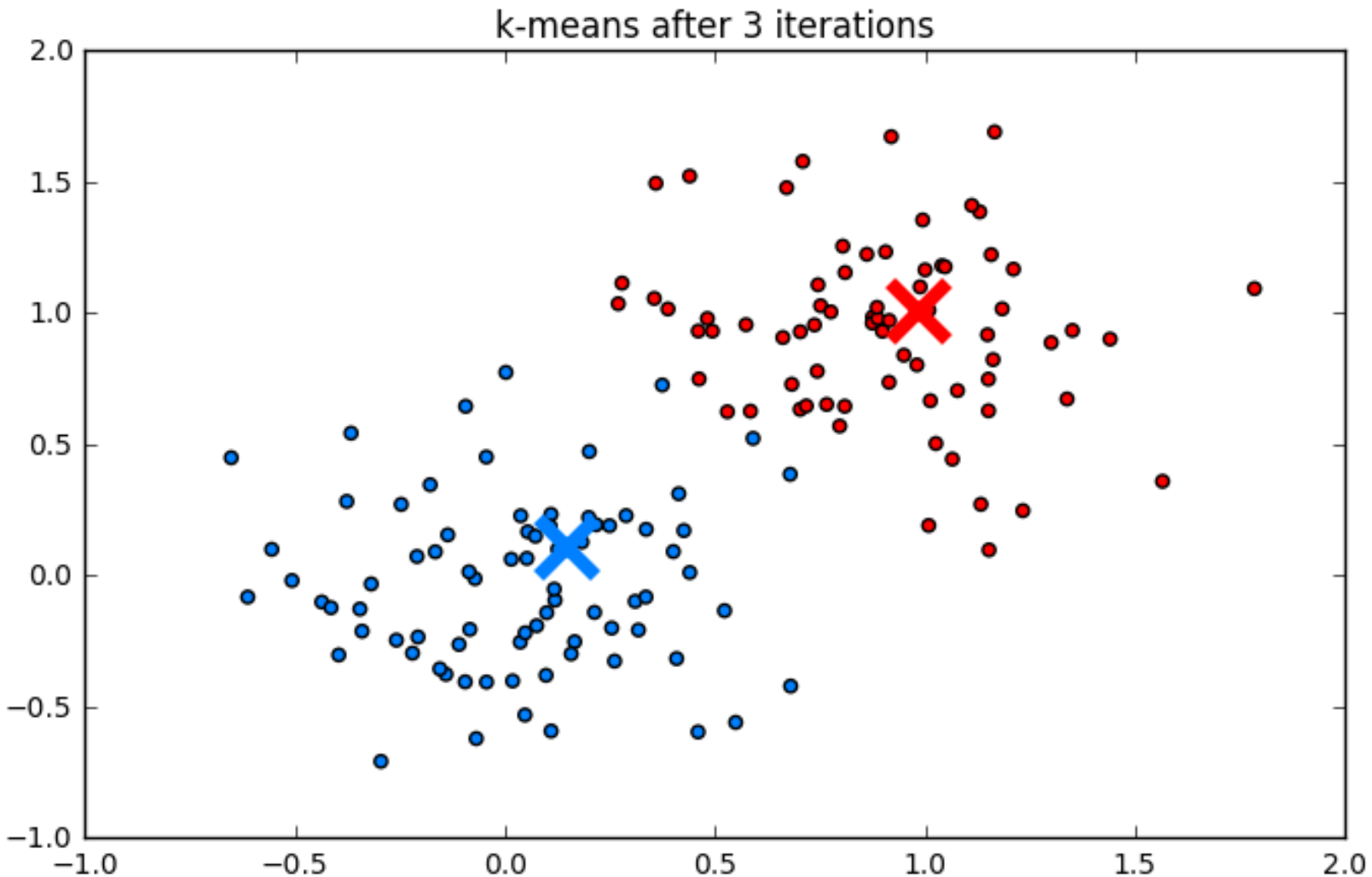
Example of K-means



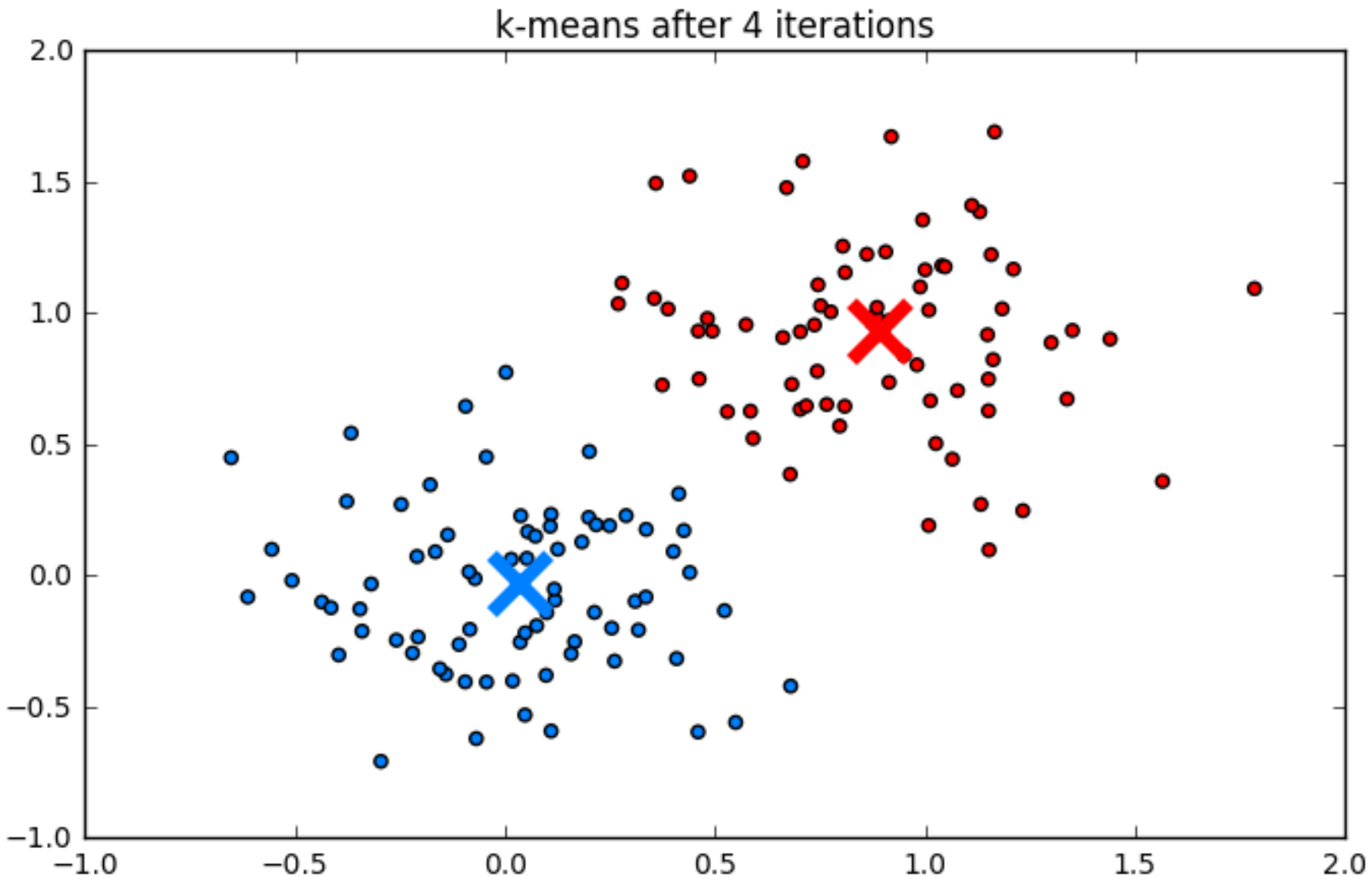
Example of K-means



Example of K-means

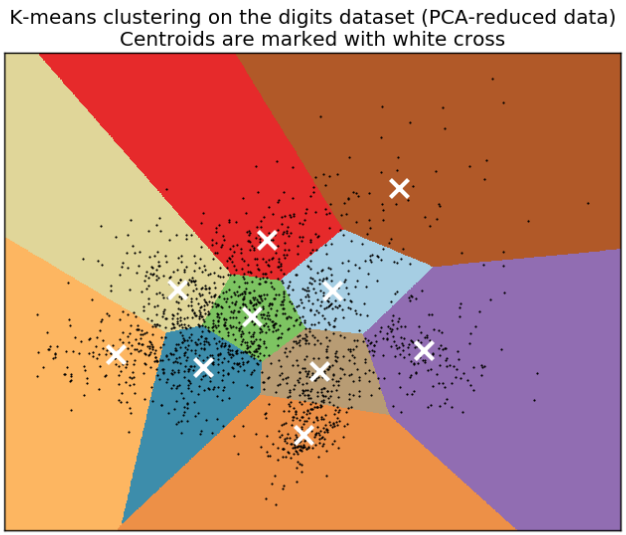


Example of K-means



