Clustering

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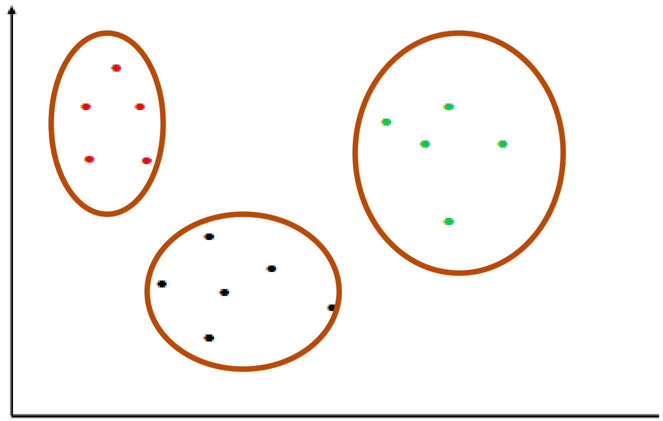
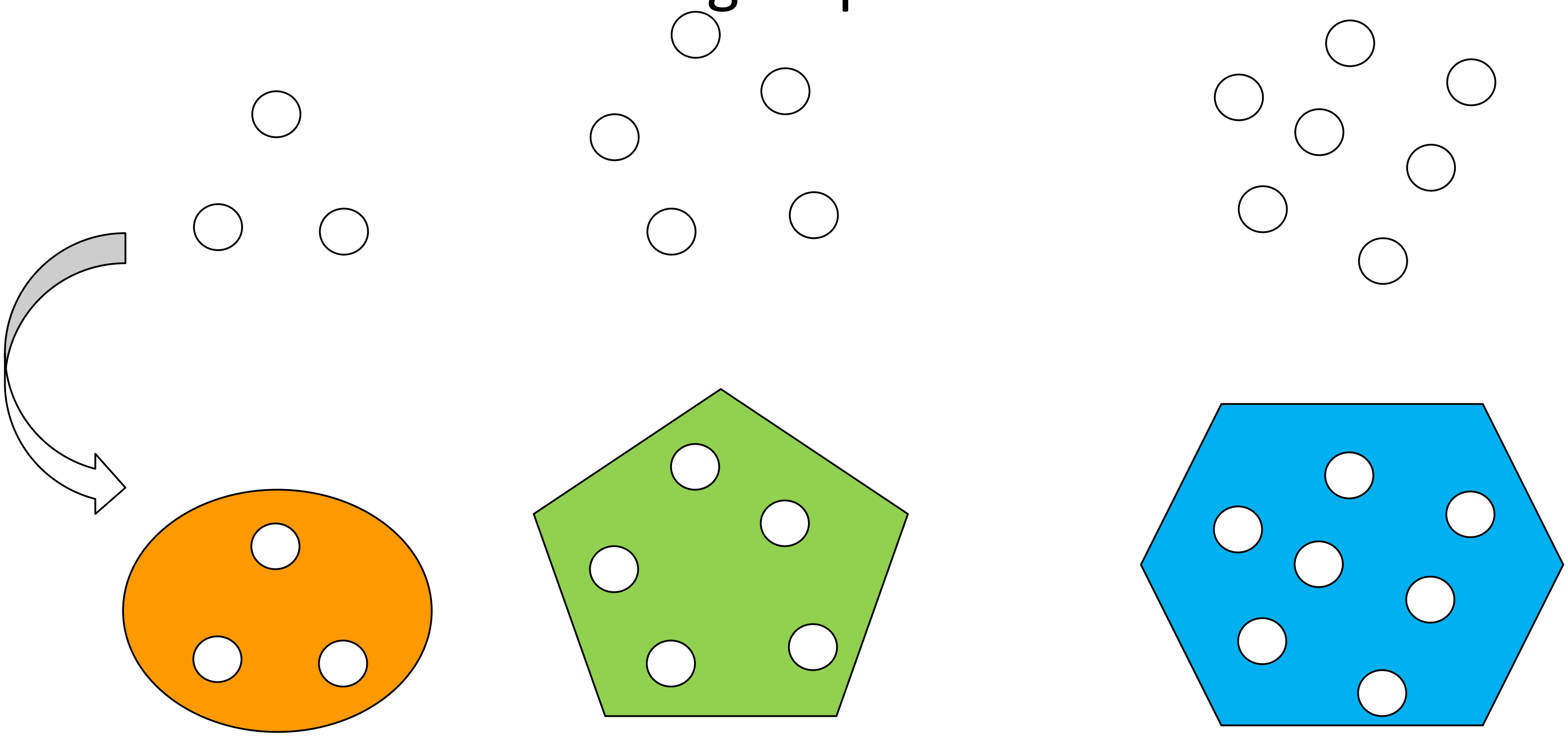


- Are there any groups in the data?
- How to group?
- How many groups?

