Machine Learning

(Học máy – IT3190E)

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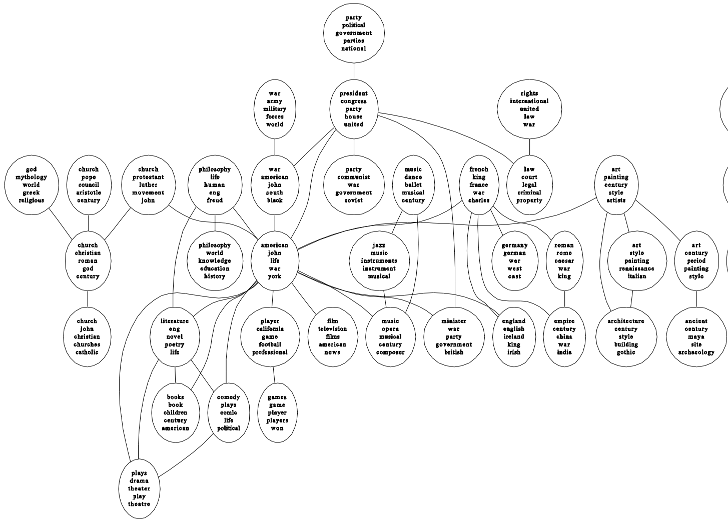
Contents

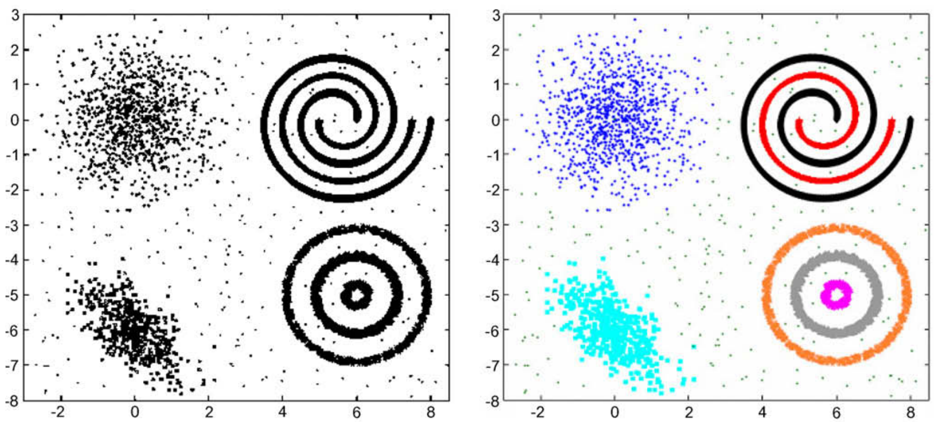
1. Basic learning problems

- **Supervised learning:** learn a function $y = f(x)$ from a given training set $\{\{x_1, x_2, \ldots, x_N\}; \{y_1, y_2, \ldots, y_N\}\}$ so that $y_i \cong f(x_i)$ for every i.
  - Each training instance has a label/response.
- **Unsupervised learning:** learn a function $y = f(x)$ from a given training set $\{x_1, x_2, \ldots, x_N\}$.
  - No response is available
  - Our target is the hidden structure in data.

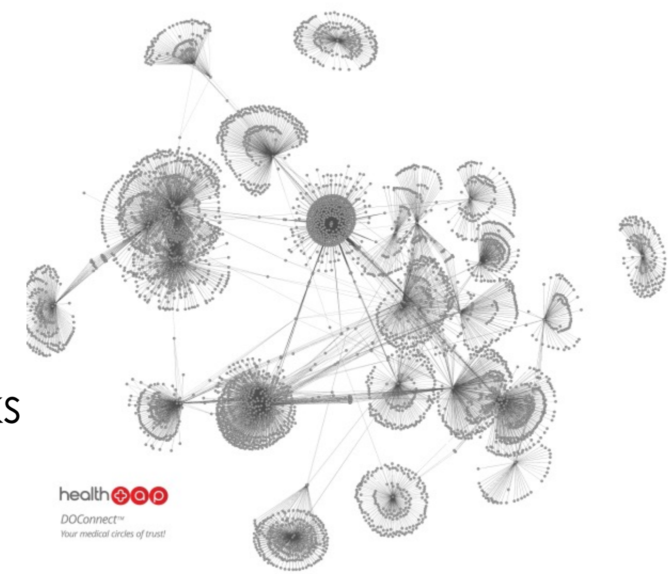


Unsupervised learning: examples (1)

