Clustering

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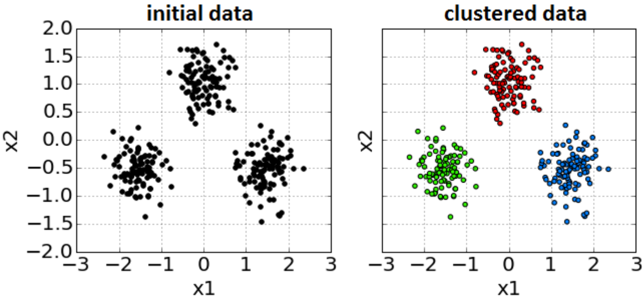
Aim of clustering

- 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 $\mu_1,...\mu_K$:

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

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

Generic algorithm

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

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

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

return $z_1, ...z_N$

- Comments:
  - different distance functions lead to different algorithms:
    - $\rho(x, x') = \|x - x'\|_2^2$=> K-means
    - $\rho(x, x') = \|x - x'\|_1$=> 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

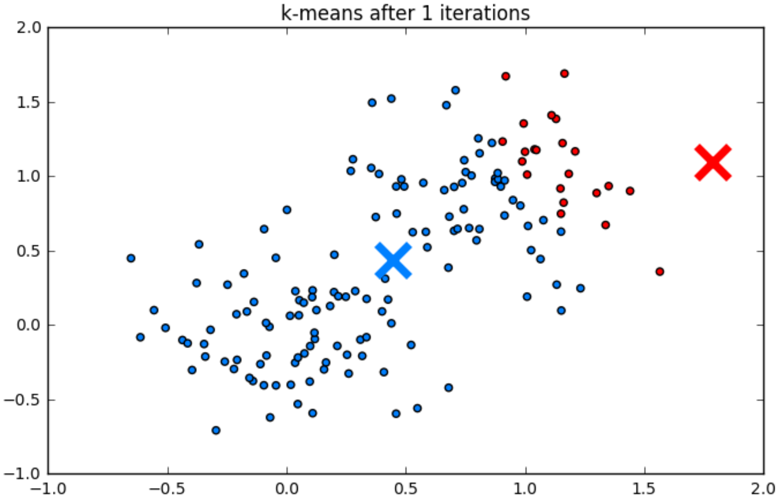
Optimality:

- 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).

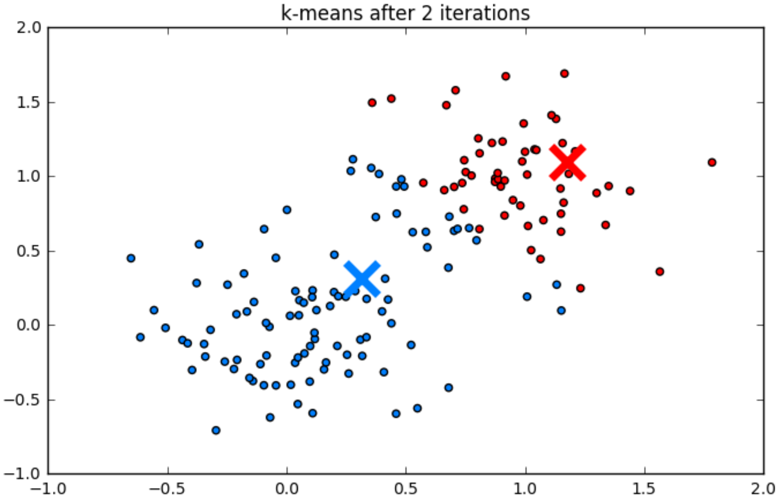
Complexity: $O(NDKI)$, where K is the number of clusters and I is the number of iterations.

- Usually algorithm converges in small number of iterations I.

