Clustering

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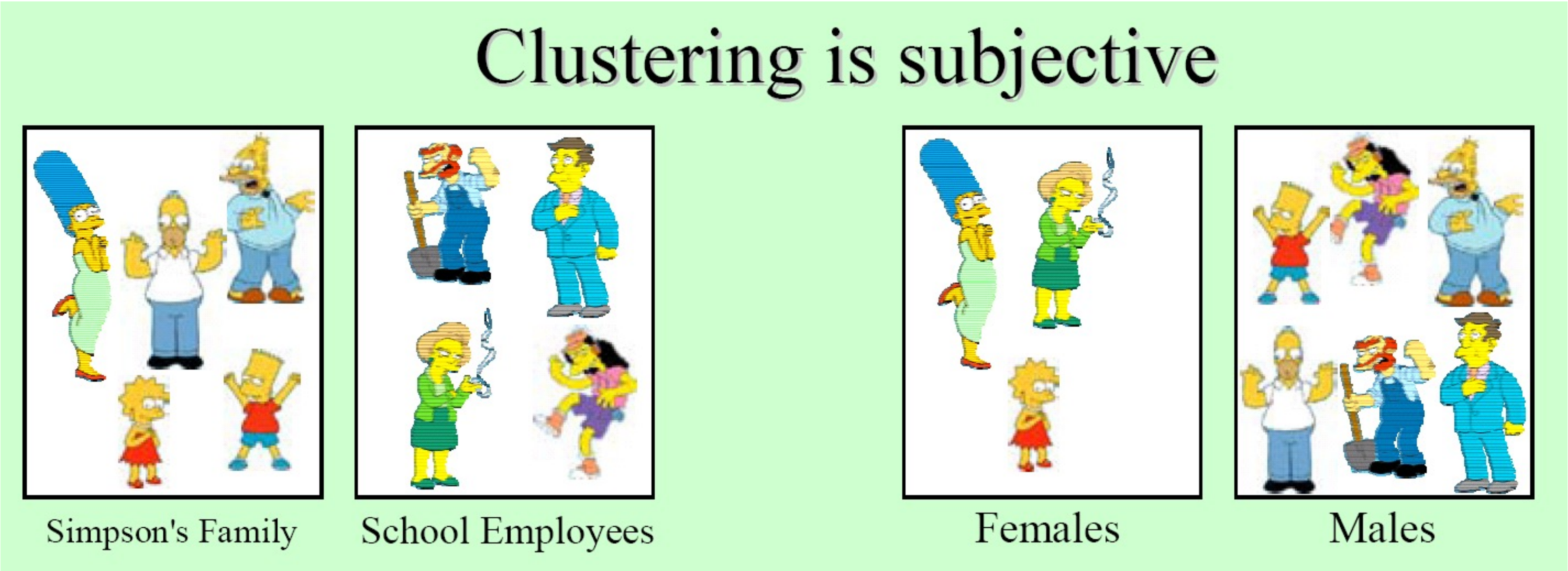
Some slides courtesy of Eric Xing, Carlos Guestrin

What is clustering?

- Clustering: the process of grouping a set of objects into classes of similar objects
  - high intra-class similarity
  - low inter-class similarity
  - It is the most common form of unsupervised learning



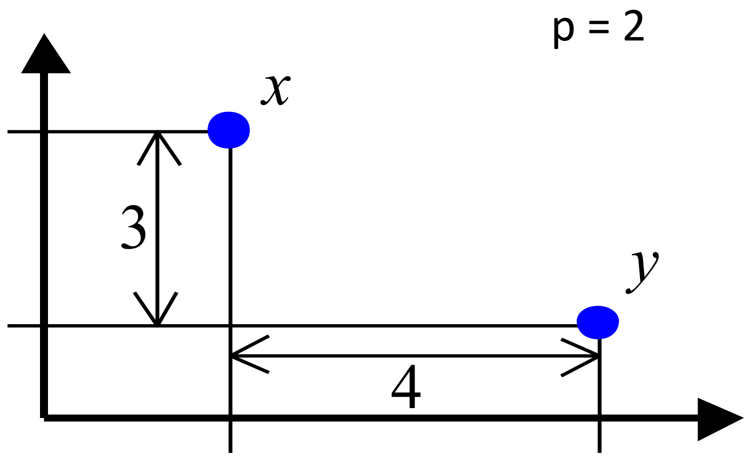
What is Similarity?