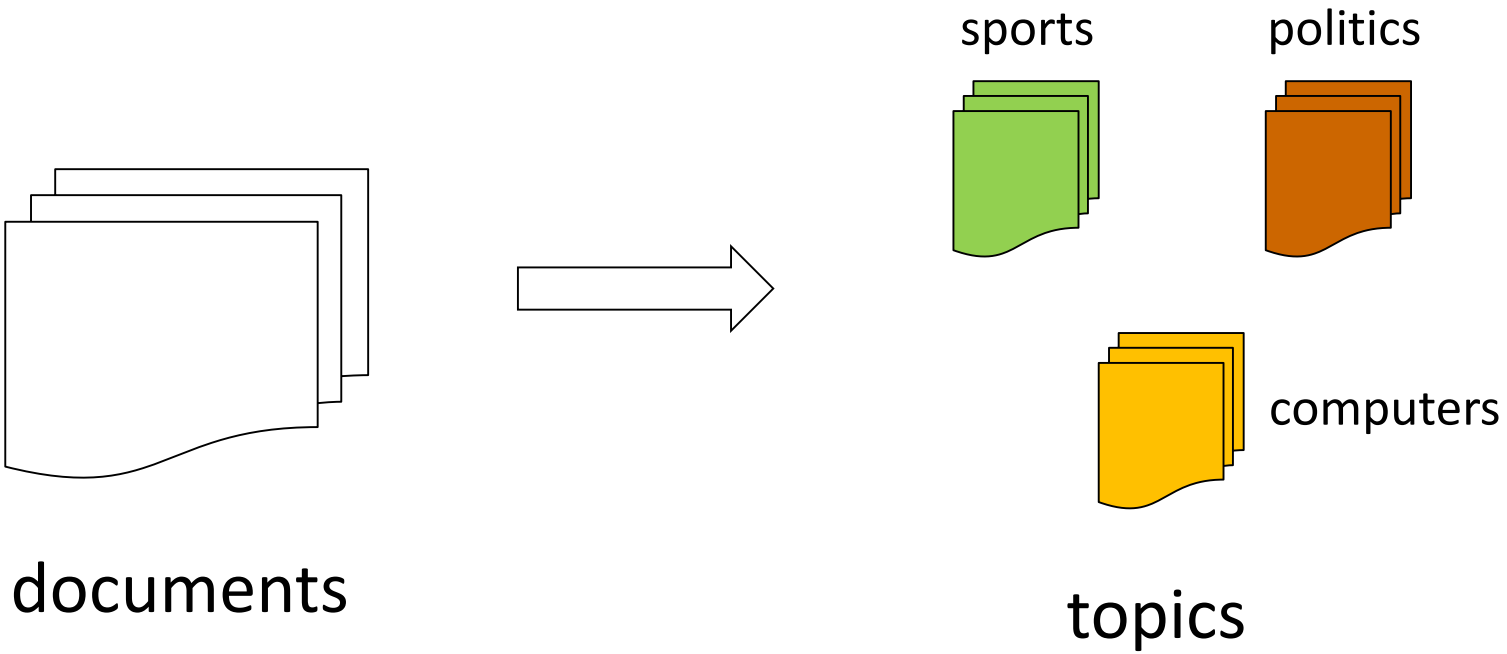
Unsupervised Learning

- **Clustering:** most common form of unsupervised learning
  - Given a collection of unlabeled examples (objects), discover self-similar groups in the data



Unsupervised Learning

- **Text Clustering**



Unsupervised Learning

- **Image Segmentation**

Clustering Applications

- Find genes that are similar in their functions
- Group documents based on topics
- Categorize customers based on their buying habit
- Group images based on their contents

Clustering Issues

- What is a natural grouping among these objects?
  - Definition of "group“
- What makes objects “related”?
  - Definition of "similarity/distance“
- Representation for objects
  - Vector, normalization?
- How many clusters?
  - Fixed a priori?
  - Completely data driven?
  - Avoid “trivial” clusters - too large or small

What is a natural grouping?

