Clustering

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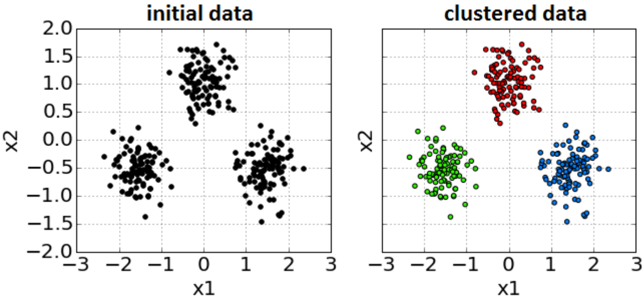
Aim of clustering

- 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, cluster average target, 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?
- 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 representative μ_k, $k = 1, 2, ...K$.
- Criterion to find representatives $\mu_1, ...\mu_K$:

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

Generic algorithm

```
initialize μ_1,...μ_K from
random training objects

WHILE not converged:
    FOR n = 1,2,...N:
        z_n = arg min_k ρ(x_n, μ_k)

    FOR k = 1,2,...K:
        μ_k = arg min_μ Σ_{n:z_n=k} ρ(x_n, μ)

RETURN z_1,...z_N
```

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 or constrained to be existing objects
- 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

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.

WHILE not converged:

    FOR i = 1,2,...N:
        find cluster number of x_i:
        z_i = arg min_{j∈{1,2,...K}} ||x_i − μ_j||_2^2