Hard to define! But *we know it when we see it*

- The real meaning of similarity is a philosophical question. We will take a more pragmatic approach - think in terms of a distance (rather than similarity) between vectors or correlations between random variables.

Distance metrics

$x = (x_1, x_2, \ldots, x_p)$
$y = (y_1, y_2, \ldots, y_p)$



Euclidean distance $$d(x,y) = \sqrt[2]{\sum_{i=1}^{p} |x_i - y_i|^2}$$ **5**

Manhattan distance $$d(x,y) = \sum_{i=1}^{p} |x_i - y_i|$$ **7**

Sup-distance $$d(x,y) = \max_{1 \le i \le p} |x_i - y_i|$$ **4**

Correlation coefficient

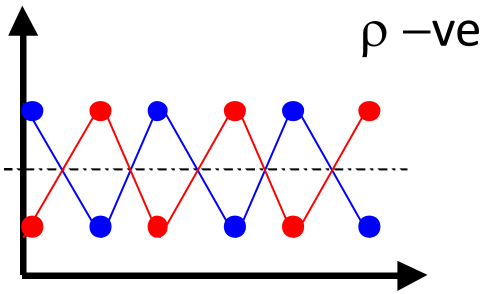
$x = (x_1, x_2, \ldots, x_p)$
$y = (y_1, y_2, \ldots, y_p)$

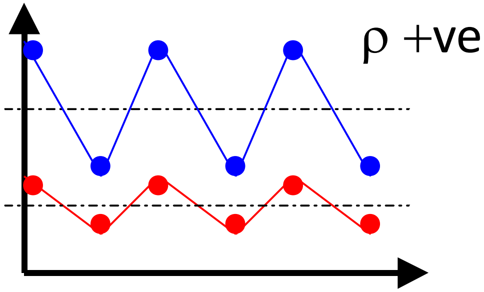
Random vectors (e.g. expression levels of two genes under various drugs)

Pearson correlation coefficient

$$\rho(x,y) = \frac{\sum_{i=1}^{p} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{p} (x_i - \bar{x})^2 \times \sum_{i=1}^{p} (y_i - \bar{y})^2}}$$

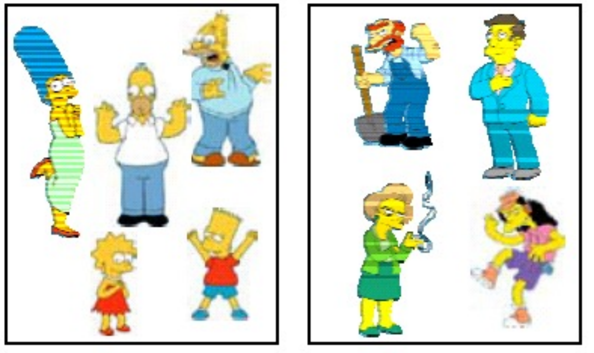
where $\bar{x} = \frac{1}{p}\sum_{i=1}^{p} x_i$ and $\bar{y} = \frac{1}{p}\sum_{i=1}^{p} y_i$.



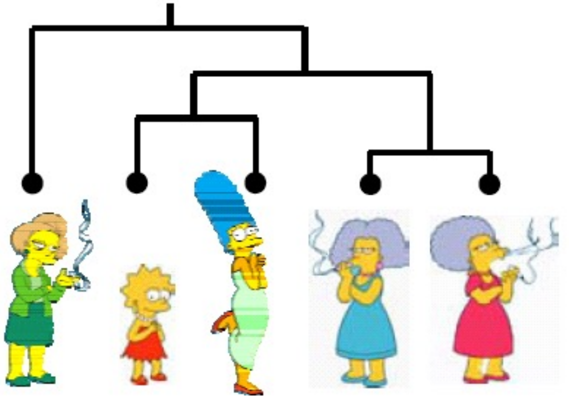


Clustering Algorithms

- **Partition algorithms**
  - K means clustering
  - Mixture-Model based clustering