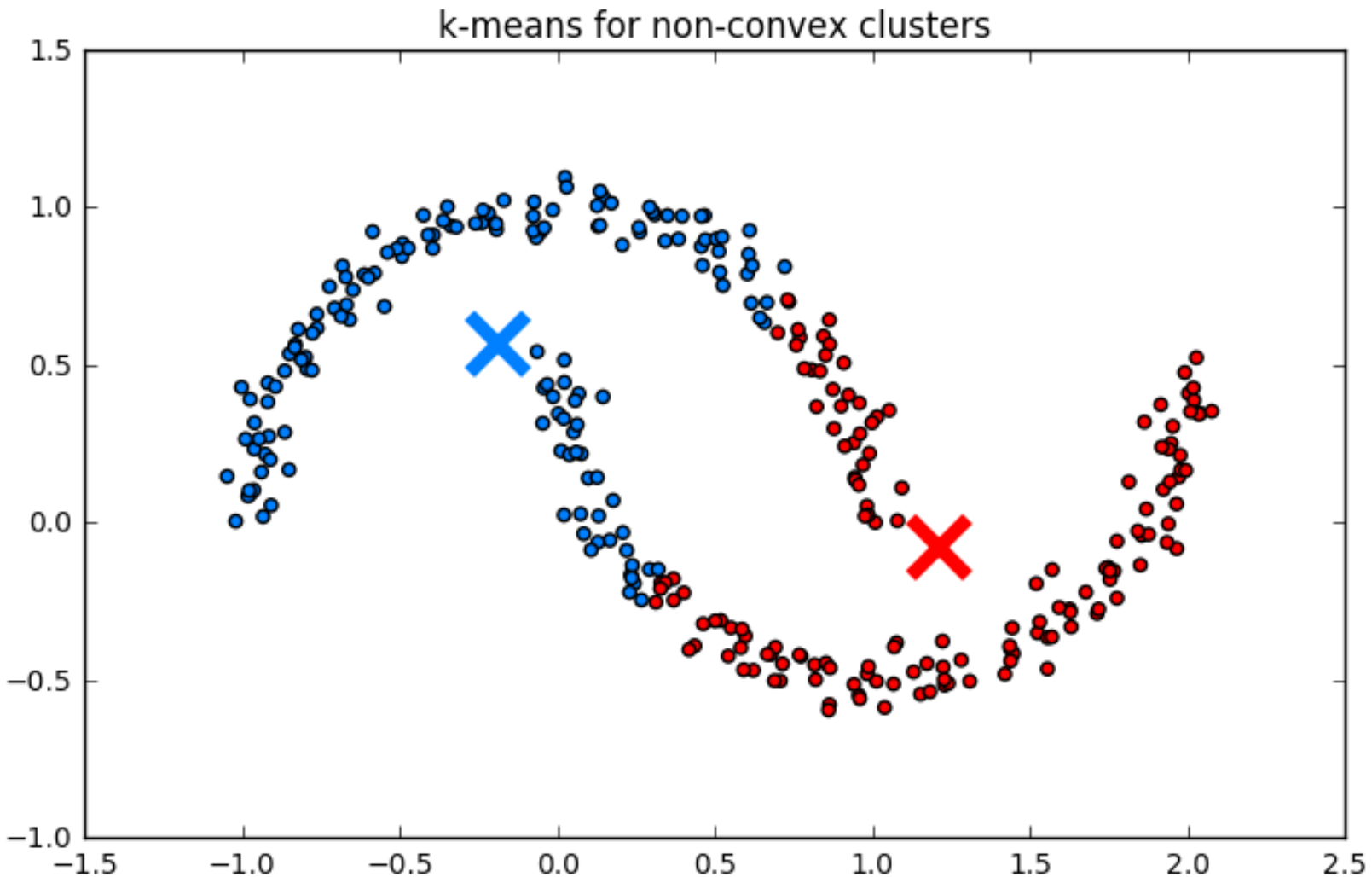
Gotchas

- K-means assumes that clusters are convex:

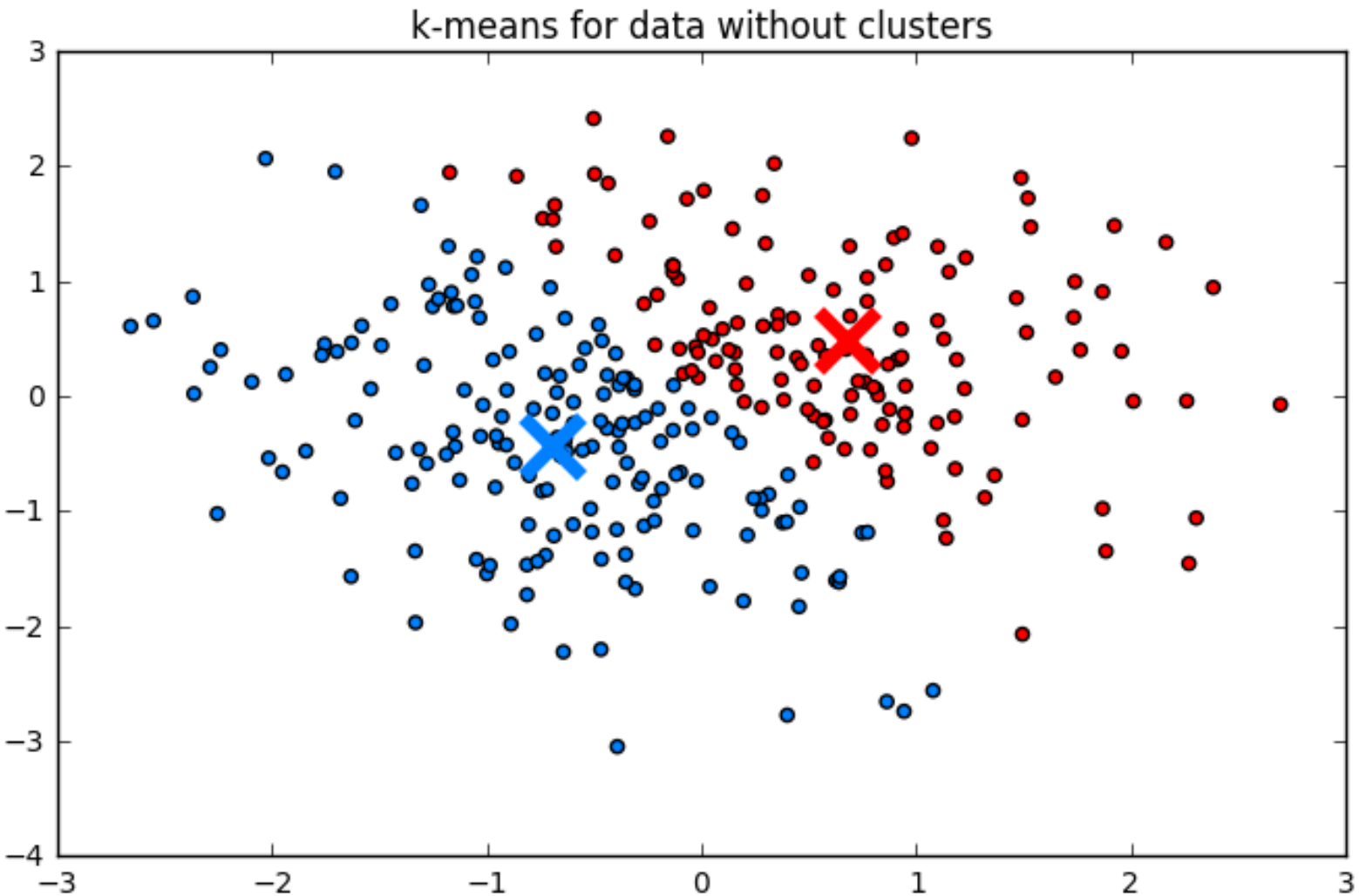


- It always finds clusters even if none actually exist
  - need to control cluster quality metrics