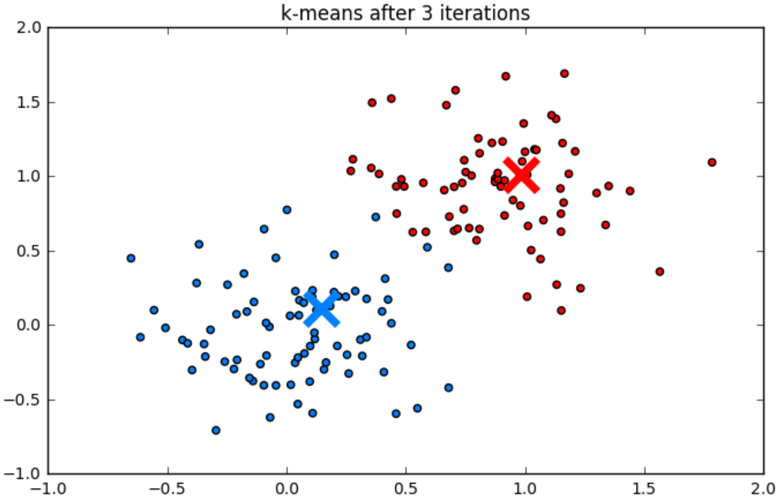
Example of K-means



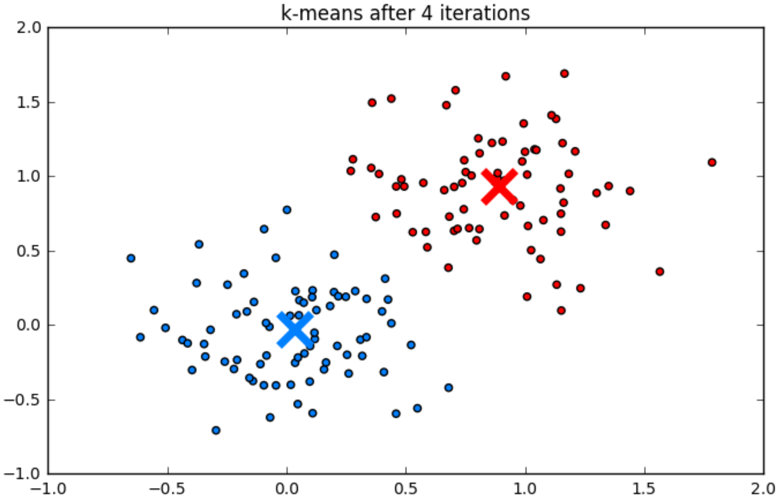
Example of K-means



Example of K-means



Example of K-means



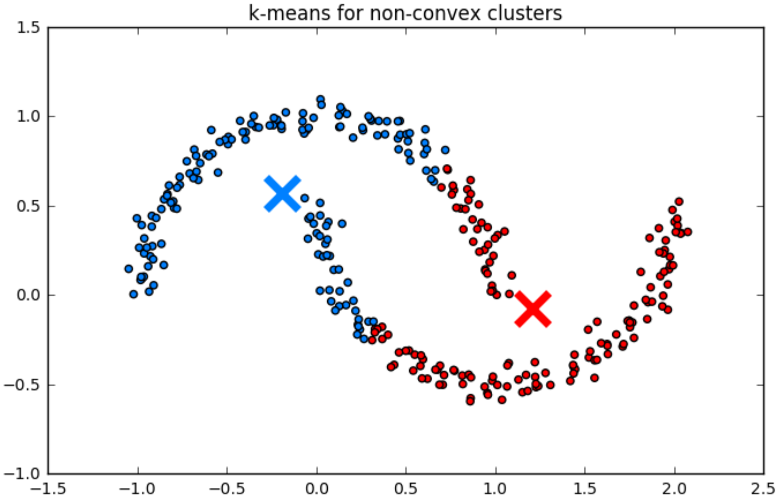
Gotchas

- K-means assumes that clusters are convex:

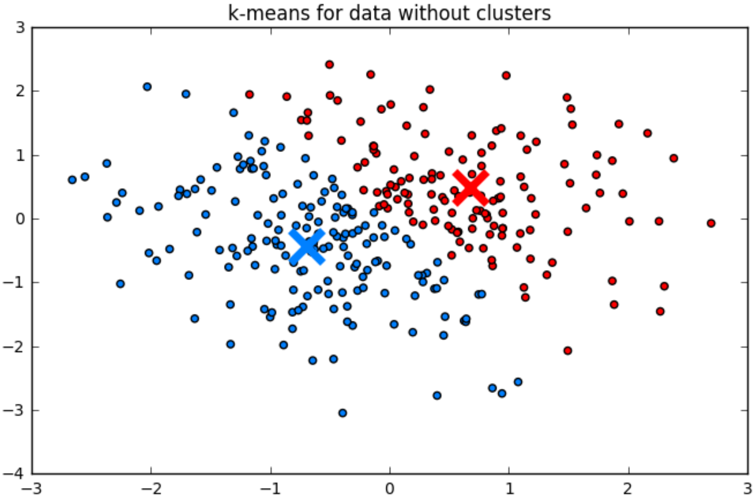
K-means clustering on the digits dataset (PCA-reduced data)
Centroids are marked with white cross