- By color? By pattern? By weight?
- The definition of natural grouping is subjective
- This is why we call clustering ***<u>exploratory</u>*** data analysis

What is similarity?

- This is a philosophical question. We will take a more pragmatic approach.
  - Depends on representation and algorithm. For many representations/algorithms, it is easier to think in terms of a distance (rather than similarity) between vectors

Hard to define but

We know it when we see it

Properties of a distance measure?

- **D must be Symmetric**
  - $D(A, B) = D(B, A)$
  - Otherwise, we can say A looks like B but B does not look like A

- **Positivity, and self-similarity**
  - $D(A, B) \geq 0$, and $D(A, B) = 0$ iff $A = B$
  - Otherwise, there will different objects that we cannot tell apart

- **Must satisfy triangle inequality**
  - $D(A, B) + D(B, C) \geq D(A, C)$
  - Otherwise, one can say “A is like B, B is like C, but A is not like C at all”

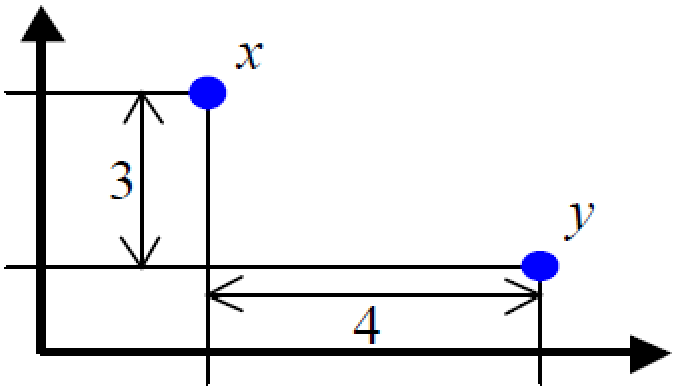
Distance Measures: Minkowski Metric

- Suppose two object x and y both have d features
  - $x = (x_1, \cdots, x_d), y = (y_1, \cdots, y_d)$
- The Minkowski metric of order r is defined by

$$d(x,y) = \sqrt[r]{\sum_i |x_i - y_i|^r}$$

- Common Minkowski metrics:
  - Euclidean(r=2): $d(x,y) = \sqrt[2]{\sum_i (x_i - y_i)^2}$, also called L_2 distance
  - Manhattan distance(r=1) : $d(x,y) = \sum_i |x_i - y_i|$, also called L_1 distance
  - “Sup” distance(r = +∞): $d(x,y) = \max_i |x_i - y_i|$, also called L_∞ distance

A simple example



1 : Euclidean distance : $\sqrt[2]{4^2+3^2}=5.$

2 : Manhattan distance : $4+3=7.$

3 : "sup" distance : $\max\{4,3\}=4.$

Similarities

- Cosine similarity – commonly used to measure document similarity

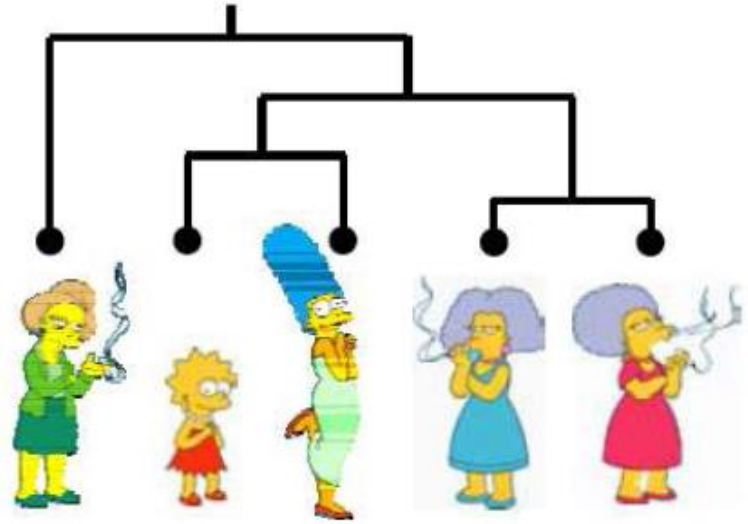
$$cos(\mathrm{x}, \mathrm{x}') = \frac{<\mathrm{x} \cdot \mathrm{x}'>}{|\mathrm{x}| \cdot |\mathrm{x}'|}$$