    FOR j = 1,2,...K:
        μ_j = 1/(∑_{n=1}^N 𝕀[z_n=j]) ∑_{n=1}^N 𝕀[z_n = j] x_i
```

Initialize μ_j, $j = 1, 2, ...K$.

WHILE not converged:

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 $j = 1, 2, ...K$:

$$\mu_j = \frac{1}{\sum_{n=1}^{N} \mathbb{I}[z_n = j]} \sum_{n=1}^{N} \mathbb{I}[z_n = j] x_i$$

K-means properties

Convergence conditions:

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

Initialization:

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

K-means properties

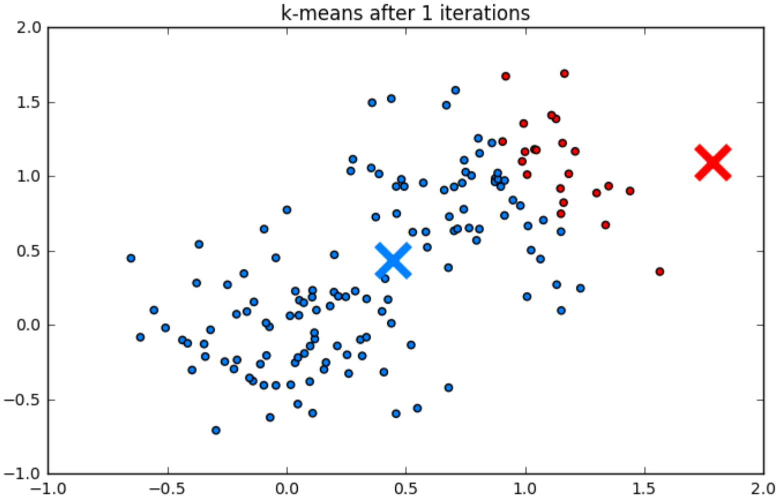
Optimality:

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

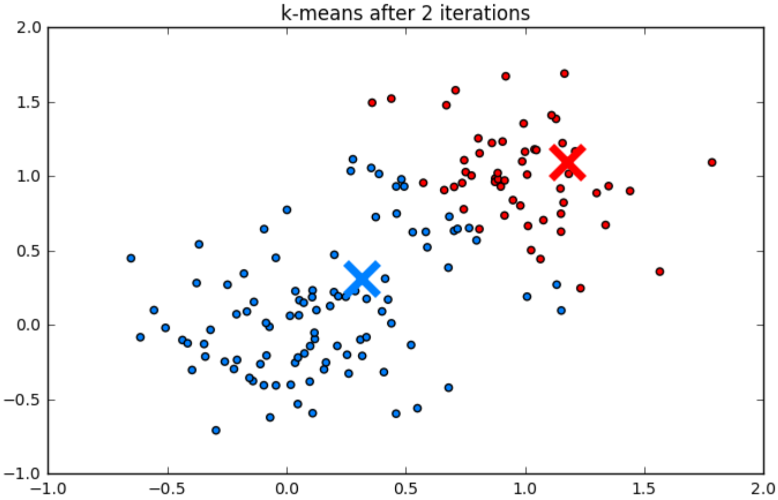
Complexity: $O(NDKI)$

- K is the number of clusters
- I is the number of iterations.
    - usually few iterations are enough for convergence.

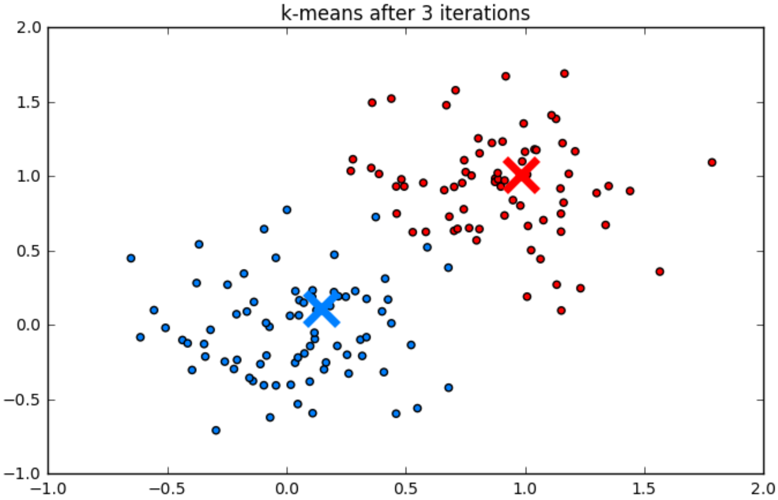
Example of K-means



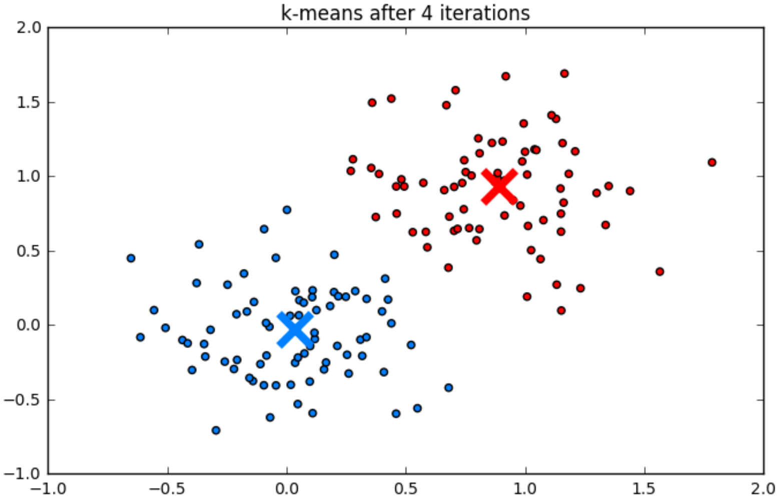
Example of K-means



Example of K-means

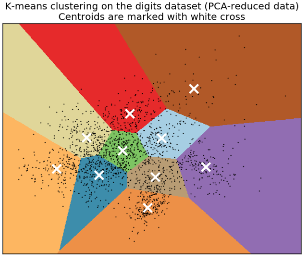


Example of K-means



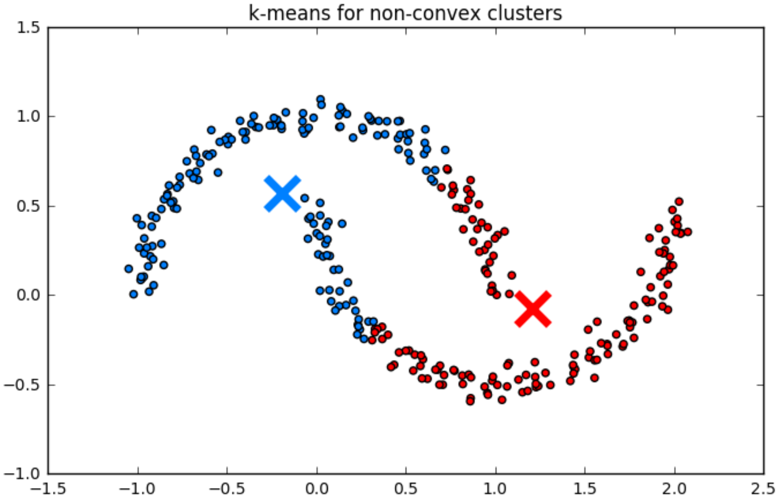
Gotchas

- K-means assumes that clusters are convex:

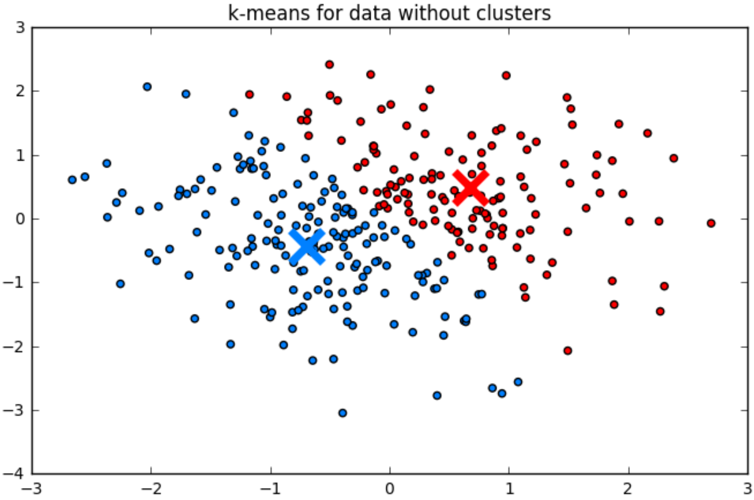


- It always finds clusters even if none actually exist
  - need to control cluster quality metrics

K-means for non-convex clusters



K-means for data without clusters



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

Algorithm

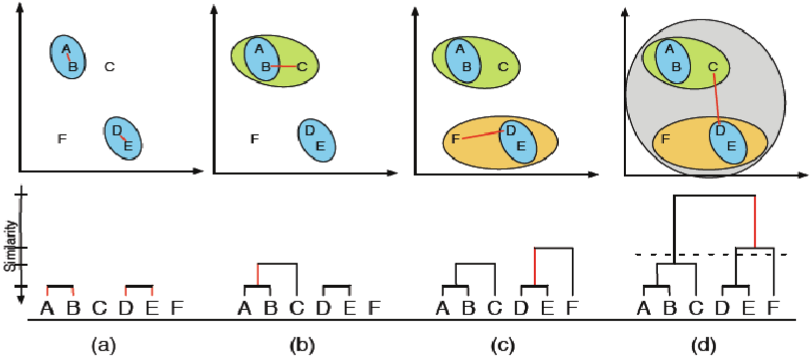
```
INPUT:
data D, flat clustering algorithm A
leaf selection criterion, termination criterion