- Clustering data into clusters
  - Discover the data groups/clusters

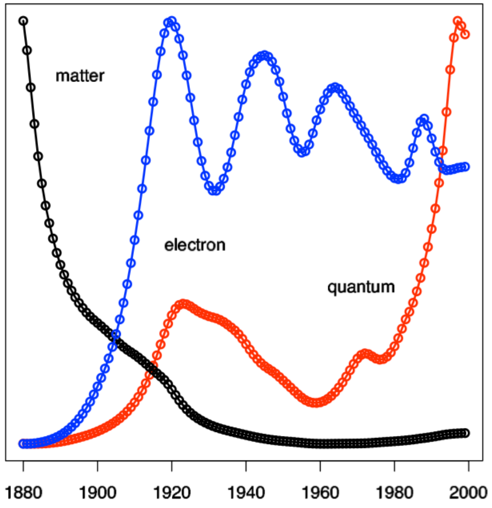


- Community detection
  - Detect communities in online social networks

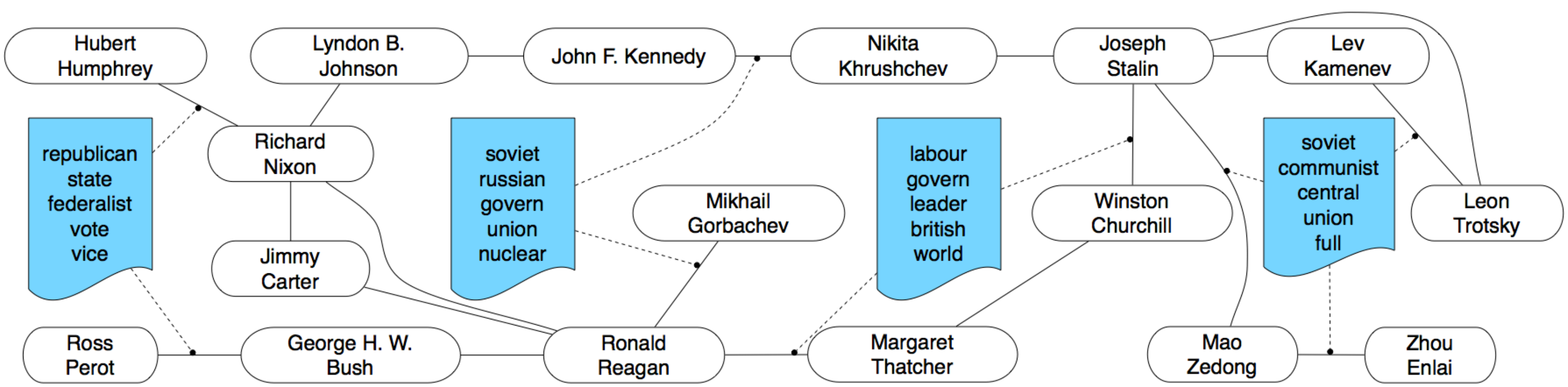


Unsupervised learning: examples (2)

- Trends detection
  - Discover the trends, demands, future needs of online users

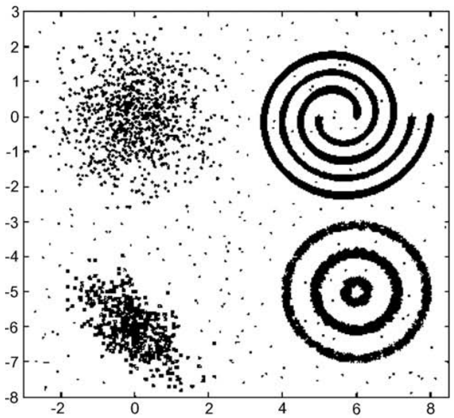


- Entity-interaction analysis

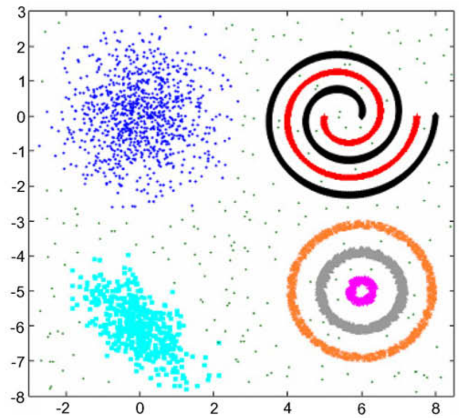


2. Clustering

- Clustering problem:
  - Input: a training set without any label.
  - Output: clusters of the training instances
- A cluster:
  - Consists of similar instances in some senses.
  - Two clusters should be different from each other.