- 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∈{1,2,...g}} ||x_i − μ_j||
   for j = 1,2,...K:
      μ_j = 1/(Σ_{n=1}^N 𝕀[z_n=j]) Σ_{n=1}^N 𝕀[z_n = j] x_i
```

- K-means is EM-algorithm when:

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∈{1,2,...g}} ||x_i − μ_j||
   for j = 1,2,...K:
      μ_j = (1 / Σ_{n=1}^N 𝕀[z_n=j]) Σ_{n=1}^N 𝕀[z_n = j] x_i
```

- 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 $C_1, ... C_K$

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

return $z_1, ... z_N$

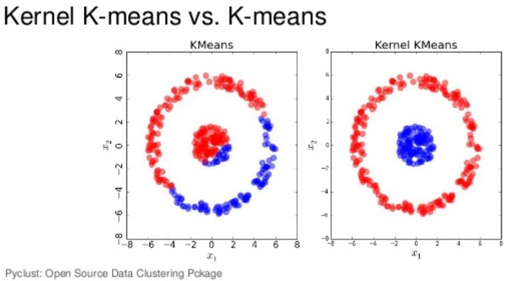
Intuition

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

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

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. $\frac{1}{|C_k|^2}\sum_{i,j\in C_k}e^{-\gamma\left\|x_i-x_j\right\|^2}$ - 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
   - K-means
   - Kernel K-means
   - Mahalanobis distance
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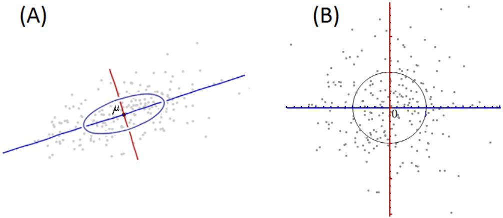
Mahalanobis distance

- 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 $F(\mu, \Sigma)$:

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

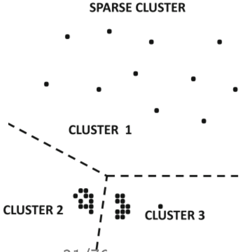


Mahalanobis distance clustering

- 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
    - Kernel K-means
    - Mahalanobis distance
    - K-medoids

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 $\mu_1, ...\mu_K$ 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 $n = 1, 2, ...N$:
  $z_n = \arg\min_k \rho(x_n, \mu_k)$

return $z_1, ...z_N$

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
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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

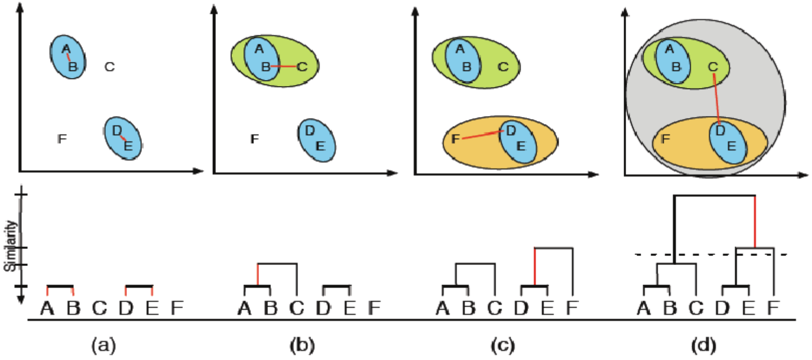
Hierarchical clustering

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.

Variance based clustering

- For each cluster i keeps statistics:

$$m_i = |C_i|, \; F_i^d = \sum_{k \in C_i} x_k^d, \; S_i^d = \sum_{k \in C_i} \left(x_k^d\right)^2$$

- Using statistics we can calculate in-cluster variance

$$V_i = \sum_{d=1}^{D} \left[\frac{S_i^d}{m_i} - \left(\frac{F_i^d}{m_i} \right)^2 \right]$$

- After merge variance always $\uparrow$, distance:

$$\rho(A, B) = V_{A \cup B} - V_A - V_B$$

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,...L_K
   add L_1,...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 $\phi_j, \mu_j$ and $\Sigma_j$, $j = 1, 2, ...g$.

repeat while stopping condition not satisfied:
   E-step. Calculate correspondences of $x_n$
            to component $z$:
      for $n = 1, 2, ...N$:
         for $z = 1, 2, ...Z$:
            $w_{nz} = \frac{\phi_z N(x_n; \mu_z, \Sigma_z)}{\sum_k \phi_k N(x_n; \mu_k, \Sigma_k)}$   # =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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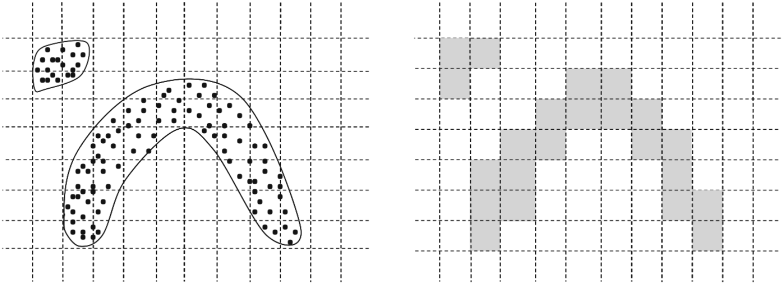
Grid-based clustering