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
    - result: balanced tree by height
  - split leaf with maximum elements
    - result: balanced tree by cluster size
- Building hierarchy top-down is more natural for a human

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

Bottom-up clustering demo



Algorithm

```
initialize distance matrix M ∈ ℝ^{NxN} 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 $m_U = median_{x \in U}\{x\}$

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General approaches

- Evaluate on the quality criterion of the final task
- Evaluate using "golden rule" clustering
    - invariant to cluster naming
    - makes sence for small golden rule set
        - otherwise reduces to classification
- Unsupervised criterion
    - based on intuition:
        - objects from same cluster should be similar
        - objects from different clusters should be different

Silhuette coefficient[1]

For each object x_i define:

- s_i-mean distance to objects in the same cluster
- d_i-mean distance to objects in the next nearest cluster

Silhouette coefficient for x_i:

$$Silhouette_i = \frac{d_i - s_i}{\max\{d_i, s_i\}}$$

Silhouette coefficient for $x_1, ...x_N$:

$$Silhouette = \frac{1}{N}\sum_{i=1}^{N}\frac{d_i - s_i}{\max\{d_i, s_i\}}$$

[1] Peter J. Rousseeuw (1987). "Silhouettes: a Graphical Aid to the Interpretation and Validation of Cluster Analysis". Computational and Applied Mathematics 20: 53–65.

Discussion

- Advantages
  - The score is bounded between -1 for incorrect clustering and +1 for highly dense clustering.
  - Scores around zero indicate overlapping clusters.
  - The score is higher when clusters are dense and well separated.
- Disadvantages
  - complexity $O(N^2 D)$
    - use feature space indexing or random subsampling
  - favours convex clusters

Calinski-Harabaz Index[2]

- Consider K clusters. For cluster $k = 1, 2, ...K$ define
  - n_k - number of objects, I_k - indexes of objects
  - c_k - centroid, $c = \frac{\sum_{k=1}^{K} n_k c_k}{\sum_{k=1}^{K} n_k}$

[2] Caliński, T., & Harabasz, J. (1974). "A dendrite method for cluster analysis". Communications in Statistics-theory and Methods 3: 1-27.

Calinski-Harabaz Index

- Within cluster covariance matrix

$$W = \frac{1}{N-K}\sum_{k=1}^{K}\sum_{x\in I_k}(x-c_k)(x-c_k)^T$$

- Between cluster covaraince matrix

$$B = \frac{1}{K-1}\sum_{k=1}^{K} n_k(c_k-c)(c_k-c)^T$$

- Calinski-Harabaz Index:

$$I = \frac{\operatorname{tr} B}{\operatorname{tr} W}$$

Discussion

- Advantages
  - The score is higher when clusters are dense and well separated.
  - Complexity $O(ND)$
- Drawbacks
  - Index favours convex clusters

Example

Metrics will not be large here.