After clustering



Clustering

- Approaches to clustering
  - Partition-based clustering
  - Hierarchical clustering
  - Mixture models
  - Deep clustering
  - …
- Evaluation of clustering quality
  - Distance/difference between any two clusters should be large. (inter-cluster distance)
  - Difference between instances inside a cluster should be small.

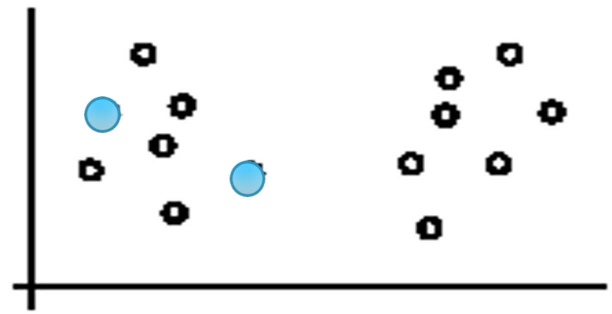
3. K-means for clustering

- K-means was first introduced by Lloyd in 1957.
- K-means is the most popular method for clustering, which is partition-based.
- Data representation: D = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_r$}, each $\mathbf{x}_i$ is a vector in the n-dimensional Euclidean space.
- K-means partitions D into K clusters:
  - Each cluster has a central point which is called **centroid**.
  - K is a pre-specified constant.

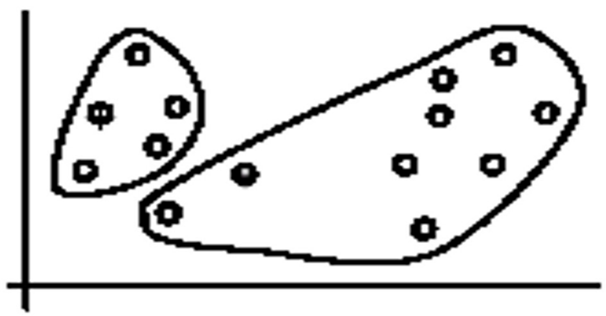
K-means: main steps

- *Input:* training data **D**, number K of clusters, and distance measure d(x,y).
- *Initialization:* select randomly K instances in **D** as the initial centroids.
- Repeat the following two steps <u>until convergence</u>
  - *Step 1:* for each instance, assign it to the cluster with nearest centroid.
  - *Step 2:* for each cluster, <u>recompute its controid</u> from all the instances assigned to that cluster.

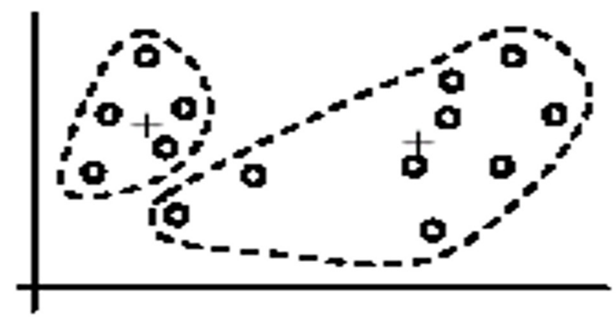
K-means: example (1)