- Kernels: RBF (Gaussian) Kernel

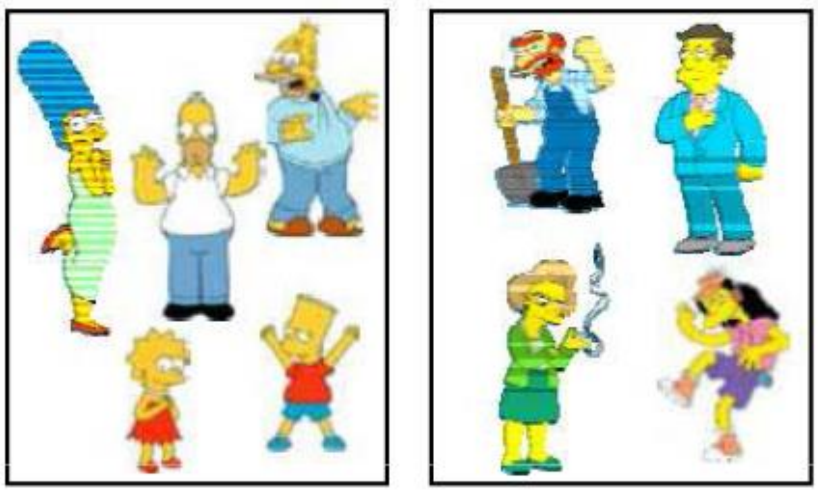
$$K(X, X') = \exp \frac{-|X - X'|^2}{2\sigma^2}$$

Clustering Algorithms

- **Hierarchical algorithms**
  - Bottom up (agglomerative)
  - Top down (divisive)

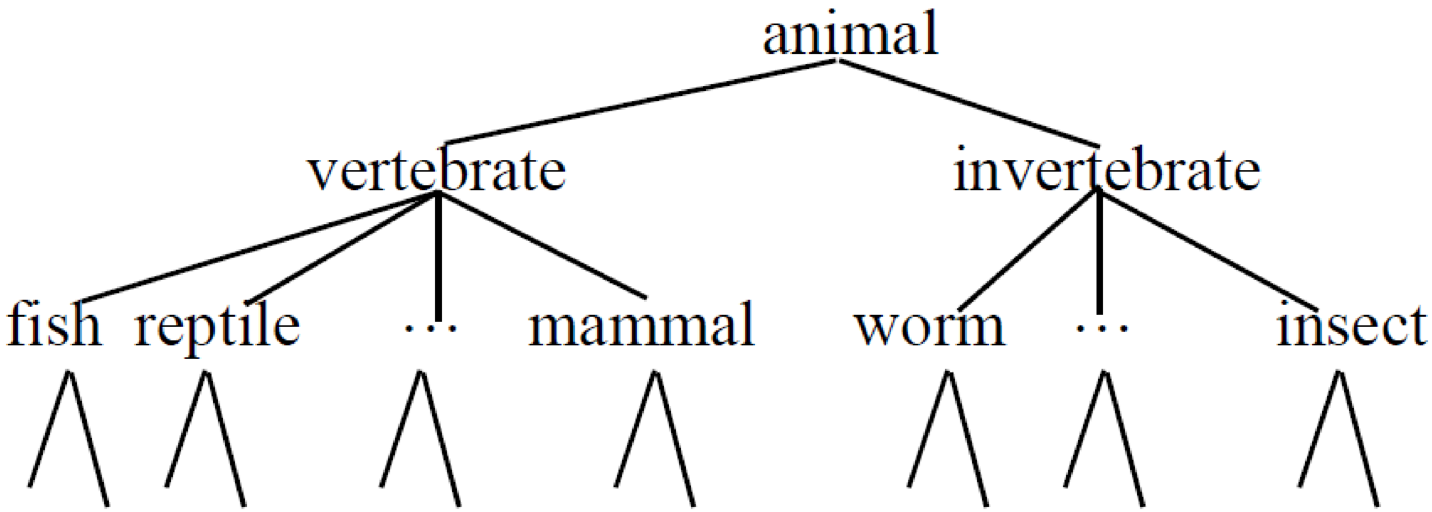


- **Partition algorithms (Flat)**
  - K-means
  - Mixture of Gaussians
  - Spectral clustering