- 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



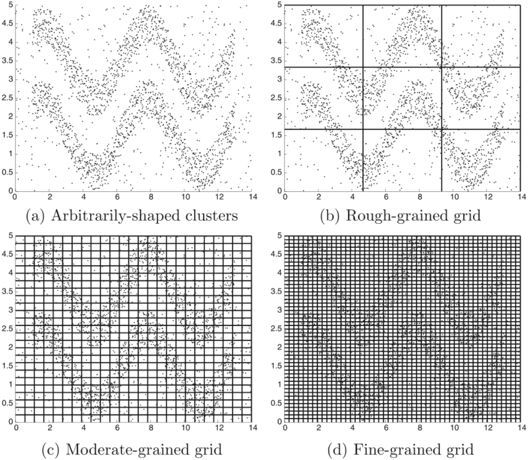
(a) Data points and grid

(b) Agglomerating adjacent grids

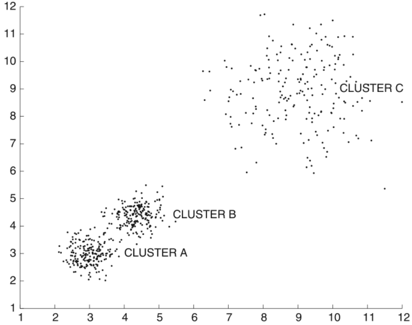
Discussion

- 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



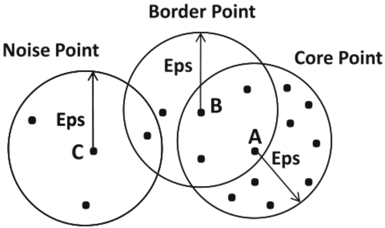
Failure for varying density



- 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

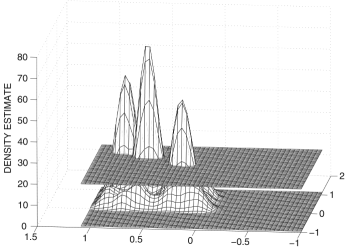
- Connecting core points - agglomerative clustering with single linkage, stopping at distance ε.
- Resistant to outliers by ignoring noise points.
- Similar to grid-based clustering:
  - automatically determines the number of clusters
  - works badly for density varying clusters
- Complexity $O(N^2 D)$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

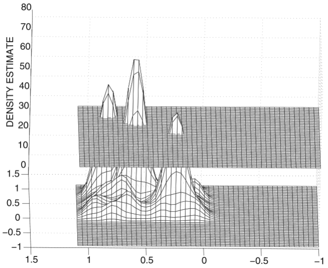
DENCLUE clustering

- INPUT: training set $x_1, ...x_N$, threshold τ.
- Construct kernel density of dataset:
  $p(x) = \frac{1}{Nh^D} \sum_{n=1}^{N} K\left(\frac{\rho(x,x_n)}{h}\right)$
- Associate each point a peak it follows to by gradient ascent:
  1. $x_0 = x$
  2. repeat while not converged: $x_{n+1} = x_n + \varepsilon \nabla p(x_n)$
- Make clusters of data points, converging to the same peak.
- Discard clusters, corresponding to peaks with $p(x) < \tau$
- Merge clusters, connected by path of data points $\left\{p(x_{i(k)})\right\}_{k=1}^{K}$, having $p(x_{i(k)}) \geq \tau \; k = 1, 2, ...K$.
- OUTPUT: cluster indices of $x_1, ...x_N$.

DENCLUE Comments

- Depending on threshold τ may obtain different number of clusters:





- Automatically determines number of clusters, given τ.
- Clusters can be of arbitrary shape
- By varying τ, we can build hierarchical clustering.