(A). Random selection of *k* centers



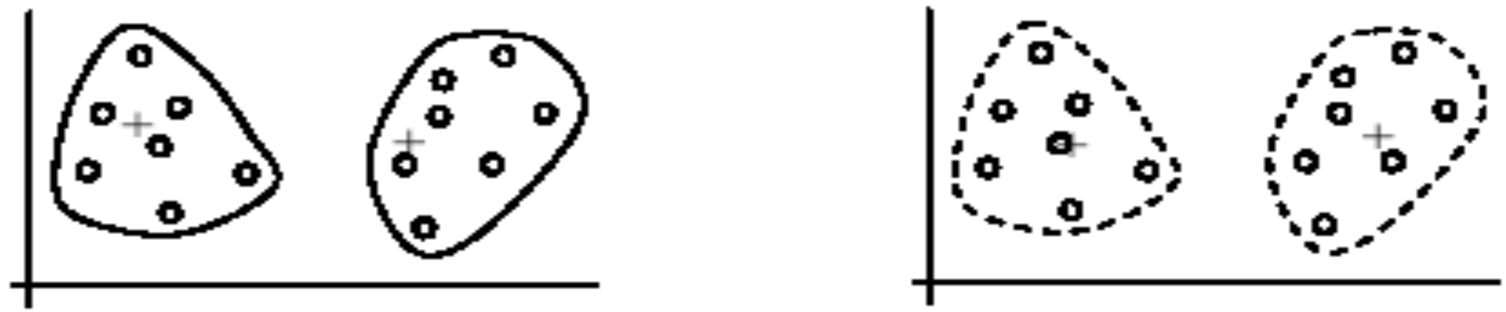
Iteration 1: (B). Cluster assignment



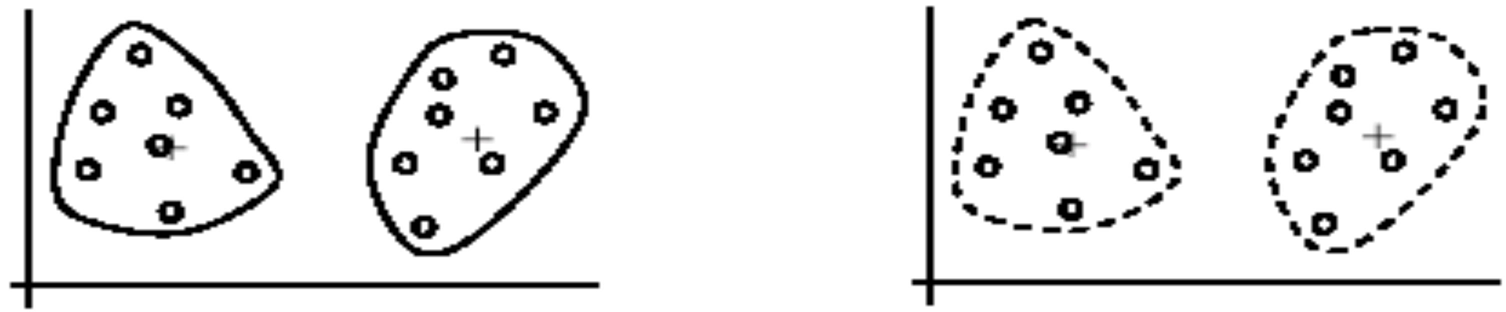
(C). Re-compute centroids

[Liu, 2006]

K-means: example (2)



Iteration 2: (D). Cluster assignment (E). Re-compute centroids



Iteration 3: (F). Cluster assignment (G). Re-compute centroids

[Liu, 2006]

K-means: convergence

- The algorithm converges if:
  - Very few instances are reassigned to new clusters, or
  - The centroids do not change significantly, or
  - The following sum does not change significantly

$$Error = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} d(\mathbf{x}, \mathbf{m_i})^2$$

  - Where C_i is the i^{th} cluster; $\mathbf{m}_i$ is the centroid of cluster C_i.

K-means: centroid, distance

- Re-computation of the centroids:

$$\mathbf{m_i} = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$

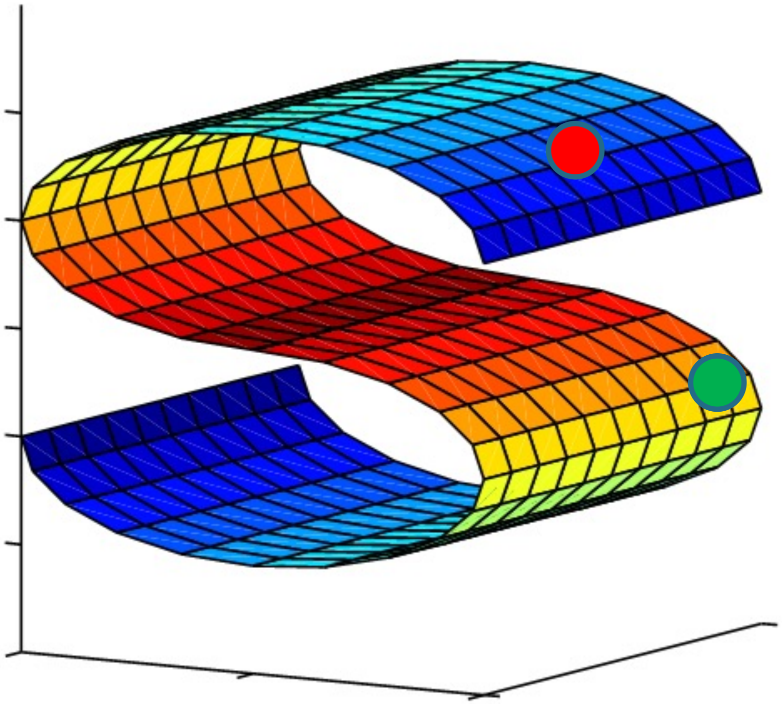
  - $\mathbf{m}_i$ is the centroid of cluster C_i. $|C_i|$ denotes the size of C_i.
- Distance measure:
  - Euclidean

$$d(\mathbf{x}, \mathbf{m_i}) = \|\mathbf{x} - \mathbf{m_i}\| = \sqrt{(x_1 - m_{i1})^2 + (x_2 - m_{i2})^2 + \ldots + (x_n - m_{in})^2}$$

  - Other measures are possible.