Hierarchical Clustering

- Given a set of objects, build a tree-based taxonomy



- Hierarchies are a convenient way for organizing information, used frequently by web-portals

Hierarchical Agglomerative Clustering (HAC)

- Start with each object in a separate cluster
- Repeatedly join the closest pair of clusters
- until there is only one cluster

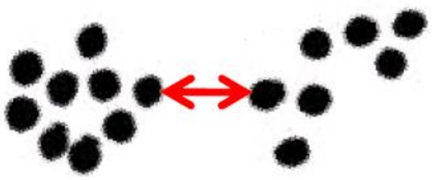
- The history of merging forms a tree of hierarchy

- ***Question***: how to measure the "**closeness**" of two clusters?

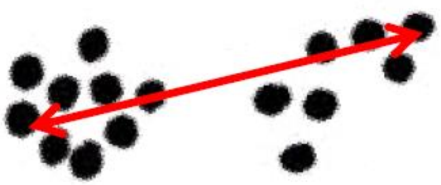
Closest Pair of Clusters?

The distance between two clusters is defined as the distance between:

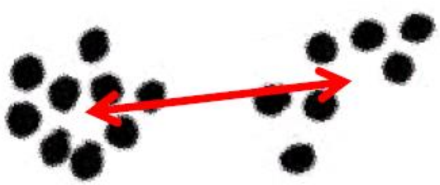
- Single-link
  - The nearest pair of points



- Complete-link
  - The farthest pair of points



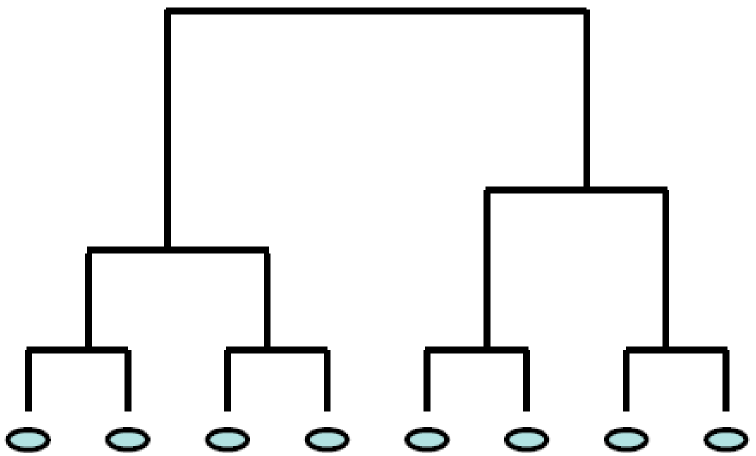
- Centroid
  - The center of gravity



- Average-link
  - Average of all cross-cluster pairs

Visualization of the hierarchy: Dendogram

- Can be used to identify the number of clusters in data
  - A horizontal cut will create a unique clustering
  - Moving the cut from root down creates more clusters
  - Large gaps between the merging nodes indicate a good cutting point



Computational Complexity

- All hierarchical clustering methods need to compute distance of all pairs of n individual instances which is $O(n^2)$
- There are n-1 iterations, at each iteration after the merge we must compute the distance between new cluster and all other clusters

$$\sum_{i=2}^{n-1} n - i = O(n^2)$$

- In order to maintain an overall $O(n^2)$ performance, distance update must be done in constant time – trivial for complete-link and single-link

Partition Clustering

- Given a data set of n points, we know that there are k clusters in the data, how to find these clusters?
- Roughly speaking there are $O(k^n)$ ways to partition the data, Which one is better?
- One intuition says that we want tight clusters, i.e., points should be in a tight ball
- This leads to the following objective function

  $\sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2$ --- squared distance between data point x and its cluster center

- Optimizing this objective is a combinatorial optimization problem
  - Exhaustive search for an optimal solution is not feasible

Combinatorial optimization: An iterative solution

- ***Initialization:*** Start with a random partition of the data
- ***Iterative step***: the cluster assignments and cluster centers are updated to improve the objective
- ***Stopping criterion***: if no improvement can be achieved.