K-means for non-convex clusters



K-means for data without clusters



K-means and EM algorithm

Initialize μ_j, $j = 1, 2, ...K$.

repeat while stop condition not satisfied:
  for $i = 1, 2, ...N$:
    find cluster number of x_i:
    $z_i = \arg\min_{j \in \{1,2,...g\}} ||x_i - \mu_j||$
  for $j = 1, 2, ...K$:
    $\mu_j = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n = j]} \sum_{n=1}^{N} \mathbb{I}[z_n = j] x_i$

- K-means is EM-algorithm when:

K-means and EM algorithm

Initialize μ_j, $j = 1, 2, ...K$.

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- K-means is EM-algorithm when:
  - applied to Gaussians
  - with equal priors
  - with unity covariance matrices
  - with hard clustering

K-means

- Not robust to outliers
  - K-medians is robust
- K-representatives may create singleton clusters in outliers if centroids get initialized with outlier
  - better to init centroids with mean of m randomly chosen objects
- Constructs spherical clusters of similar radii
  - Allows kernel version which can find non-convex clusters in original space

2 Representative-based clustering
- K-means
- Kernel K-means
- Mahalanobis distance
- K-medoids

Kernel K-means

- Let $C_k := \{n : z_n = k\}$ - indices of objects in cluster k.
- Squared dinstance to centroid:

$$\rho(x, \mu_k)^2 = \|x - \mu_k\|^2 = \langle \varphi(x) - \frac{1}{|C_k|} \sum_{i \in C_k} \varphi(x_i),\ \varphi(x) - \frac{1}{|C_k|} \sum_{i \in C_k} \varphi(x_i) \rangle$$

$$= \langle \varphi(x), \varphi(x) \rangle - 2 \langle \varphi(x),\ \frac{1}{|C_k|} \sum_{i \in C_k} \varphi(x_i) \rangle + \frac{1}{|C_k|^2} \sum_{i,j \in C_k} \langle \varphi(x_i),\ \varphi(x_j) \rangle$$

$$= K(x, x) - 2 \frac{1}{|C_k|} \sum_{i \in C_k} K(x, x_i) + \frac{1}{|C_k|^2} \sum_{i,j \in C_k} K(x_i, x_j)$$

initialize $C_1, \ldots C_K$

while not converged:
  for $n = 1, 2, \ldots N$:
    $z_n = \arg\min_k \rho(x_n, \mu_k)^2$

return $z_1, \ldots z_N$

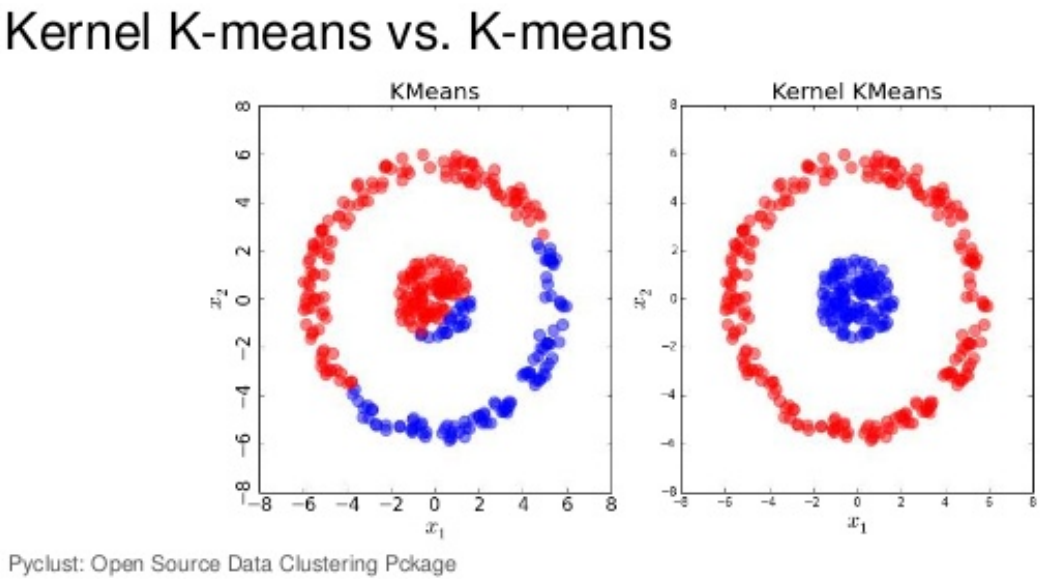
Intuition

- Consider RBF kernel $K(x,\mu) = e^{-\gamma\|x-\mu\|^2}$.

$$\rho(x,\mu_k)^2 = 1 - 2\frac{1}{|C_k|}\sum_{i\in C_k} e^{-\gamma\|x-x_i\|^2} + \frac{1}{|C_k|^2}\sum_{i,j\in C_k} e^{-\gamma\|x_i-x_j\|^2}$$

1. $\frac{1}{|C_k|}\sum_{i\in C_k} e^{-\gamma\|x-x_i\|^2}$ - average similarity of x to points in cluster k
2. $\frac{1}{|C_k|^2}\sum_{i,j\in C_k} e^{-\gamma\|x_i-x_j\|^2}$ - constant offset for cluster k, measuring its compactness.

Kernel K-means



- Complexity: with respect to N each interation $O(N^2)$, assuming small num of iterations total $O(N^2)$.
- Centroids are not calculated directly
- Allows non-convex clustering in original feature space.

2 Representative-based clustering
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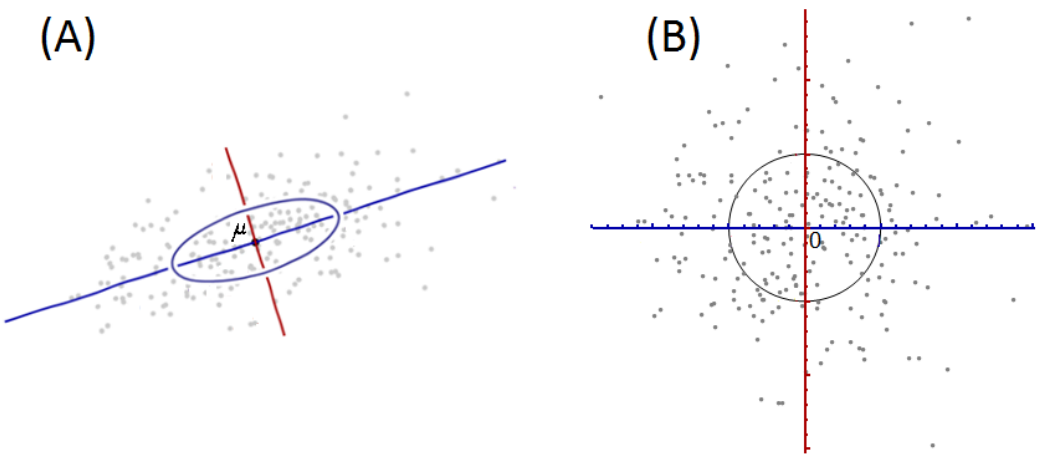
Mahalanobis distance

