Clustering

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K-means algorithm

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

$$\sum_{n=1}^{N} \rho(x_n, \mu_{z_n})^2 \to \min_{z_1,...z_N,\mu_1,...\mu_g} \tag{1}$$

  where $z_i \in \{1, 2, ...g\}$ is cluster assignment for x_i and $\mu_1, ...\mu_g$ are cluster centers.
- Direct optimization requires full search and is impractical.
- K-means is a suboptimal algorithm for optimizing (1).

K-means algorithm

```
Initialize μ_j, j = 1,2,...g.

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

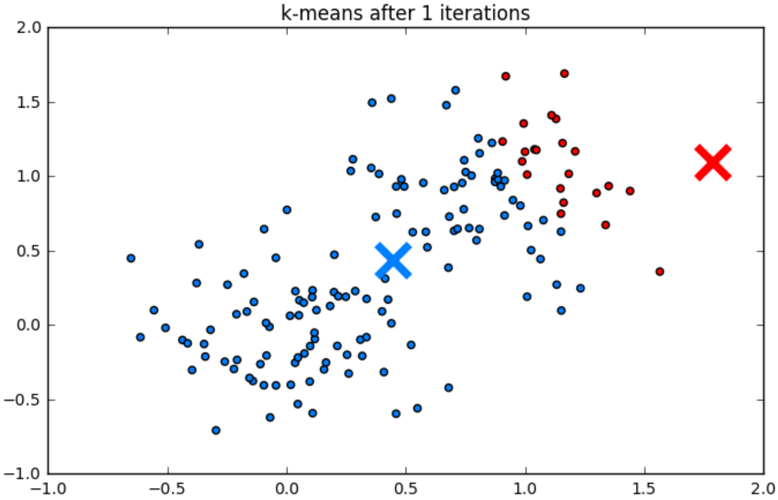
Possible stop conditions:

- cluster assignments $z_1, ...z_N$ stop to change (typical)
- maximum number of iterations reached
- cluster means $\{\mu_i,\ i = 1, 2, ...g\}$ stop changing significantly

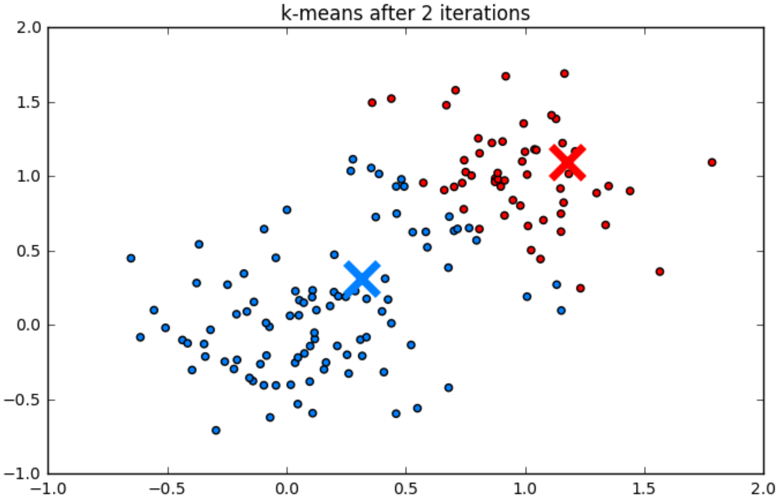
K-means properties

- Only local optimum is found
- Results depends on initialization