- Hierarchical algorithms
  - Single-linkage
  - Average-linkage
  - Complete-linkage
  - Centroid-based



Partitioning Algorithms

- Partitioning method: Construct a partition of n objects into a set of K clusters
- Given: a set of objects and the number K
- Find: a partition of K clusters that optimizes the chosen partitioning criterion
  - Globally optimal: exhaustively enumerate all partitions
  - Effective heuristic method: K-means algorithm

K-Means

Algorithm

Input – Desired number of clusters, *k*

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

Iterate –

1. Assign points to the nearest cluster centers

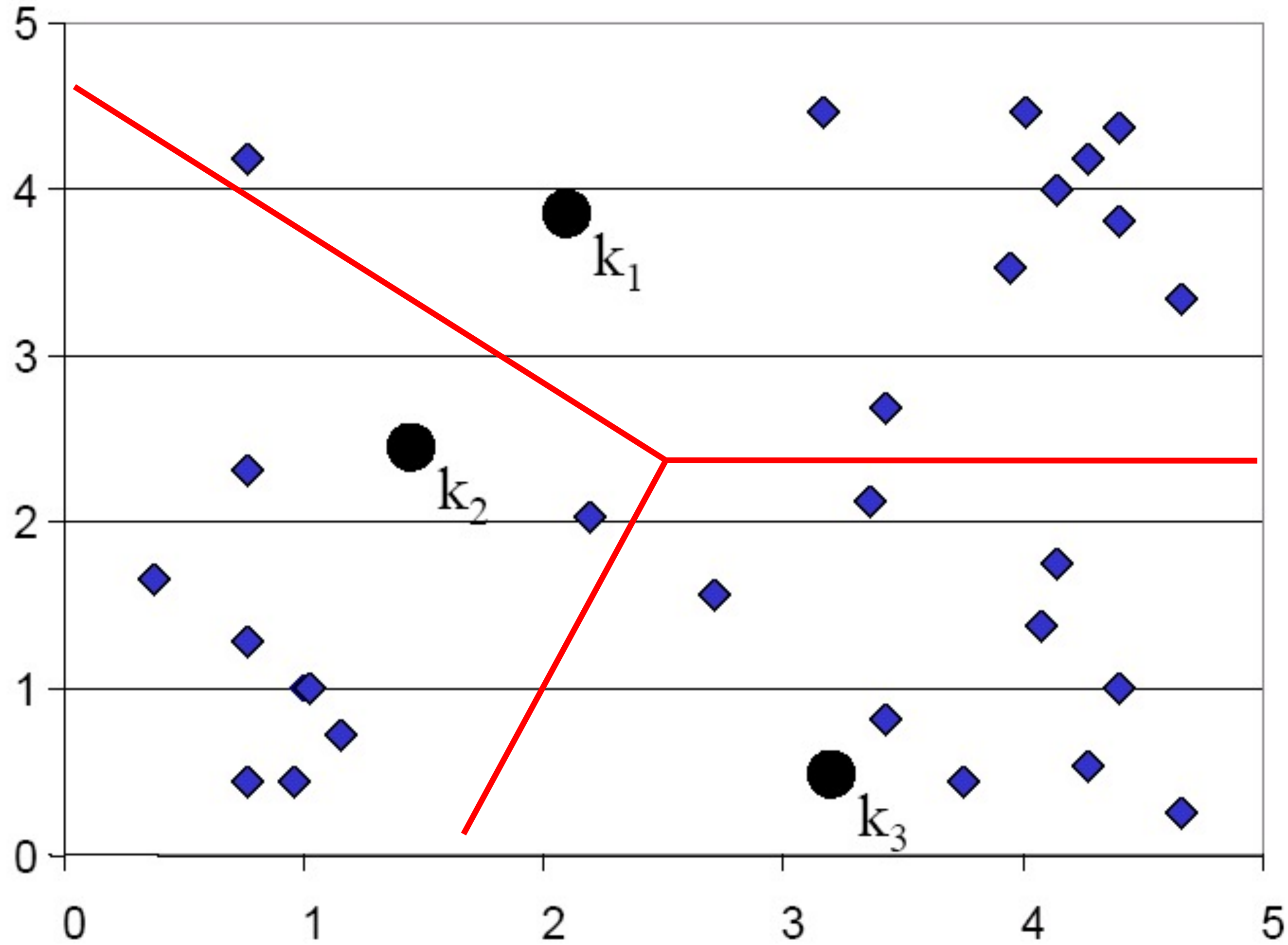
2. Re-estimate the *k* cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