Iterative greedy descent

– convergence is guaranteed, but to local optimal

K-Means

Algorithm

Input – Desired number of clusters, *k*

Initialize – the *k* cluster centers (randomly if necessary)

Iterate –

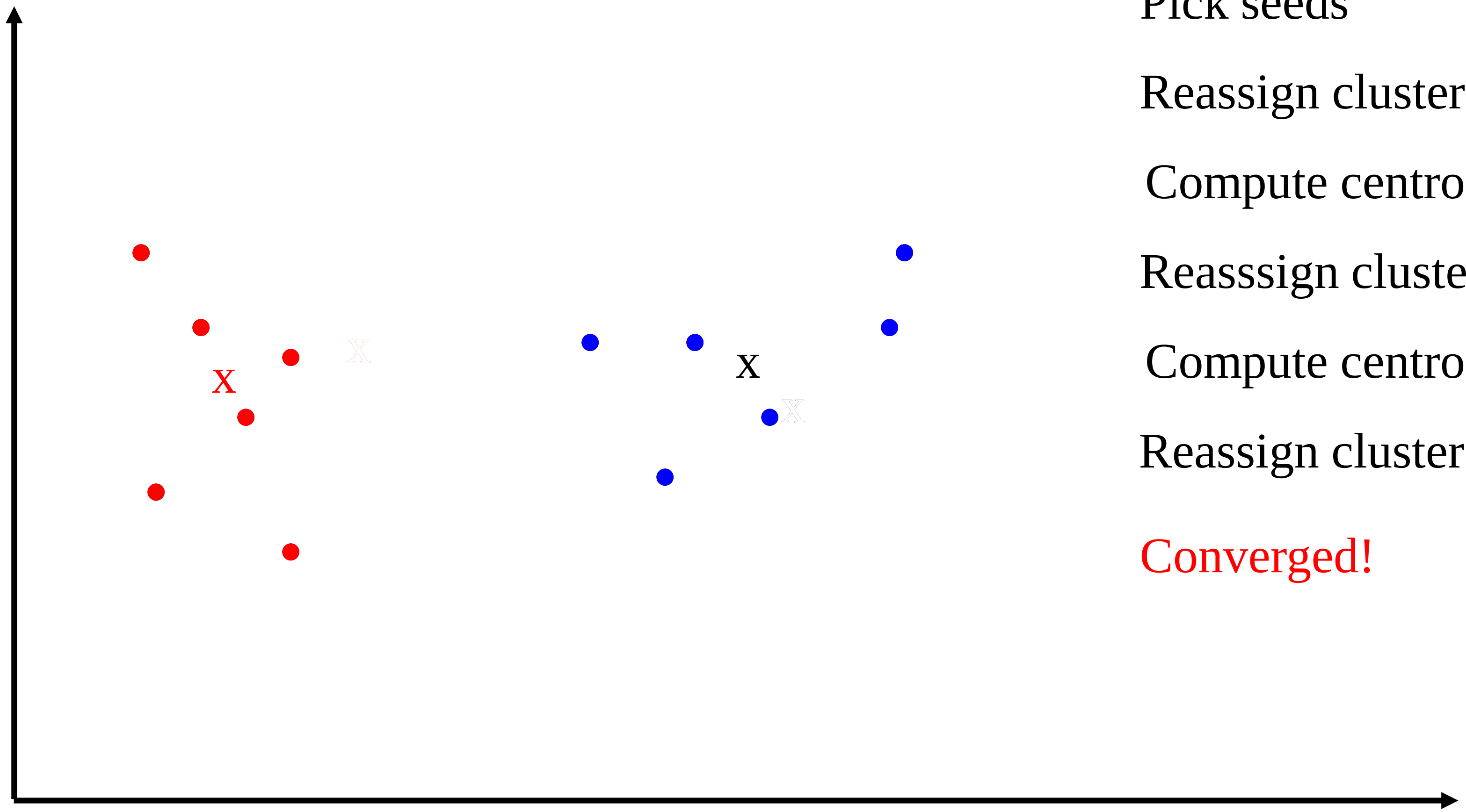
1. Assigning each of the N data points to its nearest cluster centers
2. Re-estimate the cluster center by assuming that the current assignment is correct