- Consider statistical distribution $F(\mu, \Sigma)$ with mean μ and covariance matrix Σ:
- Mahalanobis distance from x to $F(\mu, \Sigma)$:

$$\rho(x, F(\mu, \Sigma))^2 = (x - \mu)^T \Sigma^{-1} (x - \mu)$$

- Mahalanobis distance from x to another point x', given $F(\mu, \Sigma)$:

$$\rho(x, x')^2 = (x - x')^T \Sigma^{-1} (x - x')$$

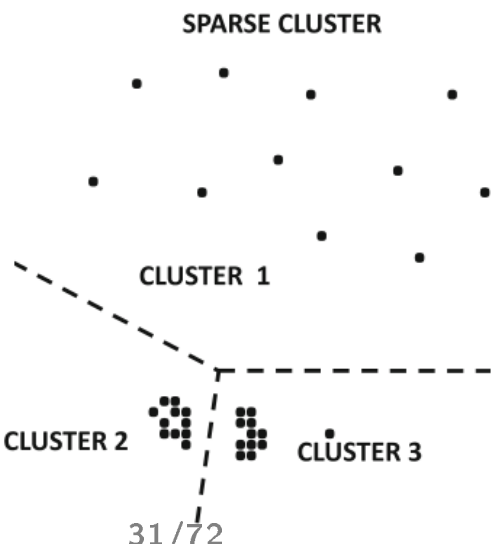


Mahalanobis distance clustering

- Mahalanobis distance in clustering:

$$\rho(x, \mu_k) = (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)$$

  - is different for each k
  - μ_k and Σ_k - sample mean and covariance matrix for objects from cluster k
- Mahalanobis distance allow modeling clusters
  - elliptically elongated
  - of different size and density



2 Representative-based clustering
- K-means
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K-medoids

- K-medoids - each cluster representative μ_k should be existing object from the training set.
- Motivation:
  - robust to outliers
  - more interpretable (representative is existing object)
  - the only option if we can calculate $\rho(x, x')$ but x, x' are incomparable elementwise
    - e.g. x_n - time series of varying length

K-medoids algorithm

initialize $\mu_1, \ldots \mu_K$ from random training objects

while not converged:
    generate replacement candidates $R = (\mu_k(i), x_n(i))_{i=1}^{I}$
    select replacement maximally improving $\sum_{n=1}^{N} \min_k \rho(x_n, \mu_k)$

    if improvement was not achived:
        fallback to previous state
        break

for $n = 1, 2, \ldots N$:
    $z_n = \arg\min_k \rho(x_n, \mu_k)$

return $z_1, \ldots z_N$

As replacement candidates we may generate all variants or random subset.

General comments on K-representatives

- Init $\{\mu_k\}_{k=1}^K$ with
  - random objects from training set
  - centroids of m randomly selected objects from training set (more robust to outliers)
- K-representatives has non-convex optimization criteria
  - depends in initialization of $\{\mu_k\}_{k=1}^K$
  - so we can restart clustering from different starting conditions and select the one, maximizing (1)
- Outliers can create singleton clusters consisting of 1 point.
  - apply outlier filtering beforehand
  - alternatively during clustering for clusters with too few points replace cluster centroids with random objects.

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- Bottom-up hierarchical clustering
- Top-down hierarchical clustering

4 Probabilistic clustering

5 Grid-based clustering

6 Spectral clustering

Motivation

- Number of clusters K not known a priory.
- Clustering is usually not flat, but hierarchical with different levels of granularity:
  - sites in the Internet
  - books in library
  - animals in nature

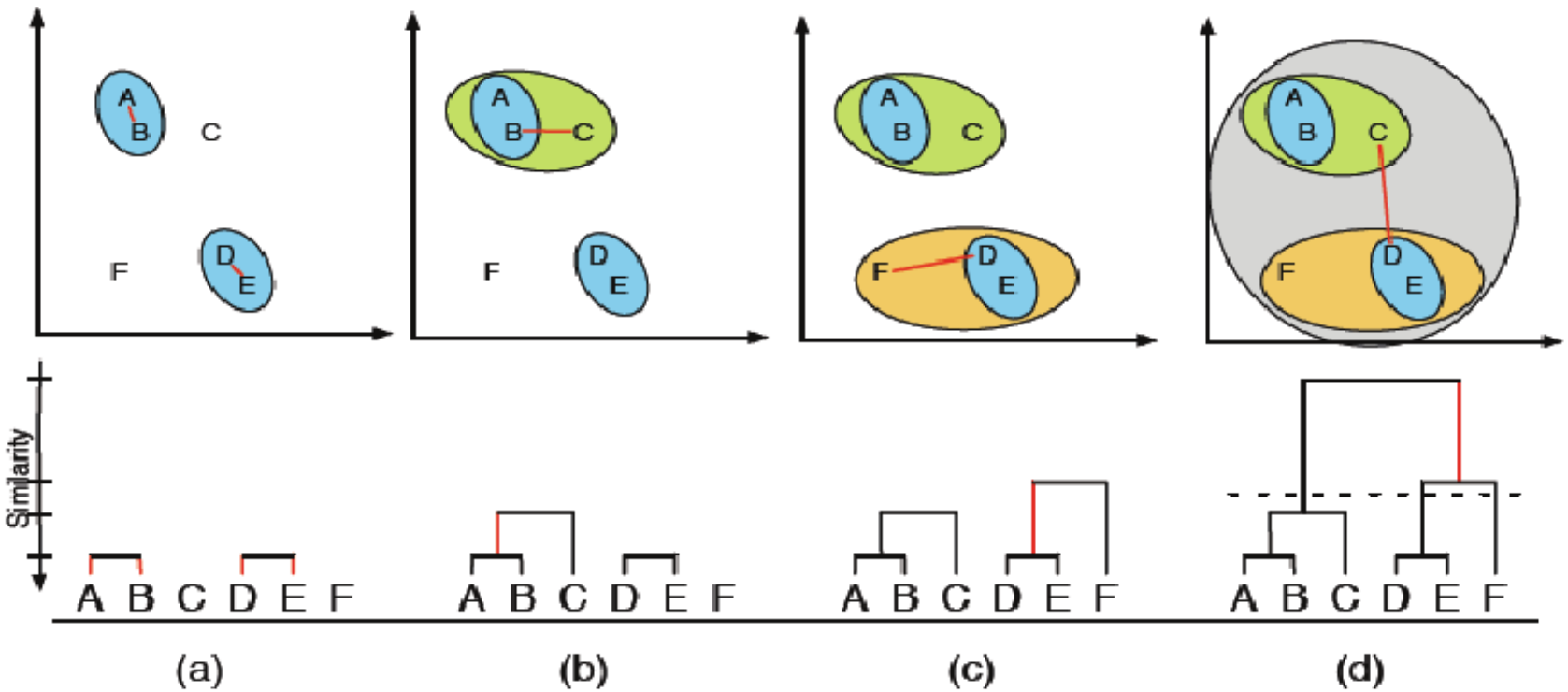
Hierarchical clustering

Hierarchical clustering may be:

- top-down
  - hierarchical K-means
- bottom-up
  - agglomerative clustering

3 Hierarchical clustering
- Bottom-up hierarchical clustering
- Top-down hierarchical clustering

Bottom-up clustering demo



Algorithm

initialize NxN distance matrix M between singleton clusters $\{x_1\}, ...\{x_N\}$

REPEAT:
1) pick closest pair of clusters i and j
2) merge clusters i and j
3) delete rows/columns i, j from M and add new row/column for merged cluster