$$\vec{\mu}_k = \frac{1}{\mathcal{C}_k} \sum_{i \in \mathcal{C}_k} \vec{x}_i$$

Termination –

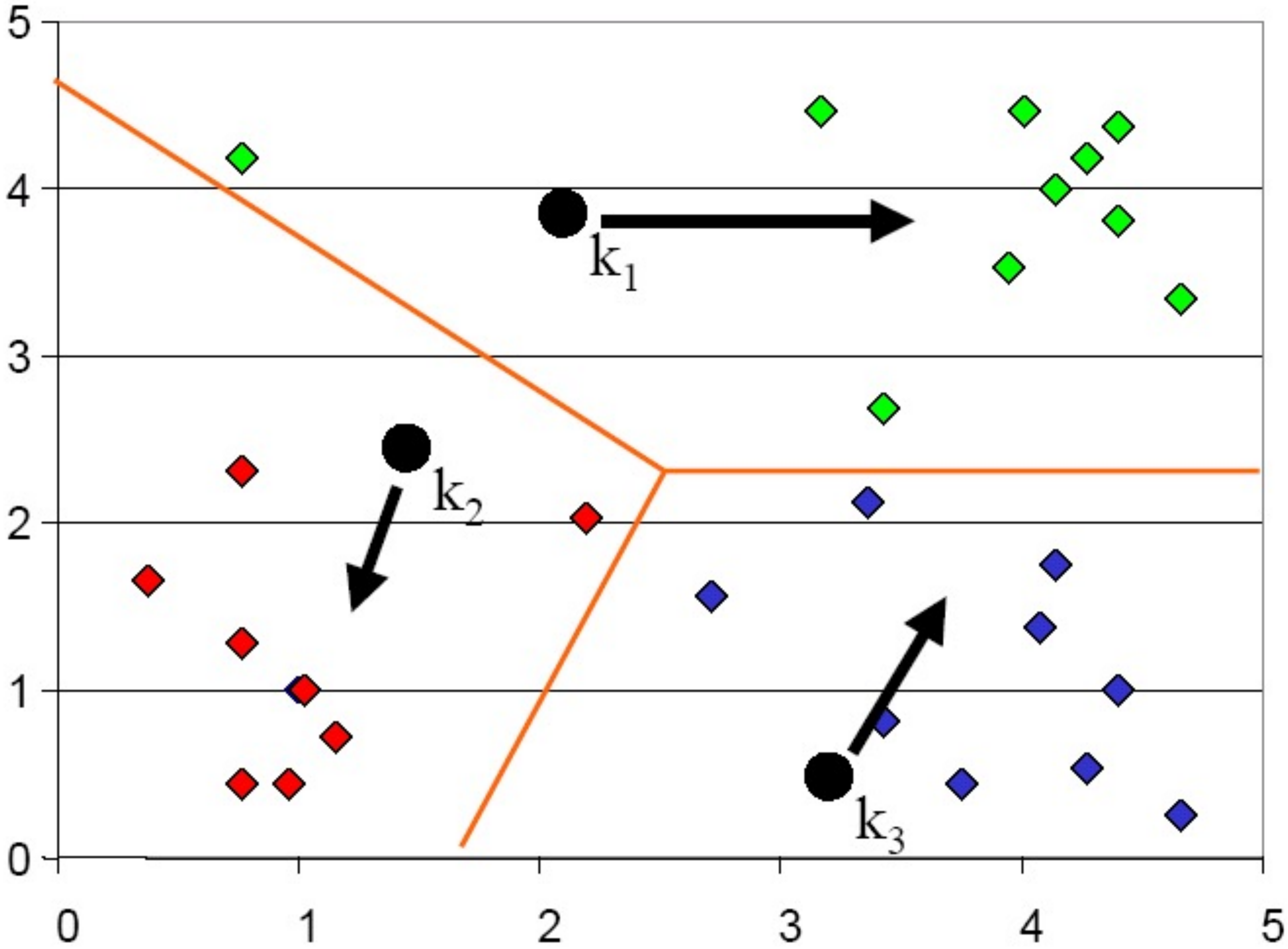
If none of the objects changed membership in the last iteration, exit. Otherwise go to 1.