DENCLUE Comments[5]

- DENCLUE becomes DBSCAN for
    - $K(\rho(x,x')) = \mathbb{I}[\rho(x,x') \le \varepsilon]$
    - $\tau = k/V_D(\varepsilon)$, where $V_D(\varepsilon)$-volume of sphere with radius ε in D-dimensional space.
- Complexity $O(N^2 I)$, I-number of iterations ig gradient ascent.
    - for N points I times need to calculate $p(x)$
    - $p(x)$ can be calculated in less than $O(N)$ by looking only at neighboright points which can be found fast with spatial index
        - using: ball trees, KD-trees, mapping: bin on the axis->objects in that bin.

[5] Gradient ascent in DENCLUE can be replaced with recursive *mean shift* method.

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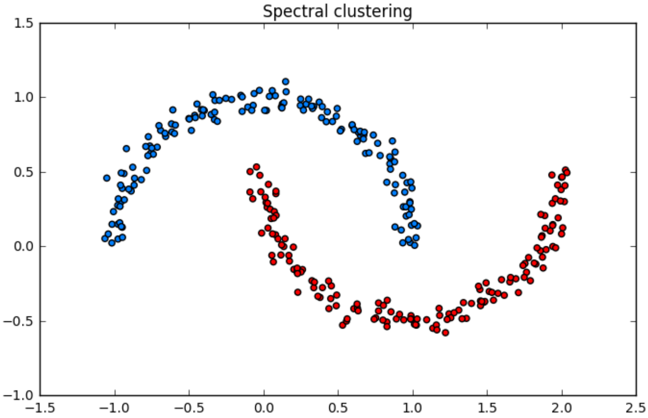
Spectral clustering - example



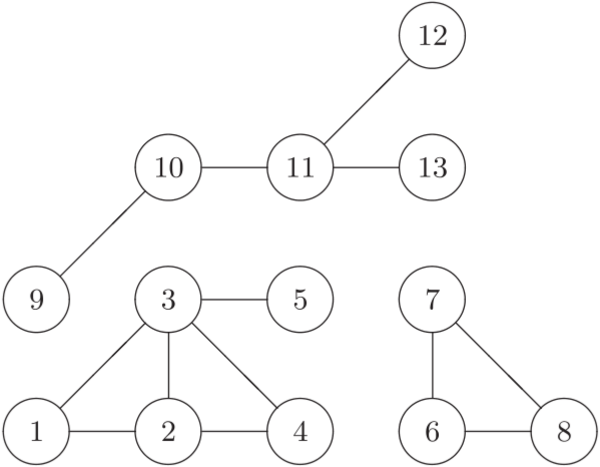
Description

- 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

- $\|x_i - x_j\| < \textit{threshold}$
- 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 $f \in \mathbb{R}^N$:

$$
\begin{aligned}
f^T L f = f^T D f - f^T W f = \sum_i d_i f_i^2 - \sum_{i,j,} f_i f_j w_{ij} = \\
\frac{1}{2}\left(\sum_i d_i f_i^2 - 2\sum_{i,j} w_{ij} f_i f_j + \sum_j d_j f_j^2\right) = \\
\frac{1}{2}\left(\sum_{i,j} w_{ij} f_i^2 - 2\sum_{i,j} w_{ij} f_i f_j + \sum_{j,i} w_{ji} f_j^2\right) = \\
\frac{1}{2}\left(\sum_{i,j} w_{ij} f_i^2 - 2\sum_{i,j} w_{ij} f_i f_j + \sum_{i,j} w_{ij} f_j^2\right) = \\
\frac{1}{2}\sum_{i,j} w_{ij}(f_i - f_j)^2 \geq 0
\end{aligned}
\tag{3}
$$

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

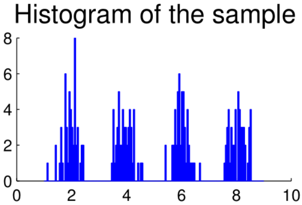
1. Find order K of singular value $\lambda = 0$ for L
2. Find set of eigenvectors $v_1, ...v_K$ corresponding to $\lambda = 0$
3. Cluster *rows* of $V = [v_1, ...v_K] \in \mathbb{R}^{NxK}$ with K-means.

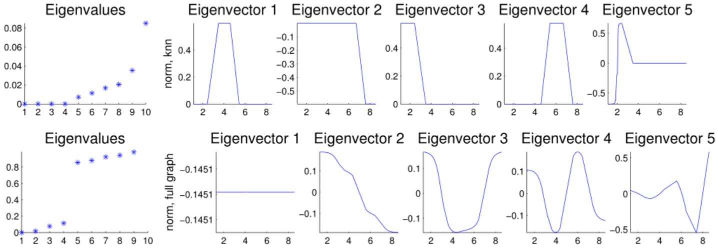
RETURN clustering for rows as clustering for initial objects $x_1, ...x_N$.

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
−0.1451