UNTIL 1 cluster is left

RETURN hiearchical clustering of objects

- Early stopping is possible when:
  - K clusters are left
  - distance between most close clusters $\geq$threshold

Agglomerative clustering - distances

- Consider clusters $A = \{x_{i_1}, x_{i_2}, ...\}$ and $B = \{x_{j_1}, x_{j_2}, ...\}$.
- We can define the following natural distances
  - nearest neighbour (or single link)

$$\rho(A,B) = \min_{a \in A, b \in B} \rho(a,b)$$

  - furthest neighbour (or complete-link)

$$\rho(A,B) = \max_{a \in A, b \in B} \rho(a,b)$$

  - group average link

$$\rho(A,B) = \text{mean}_{\ a \in A, b \in B} \rho(a,b)$$

  - closest centroid

$$\rho(A,B) = \rho(\mu_A, \mu_B)$$

    where $\mu_U = \frac{1}{|U|} \sum_{x \in U} x$ or $m_U = median_{x \in U}\{x\}$

Intercluster distance properties[3]

- Nearest neighbour
  - extracts clusters of arbitrary shape
  - may merge distinct clusters connected by mistake by outliers
  - $M_{(i\cup j)k} = \min\{M_{ik}, M_{jk}\}$
- Furthest neighbour
  - creates very compact clusters
  - diameter of clusters grows
  - $M_{(i\cup j)k} = \max\{M_{ik}, M_{jk}\}$
- Group average link[2] and closest centroid distance give the compromise between nearest and furtherst neighbour.

[2] How $M_{(i\cup j)k}$ will be recalulated for average link?

[3] Suppose we modify distance $\rho(x, x')$ with monotone transformation F: $\rho'(x, x') = F(\rho(x, x'))$. Which of the cluster distances will not be affected by this change?

Intercluster distance properties

Group average link is preferred to closest centroid distance, because

- centroid distance may lead to non-monotonous joining distance sequences in agglomerative algorithm.
- in contrast nearest neighbour , furtherst neightbour and group average link always lead to monotonous joining distance sequences
- representation of cluster by mean/median ignores cluster shape
- centroid and median distance tend to prefer larger clusters, for which means are generally closer.

Complexity

- Memory requirements: $O(N^2)$ - keep all pairwise distances.
- Computational requirements:
  - $O(D)$ - distance calculation
  - $O(N^2 D)$ - calculate all pairwise distances
  - Binary min-heap of size m: $O(\ln m)$-insert element, $O(\ln m)$-delete element, $O(1)$-find min
  - Create heap of N^2 paisewise distances: $O(N^2 \ln N)$
  - merging of clusters:
    - find minimum $O(1)$, delete $O(\ln N)$, calculate $O(N)$, insert $O(\ln N)$
    - do it N times: $O(N^2)$
  - total complexity: $(N^2 D + N^2 \ln N)$
- When N is large we can:
  - use only random subsample of objects
  - merge points with $K-$representatives to K clusters to which apply agglomerative clustering.

K-representatives+agglomerative clustering

- Efficient combination:
  1. apply K-representatives with $M > K$ clusters
  2. use agglomerative clustering to merge excessive clusters to K

  - K-means has complexity $O(N)$
  - agglomerative clustering complexity $O\left(M^2 \ln M\right)$
  - but agglomerative clustering allows non-convex clusters!

3 Hierarchical clustering
- Bottom-up hierarchical clustering
- Top-down hierarchical clustering

Algorithm

INPUT:
data D, flat clustering algorithm A
leaf selection criterion, termination criterion

Initialize tree T to root, containing all data

REPEAT
  based on selection criterion, select leaf L
  using algorithm A split L into children $L_1, \ldots L_K$
  add $L_1, \ldots L_K$ as child nodes to tree T
UNTIL termination criterion

Comments

- Leaf selection criterion:
  - split leaf most close to the root
    - balanced tree by height
  - split leaf with maximum elements
    - balanced tree by cluster weight
- Building hierarchy top-down is more natural for a human

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EM-algorithm for normal mixtures

Initialize ϕ_j, μ_j and Σ_j, $j = 1, 2, ...g$.

repeat while stopping condition not satisfied:

E-step. Calculate correspondences of x_n to component z:

for $n = 1, 2, ...N$:

for $z = 1, 2, ...Z$:

$$w_{nz} = \frac{\phi_z N(x_n; \mu_z, \Sigma_z)}{\sum_k \phi_k N(x_n; \mu_k, \Sigma_k)} \quad \text{\# =p(z|x(n))}$$

M-step. Update component parameters:

for $z = 1, 2, ...Z$:

$$\widehat{\phi}_z = \frac{1}{N} \sum_{n=1}^{N} w_{nz}$$

$$\widehat{\mu}_z = \frac{\sum_{n=1}^{N} w_{nz} x_n}{\sum_{n=1}^{N} w_{nz}}$$

$$\widehat{\Sigma}_z = \frac{1}{\sum_{n=1}^{N} w_{nz}} \sum_{n=1}^{N} w_{nz} (x_n - \widehat{\mu}_z)(x_n - \widehat{\mu}_z)^T$$

K-means versus EM clustering

- For each x_n EM algorithm gives $w_{nz} = p(z|x_n)$.
- This is soft or probabilistic clustering into Z clusters, having priors $\phi_1, ...\phi_Z$ and probability distributions $p(x;\theta_1), ...p(x;\theta_Z)$.
- We can make it hard clustering using $z_n = \arg\max_z w_{nz}$.

- EM clustering becomes K-means clustering when:
  - applied to Gaussians
  - with equal priors
  - with unity covariance matrices
  - with hard clustering

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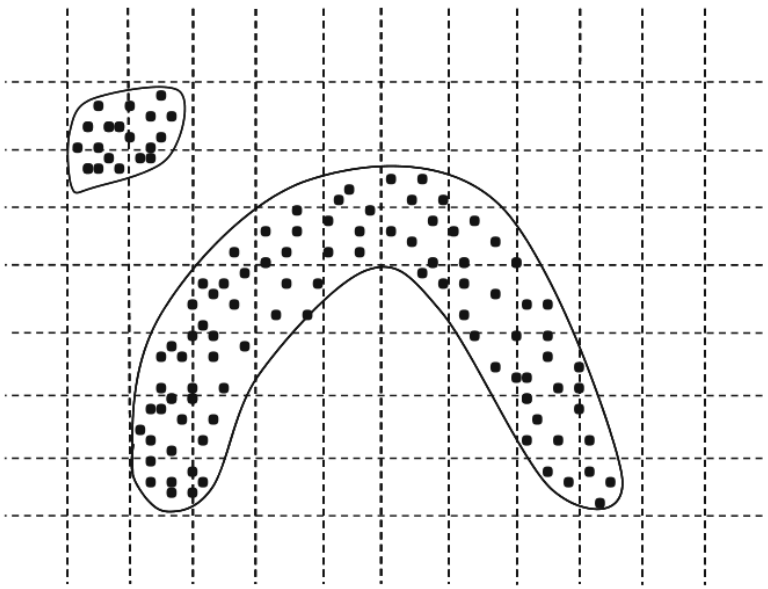
Grid-based clustering