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

Termination –

If none of the data points changed membership in the last iteration, exit. Otherwise, go to 1

K-Means Example (K=2)



Pick seeds

Reassign clusters

Compute centroids

Reasssign clusters

Compute centroids

Reassign clusters

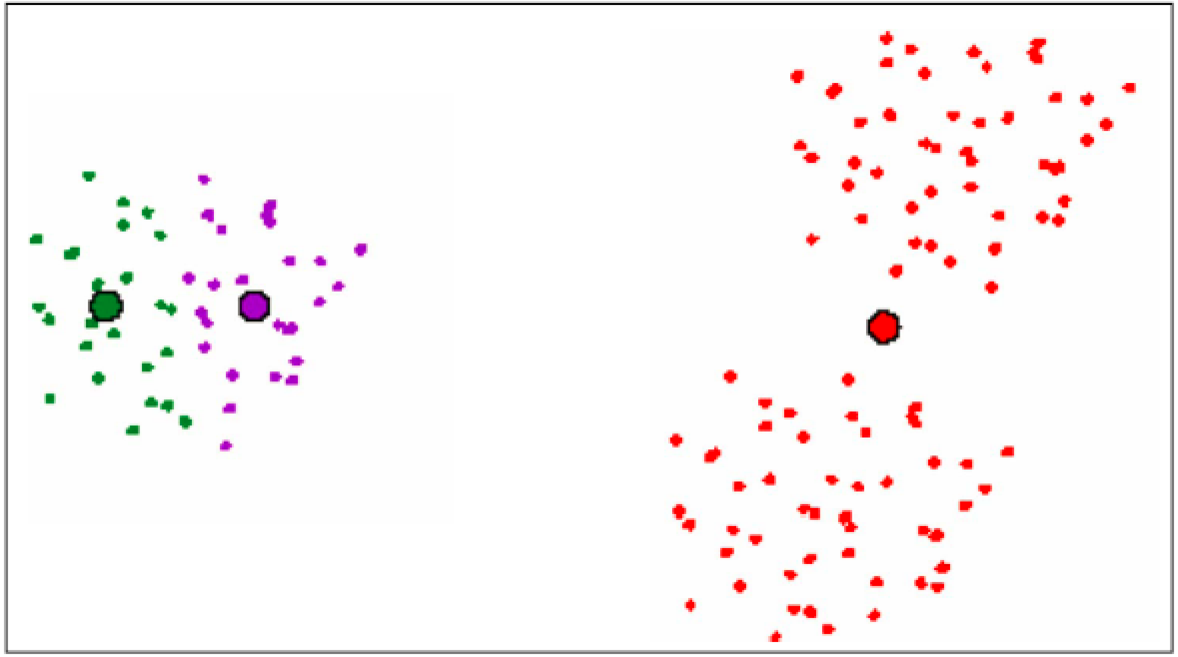
Converged!

Computational Complexity

- At each iteration:
  - Reassigning clusters: $O(kn)$ distance computations
  - Computing centroids: Each instance vector gets added once to some centroid: $O(n)$
- Assume these two steps are each done once for I iterations: $O(Ikn)$.
- Linear in all relevant factors, assuming a fixed number of iterations, more efficient than $O(n^2)$ HAC
- Does it always converge?

Impact of Initial Seeds

- Highly sensitive to the initial seeds



- Multiple random trials: choose the one with best sum of squared loss (important!)
- Heuristics for choosing better centers
  - choose initial centers to be far apart – furthest first traversal (K-Means++ algorithm)
  - Initialize with results of other clustering method

More Comments

- K-Means is exhaustive:
  - Cluster every data point, no notion of outlier
  - Outliers cause problems
    - Become singular clusters
    - Bias the centroid estimation
- K-medoids methods is more robust to outliers
  - Cluster medoid: the point that has minimum sum squared distance to all data points in the cluster
  - More expensive to compute
    - For each point: sum squared distance with all other pts in cluster $O(|C|^2)$
- Need to specify *k*: difficult in practice
  - Automatically deciding *k*? more on this later…

Soft Clustering

- Hard clustering:
  - Data point is deterministically assigned to one and only one cluster
  - But in reality clusters may overlap
- Soft-clustering:
  - Data points are assigned to clusters with certain probabilities
- Model-based clustering