K-means Clustering: Step 1

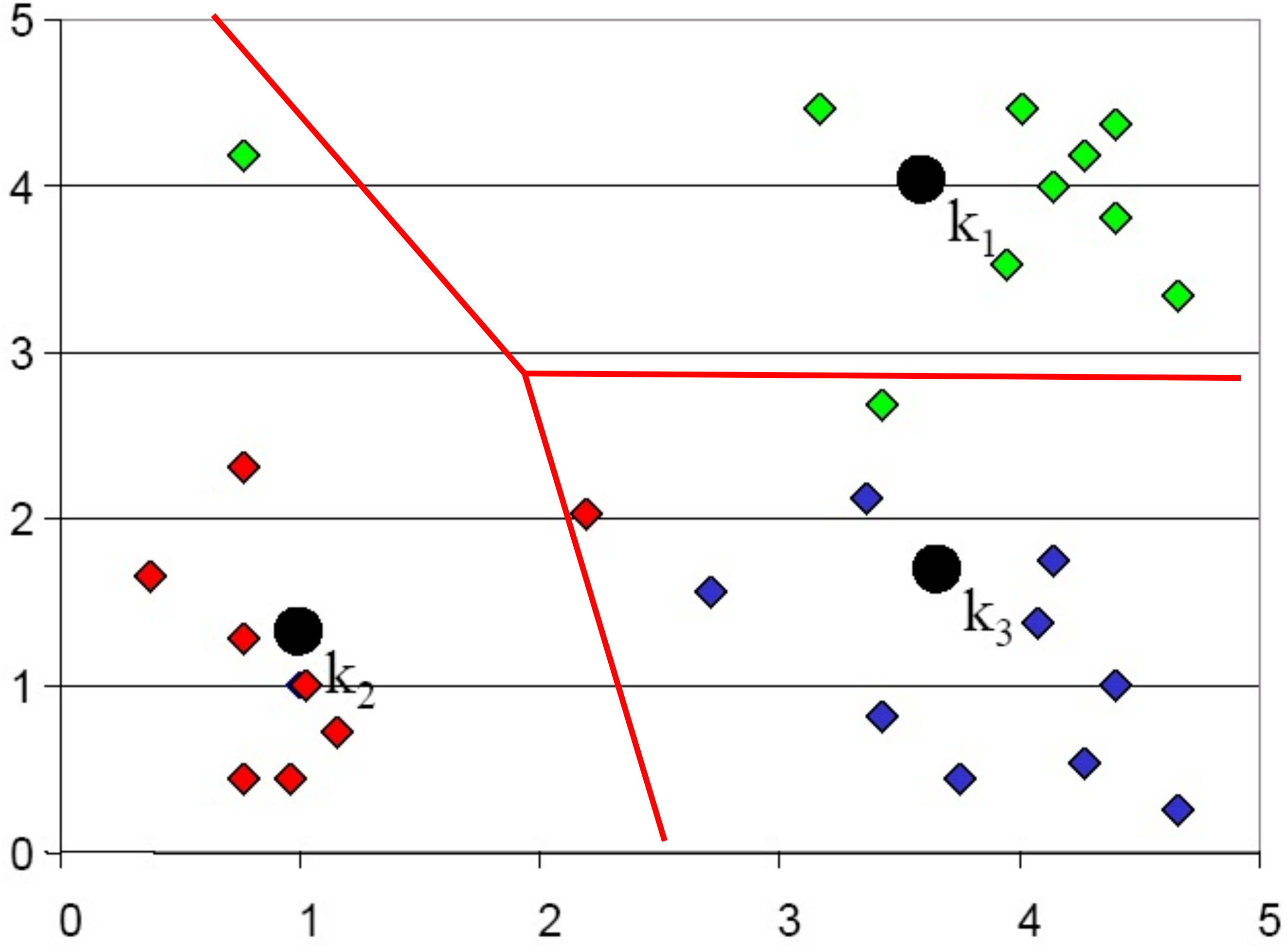