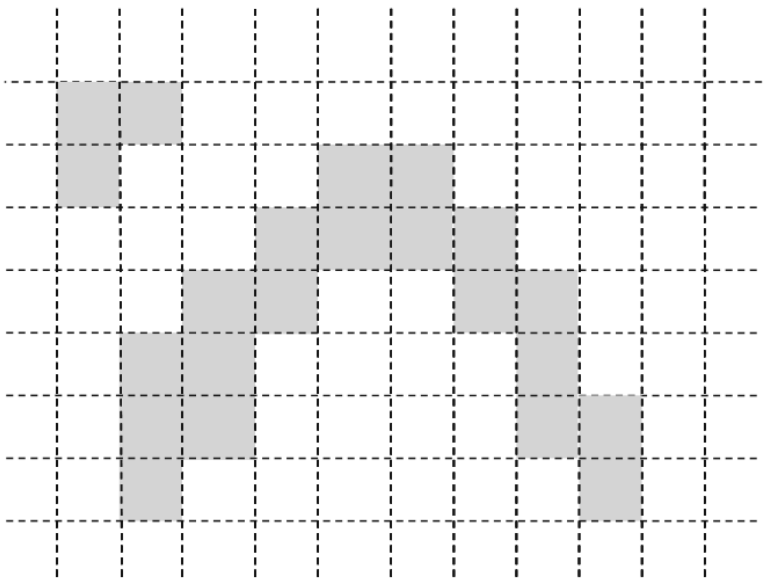
- Divide each dimension into p equal intervals
- Obtain p^D hypercubes
- Consider hypercube filled when it contains $\geq k$ points.
  - need not consider all possible hypercubes - look at data distribution along each axis.
- Consider hypercubes locally connected if they share $r < D$ common dimensions
  - r=0: corner, r=1: border, r>1: side
- Create graph:
  - node - filled hypercube
  - edges - between locally connected hypercubes
- Clusters: connected components in the graph[4]

[4] Propose an algorithm to index all objects with connected components they belong to.

Illustration



(a) Data points and grid

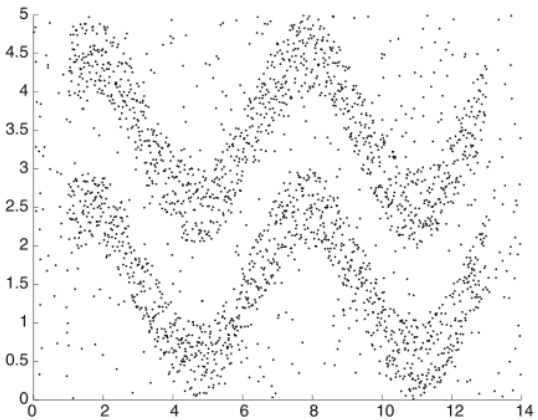


(b) Agglomerating adjacent grids

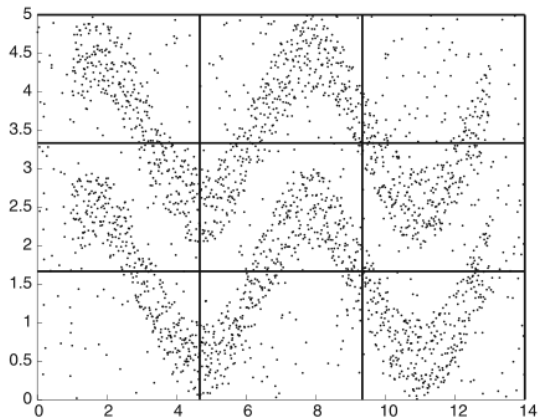
Discussion

- Number of clusters is determined automatically
- Clusters may have arbitrary shape
- Need to specify: p, k, r.
- Under what selection of p, k the algorithm will have tendency to:
  - join distinct clusters?
  - separate true cluster due to local variations in density?
- Method will fail when cluster has varying density.
  - K-representatives - not, but it will fail for clusters of different size
  - mixture of Gaussians - not, but it will fail for non-elliptic clusters

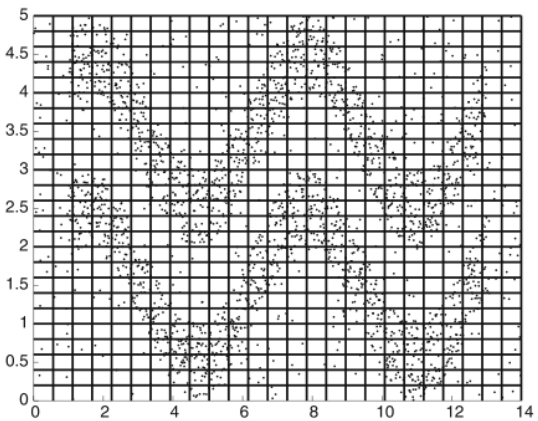
Selection of p



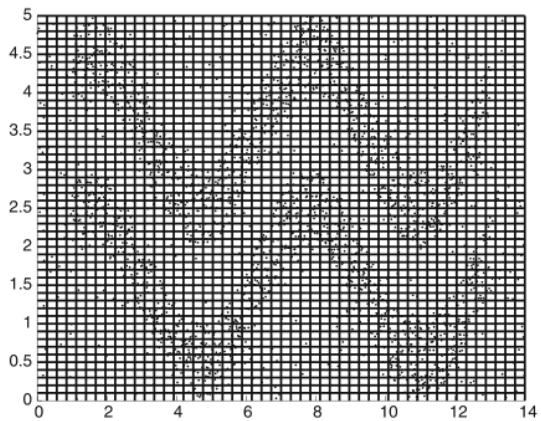
(a) Arbitrarily-shaped clusters



(b) Rough-grained grid

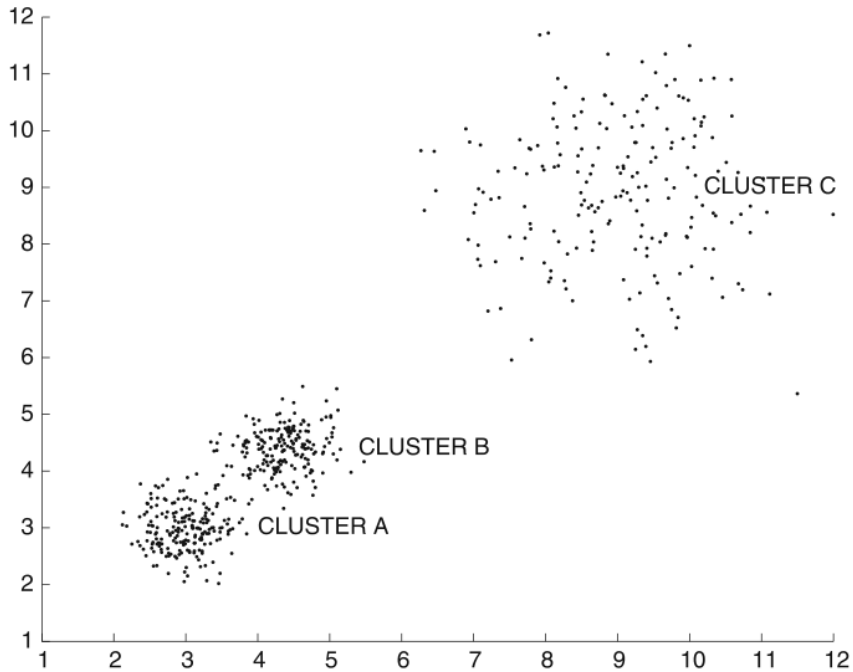


(c) Moderate-grained grid



(d) Fine-grained grid

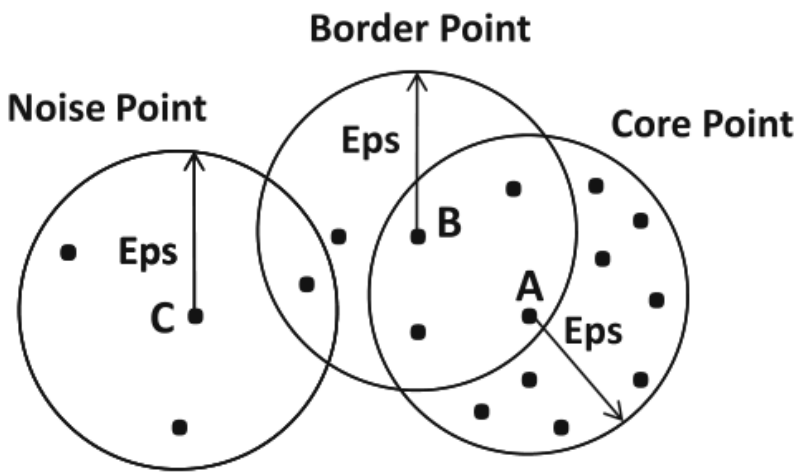
Failure for varying density



- Large k: cluster C is missed
- Small k: clusters A and B get merged

DBScan

- Core point: point having $\geq k$ points in its ε neighbourhood
- Border point: not core point, having at least 1 core point in its ε neighbourhood
- Noise point: neither a core point nor a border point



- k, ε - parameters of the method.