K-means: about distance

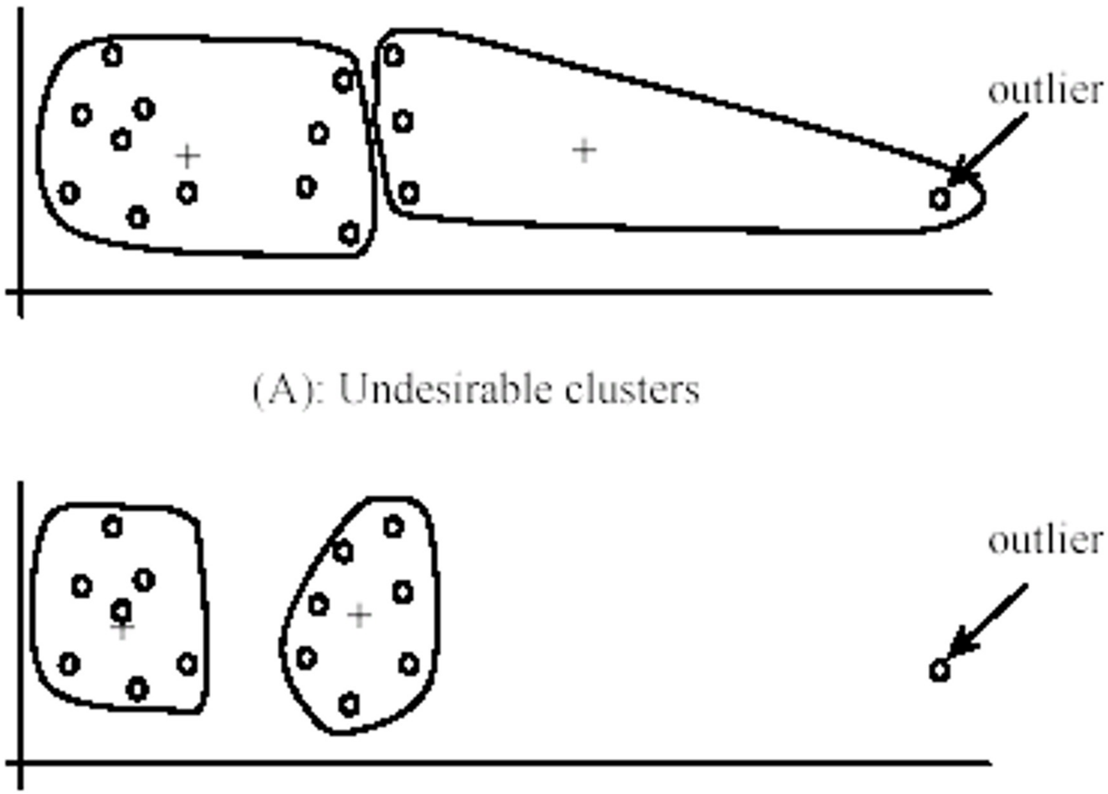
- Distance measure
  - Each measure provides a view on data
  - There are infinite number of distance measures
  - Which distance is good?
- Similarity measures can be used
  - Similarity between two objects



K-means: affects of outliers

- *K-means is sensitive with outliers*, i.e., outliers might affect significantly on clustering results.
  - Outliers are instances that significantly differ from the normal instances.
  - The attribute distributions of outliers are very different from those of normal points.
  - Noises or errors in data can result in outliers.

K-means: outlier example



(A): Undesirable clusters

(B): Ideal clusters

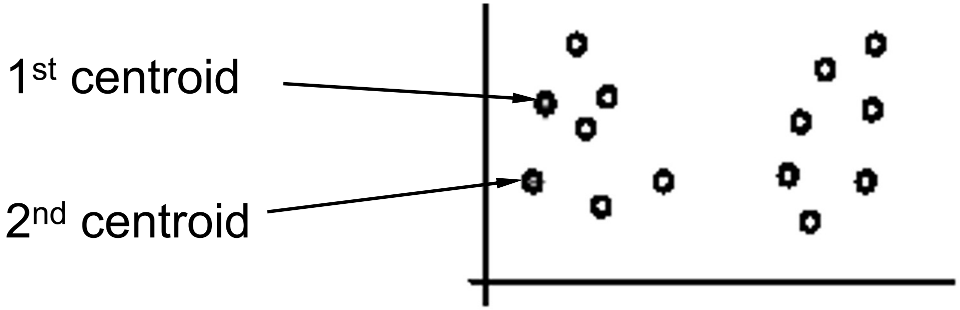
[Liu, 2006]