  - It is common to run algorithm multiple times with different initializations and then select the result minimizing criterion in (1).
- *Complexity: $O(NDgI)$, where g is the number of clusters and I is the number of iterations. Why?*
  - If clusters exist, algorithm converges with few iterations and complexity is $O(NDg)$

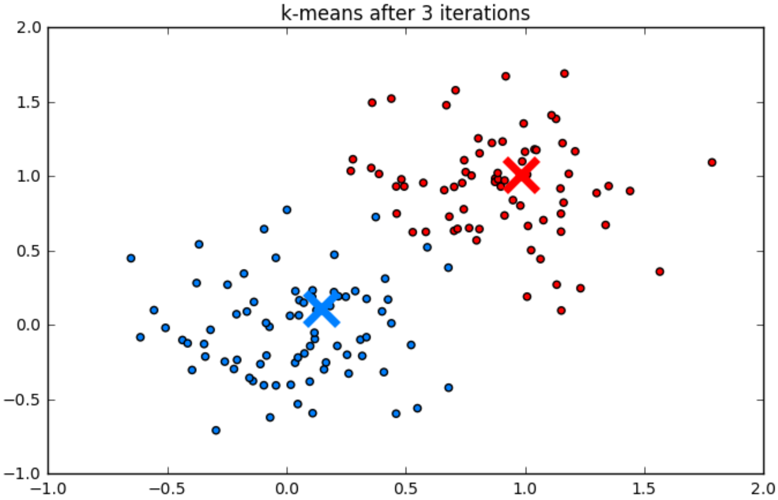
Example of K-means



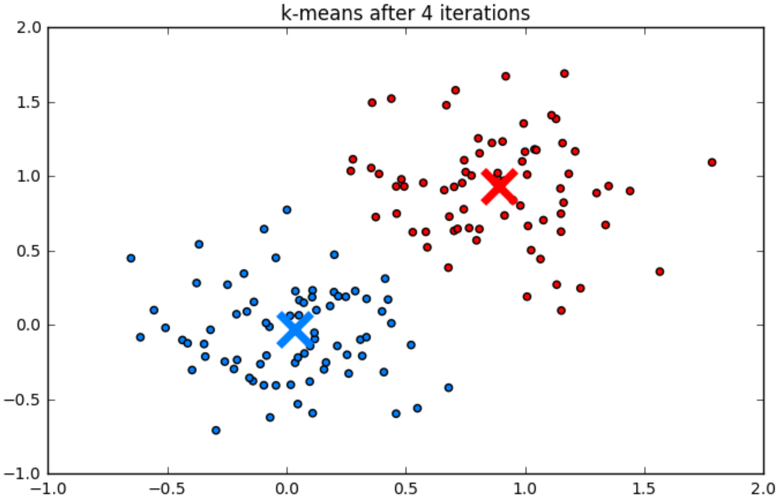
Example of K-means



Example of K-means

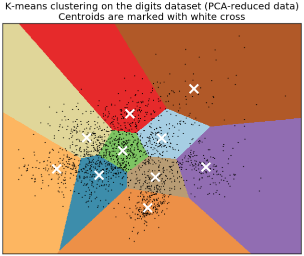


Example of K-means



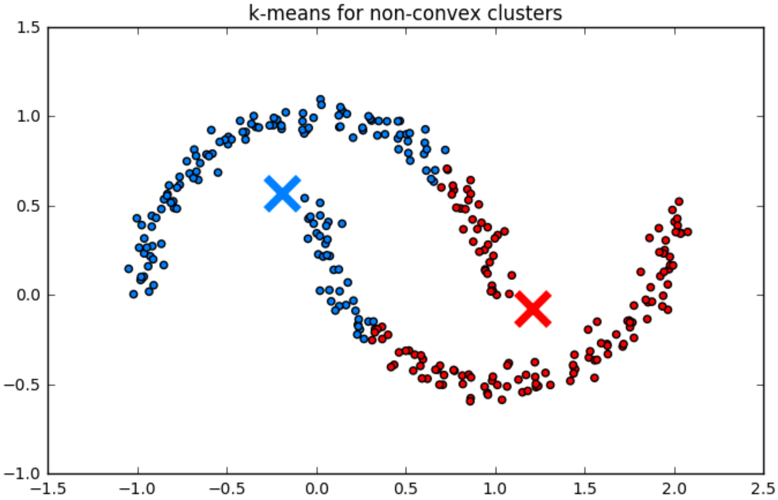
Gotchas

- K-means assumes that clusters are convex:

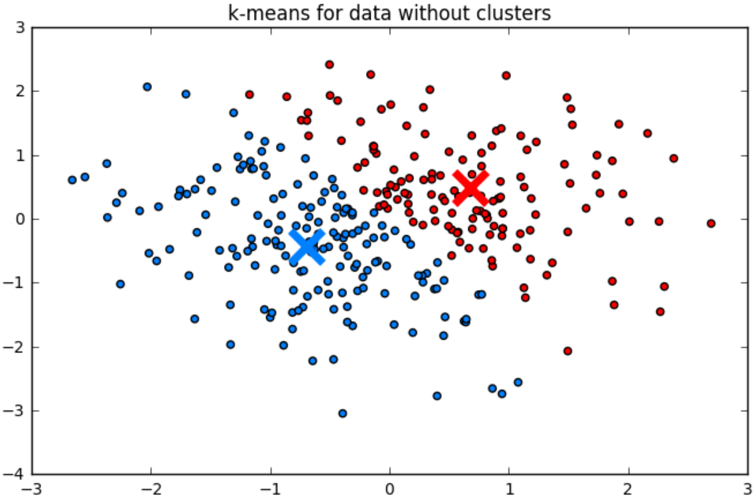


- It always finds clusters even if none actually exist
    - need to control cluster quality metrics

K-means for non-convex clusters



K-means for data without clusters



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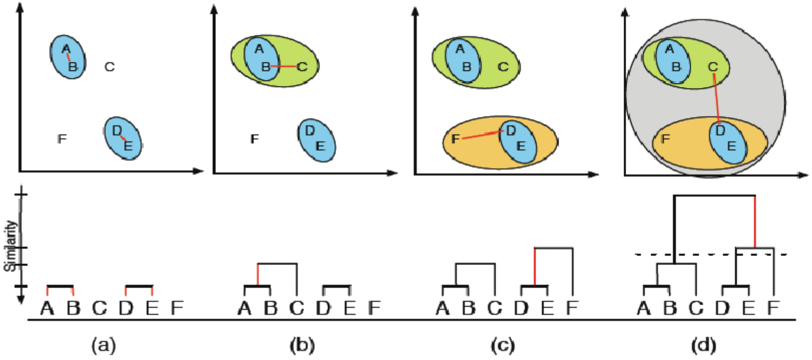
Hierarchical clustering

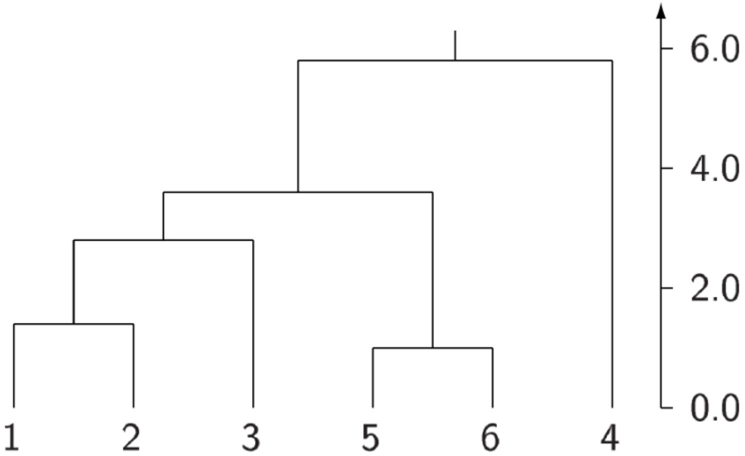
Hierarchical clustering may be:

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

Bottom-up clustering demo



Agglomerative clustering



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

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

  - centroid distance ($\mu_U = \frac{1}{|U|} \sum_{x \in U} x$)

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

  - median distance ($m_U = median_{x \in U}\{x\}$)

$$\rho(A, B) = \rho(m_a, m_b)$$

Agglomerative clustering - distance properties[1]

- nearest neighbour may create stretched clusters
- furtherst neighbour creates very compact clusters.
- group average link, centroid and median distance give the compromise.
    - however centroid and median distance may lead to non-monotonous joining distance sequences in agglomerative algorithm.
    - so average link is apriori preferred

[1] How similarity matrix is modified on each merge of 2 clusters for single/complete/group average link distances?