Algorithm

INPUT: training set, parameters ε, k.

1) Determine core, border and noise points with ε, k.
2) Create graph in which core points are connected if they are within ε of one another
3) Determine connected components in the graph
4) Assign each border point to connected component with which it is best connected

RETURN points in each connected component as a cluster

Comments

- Connecting core points - agglomerative clustering with single linkage, stopping at distance ε.
- Resistant to outliers by ignoring noise points.
- Similar to grid-based clustering:
  - automatically determines the number of clusters
  - works badly for density varying clusters
- Complexity $O(N^2 D)$
  - can be reduced to $O(N \ln N)$ for small D with spatial indexing.
  - grid-based methods find objects in the same region in $O(D)$.

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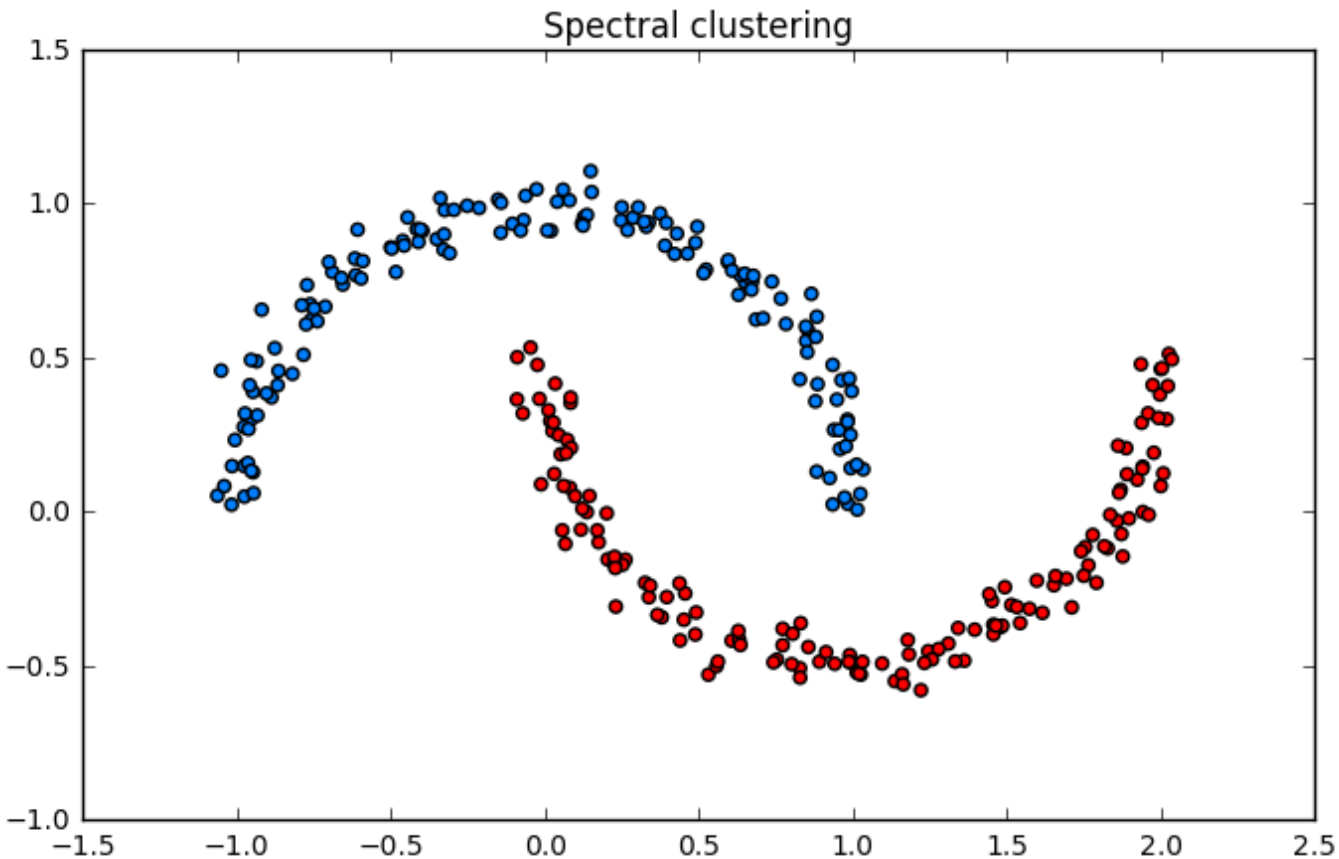
Spectral clustering - example



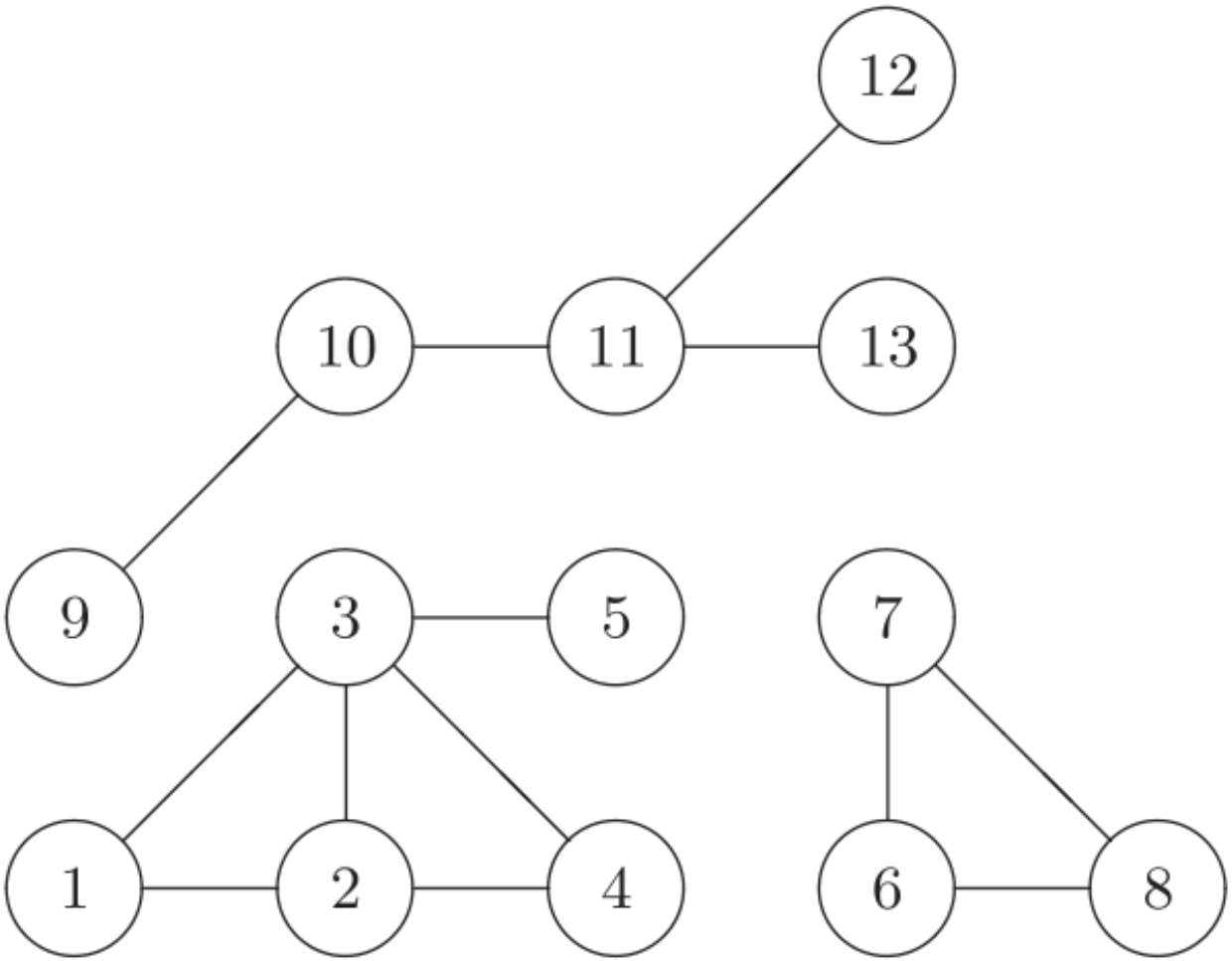
Description

- Spectral clustering relies upon similarity matrix W between objects.
- Similarity matrix <-> weighted connection graph
- Examples:
  - nodes represent people, edge weights - how much they communicate
  - nodes represent web-pages, edge weights - scalar products of $TF - IDF$