K-means: outlier solutions

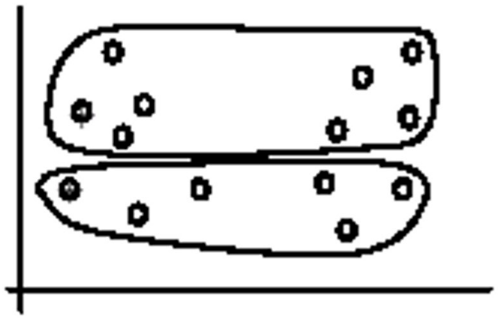
- *Outlier removal:* we may remove some instances that are significantly far from the centroids, compared with other instances.
  - Removal can be done a priori or when learning clusters.
- *Random sampling:* instead of clustering all data, we take a random sample S from the whole training data.
  - S will be used to learn K clusters. Note that S often contains fewer noises/outliers than the original training data.
  - After learning, the remaining data will be assigned to the learned clusters.

K-means: initialization

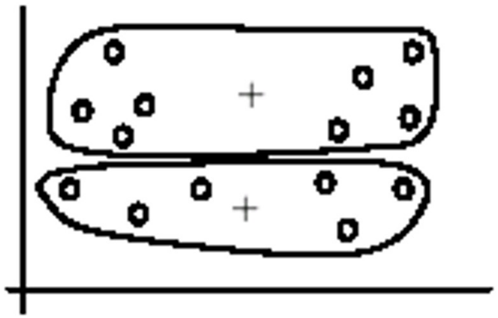
- Quality of K-means depends much on the initial centroids.



(A). Random selection of seeds (centroids)



(B). Iteration 1

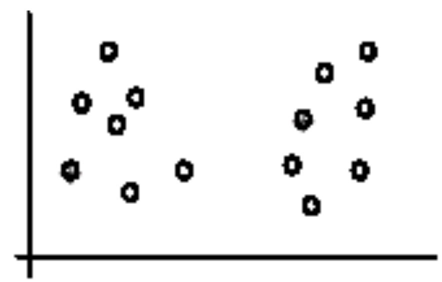


(C). Iteration 2

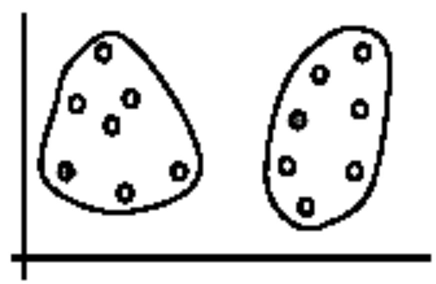
[Liu, 2006]

K-means: initialization solution (1)

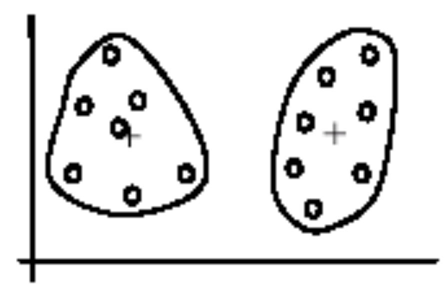
- We repeat K-means many times
  - Each time we initialize a different set of centroids.
  - After learning, we combine results from those runs to obtain a unified clustering.



(A). Random selection of *k* seeds (centroids)