Similarity matrix calculation

- $\|x_i - x_j\| < threshold$
- RBF
- based on nearest neighbours

Graph with disjoint components



Graph Laplacian

- $W = W^T$, $w_{ij} \geq 0$ - the similarity between object i and object j.
- Define $D = \text{diag}\{d_1, ...d_N\}$, where $d_i = \sum_{j=1}^{N} w_{ij}$-weighted degree of node i.
- Define graph Laplacian

$$L = D - W$$

- Properties of graph Laplacian:
  - it is symmetric
  - *It has eigenvector* $\mathbf{1} \in \mathbb{R}^N$ *consisting of ones with eigenvalue 0. Why?*
  - it is positive semi-definite: $\forall f \in \mathbb{R}^N : f^T L f \geq 0$.
  - L has eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N = 0$

Positive semi-definiteness of Laplacian

Consider arbitrary $f \in \mathbb{R}^N$:

$$f^T Lf = f^T Df - f^T Wf = \sum_i d_i f_i^2 - \sum_{i,j,} f_i f_j w_{ij} =$$

$$\frac{1}{2}\left(\sum_i d_i f_i^2 - 2\sum_{i,j} w_{ij} f_i f_j + \sum_j d_j f_j^2\right) =$$

$$\frac{1}{2}\left(\sum_{i,j} w_{ij} f_i^2 - 2\sum_{i,j} w_{ij} f_i f_j + \sum_{j,i} w_{ji} f_j^2\right) = \quad (3)$$

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

$$\frac{1}{2}\sum_{i,j} w_{ij}(f_i - f_j)^2 \geq 0$$

Eigenvectors of Laplacian

- Consider eigenvector f corresponding to eigenvalue $\lambda = 0$.
  - $f^T L f = \lambda f^T f = 0$
- Using (3) we have that

$$0 = f^T L f = \frac{1}{2} \sum_{i,j} w_{i,j} (f_i - f_j)^2 \tag{4}$$

- If objects i and j are connected on the graph, there exists a path with $w_{uv} > 0$ along the path and from (4) it should be that $f_i = f_j$.
- So the set of eigenvectors of L is spanned by indicator vectors $I_{A_1}, I_{A_2}, ...I_{A_K}$ where A_i is i-th isolated region on the graph.
- Order of $\lambda = 0$ gives the number of isolated components.

Spectral clustering algorithm

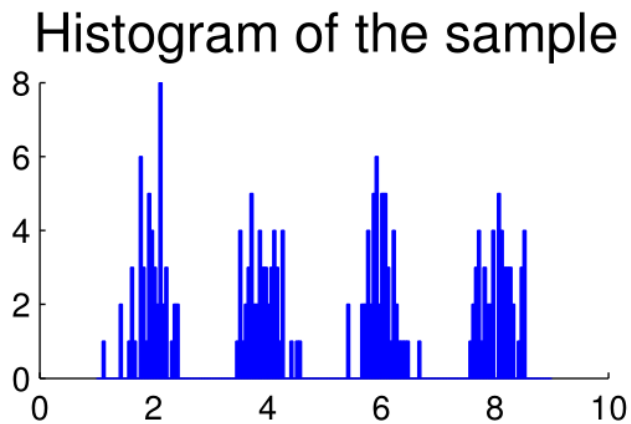
1. Find order K of singular value $\lambda = 0$ for L
2. Find set of eigenvectors $v_1, ...v_K$ corresponding to $\lambda = 0$
3. Cluster *rows* of $V = [v_1, ...v_K] \in \mathbb{R}^{NxK}$ with K-means.

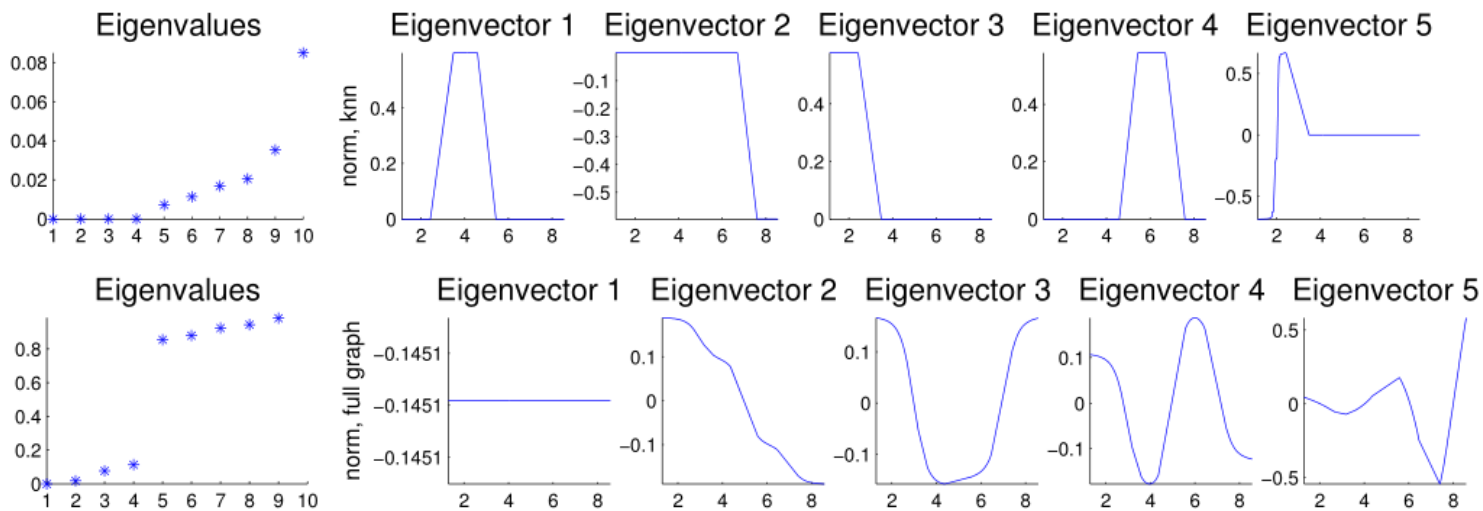
RETURN clustering for rows as clustering for initial objects $x_1, ...x_N$.

Practical application

- $L' = D^{-1}L$ is considered instead of L ("normalized" Laplacian)
  - to account for different connectivity levels of different nodes
- Most often singular values of L' are not exactly zero, but close to zero. So we select K almost-zero eigenvalues and corresponding K eigenvectors.

Example


Histogram of the sample
8
6
4
2
0
0
2
4
6
8
10


Eigenvalues
Eigenvector 1
Eigenvector 2
Eigenvector 3
Eigenvector 4
Eigenvector 5
norm, knn
Eigenvalues
Eigenvector 1
Eigenvector 2
Eigenvector 3
Eigenvector 4
Eigenvector 5
norm, full graph