(B). Iteration 1



(C). Iteration 2

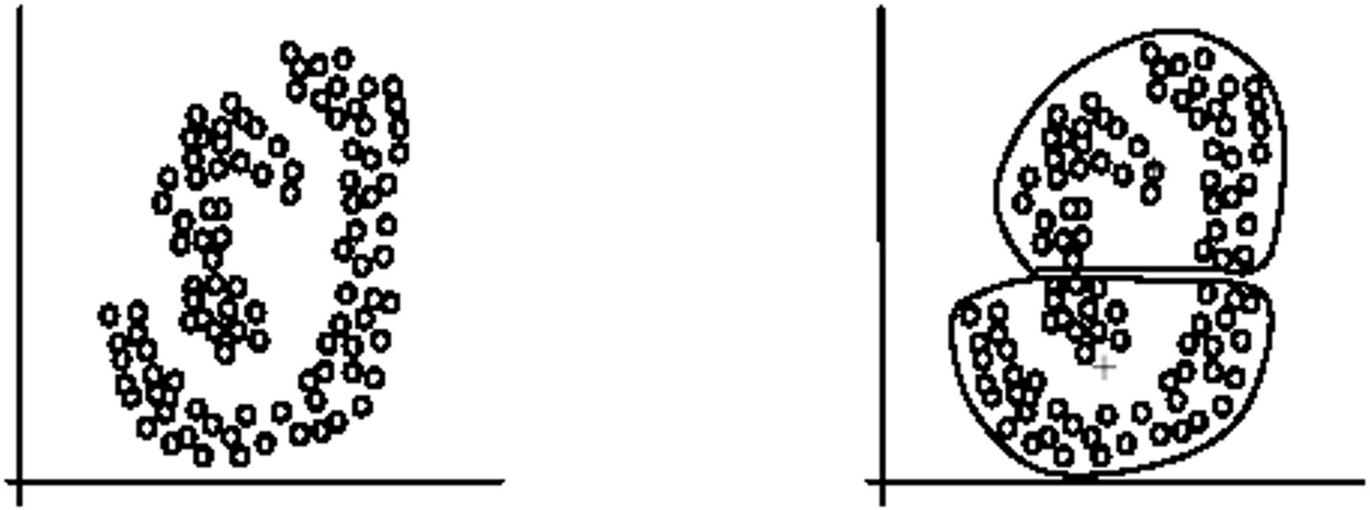
[Liu, 2006]

K-means: initialization solution (2)

- ***K-means++***: to obtain a good clustering, we can initialize the centroids from **D** in sequence as follows
  - Select randomly the first centroid $\mathbf{m}_1$.
  - Select the second centroid which are farthest to $\mathbf{m}_1$.
  - …
  - Select i^{th} centroid which are farthest from $\{\mathbf{m}_1, \ldots, \mathbf{m}_{i-1}\}$.
  - …
- By using this initialization scheme, K-means can converge to a near optimal solution [Arthur, D.; Vassilvitskii, 2007]

K-means: curved clusters

- When using Euclidean distance, K-means cannot detect non-spherical clusters.
  - How to deal with those cases?



(A): Two natural clusters (B): *k*-means clusters

[Liu, 2006]

K-means: summary

- Advantages:
  - Be very simple,
  - Be efficient in practice,
  - Converges in expected polynomial time [Manthey & Röglin, JACM, 2011]
  - Be flexible in choosing the distance measures.
- Limitations:
  - Choose a good similarity measure for a domain is not easy.
  - Be sensitive with outliers.

4. Online K-means

- K-means:
  - We need all training data for each iteration.
  - Therefore, it cannot work with big datasets,
  - And cannot work with stream data where data come in sequence.
- *Online K-means* helps us to cluster big/stream data.
  - It is an online version of K-means [Bottou, 1998].
  - It follows the methodology from online learning and stochastic gradient.
  - At each iteration, one instance will be exploited to update the available clusters.

Revisiting K-means

- Note that K-means finds K clusters from the training instances $\{x_1, x_2, \ldots, x_M\}$ by minimizing the following loss function:

$$Q_{k-means}(w) = \frac{1}{2}\sum_{i=1}^{M} \| x_i - w(x_i) \|_2^2$$

  - Where $w(x_i)$ is the nearest centroid to x_i.
- Using its gradient, we can minimize Q by repeating the following update until convergence:

$$w_{t+1} = w_t + \gamma_t \sum_{i=1}^{M} [x_i - w_t(x_i)]$$

  - Where γ_t is a small constant, often called learning rate.
- This update will converge to a local minimum.

Online K-means: idea

- Note that each iteration of K-means requires the full gradient:

$$Q'_t = \sum_{i=1}^{M} [x_i - w_t(x_i)]$$

  - Which requires all training data.
- Online K-means minimizes Q stochastically:
  - At each iteration, we just use a little information from the whole gradient Q'.
  - Those information comes from the training instances at iteration t:

$$x_t - w_t(x_t)$$

Online K-means: algorithm

- *Initialize K centroids randomly.*
- *Update the centroids as an instance comes*
  - *At iteration t, take an instance x_t.*
  - *Find the nearest centroid w_t to x_t, and then update w_t as follows:*

$$w_{t+1} = w_t + \gamma_t (x_t - w_t)$$

- Note: the learning rates $\{\gamma_1, \gamma_2, \ldots\}$ are positive constants, which should satisfy

$$\sum_{t=1}^{\infty} \gamma_t = \infty; \sum_{t=1}^{\infty} \gamma_t^2 < \infty$$

Online K-means: learning rate

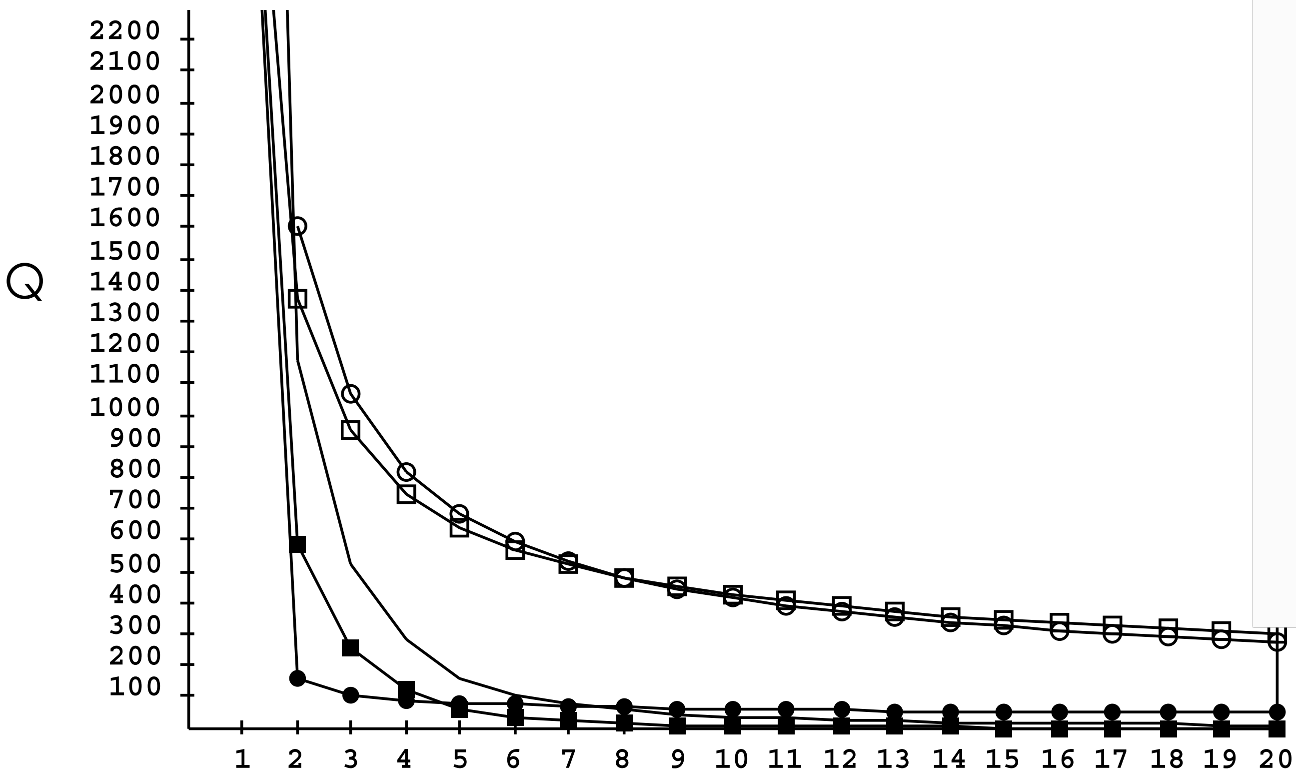
- A popular choice of learning rate:

$$\gamma_t = (t+\tau)^{-\kappa}$$

- τ, κ are possitive constants.
- κ ∈ (0.5, 1] is called *forgeting rate*. Large κ means that the algorithm remembers the past longer, and that new observations play less and less important role as *t* grows.

Convergence of Online K-means

- Objective Q decreases as t increases.



  - Online K-means (Black circles), K-means (Black squares)
  - Partial gradient (empty circles), full gradient (empty squares)

References

- Arthur, D.; Vassilvitskii, S. (2007). K-means++: the advantages of careful seeding. *Proceedings of the 18th annual ACM-SIAM symposium on Discrete algorithms*, pp. 1027–1035.
- Arthur, D., Manthey, B., & Röglin, H. (2011). Smoothed analysis of the k-means method. *Journal of the ACM (JACM)*, *58*(5), 19.
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- B. Liu. *Web Data Mining: Exploring Hyperlinks, Contents, and Usage Data.* Springer, 2006.
- Lloyd, S., 1982. Least squares quantization in PCM. IEEE Trans. Inform. Theory 28, 129–137. Originally as an unpublished Bell laboratories Technical Note (1957).
- Jain, A. K. (2010). Data clustering: 50 years beyond K-means. *Pattern recognition letters*, *31*(8), 651-666.

Exercises

- Solutions to K-means when the data distributions are not spherical?
- How to decide a suitable cluster for a new instance?