Voronoi diagram

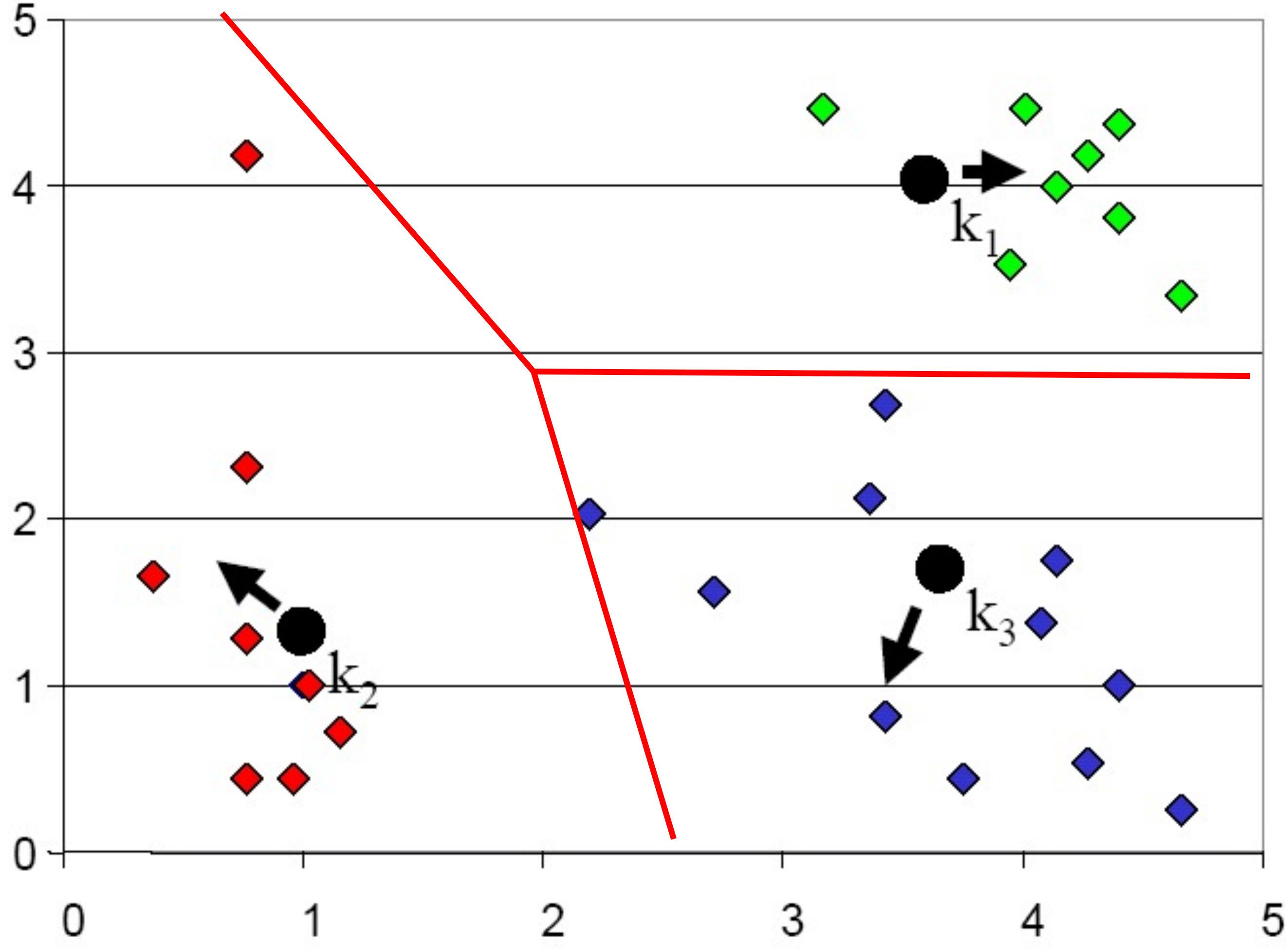
K-means Clustering: Step 2



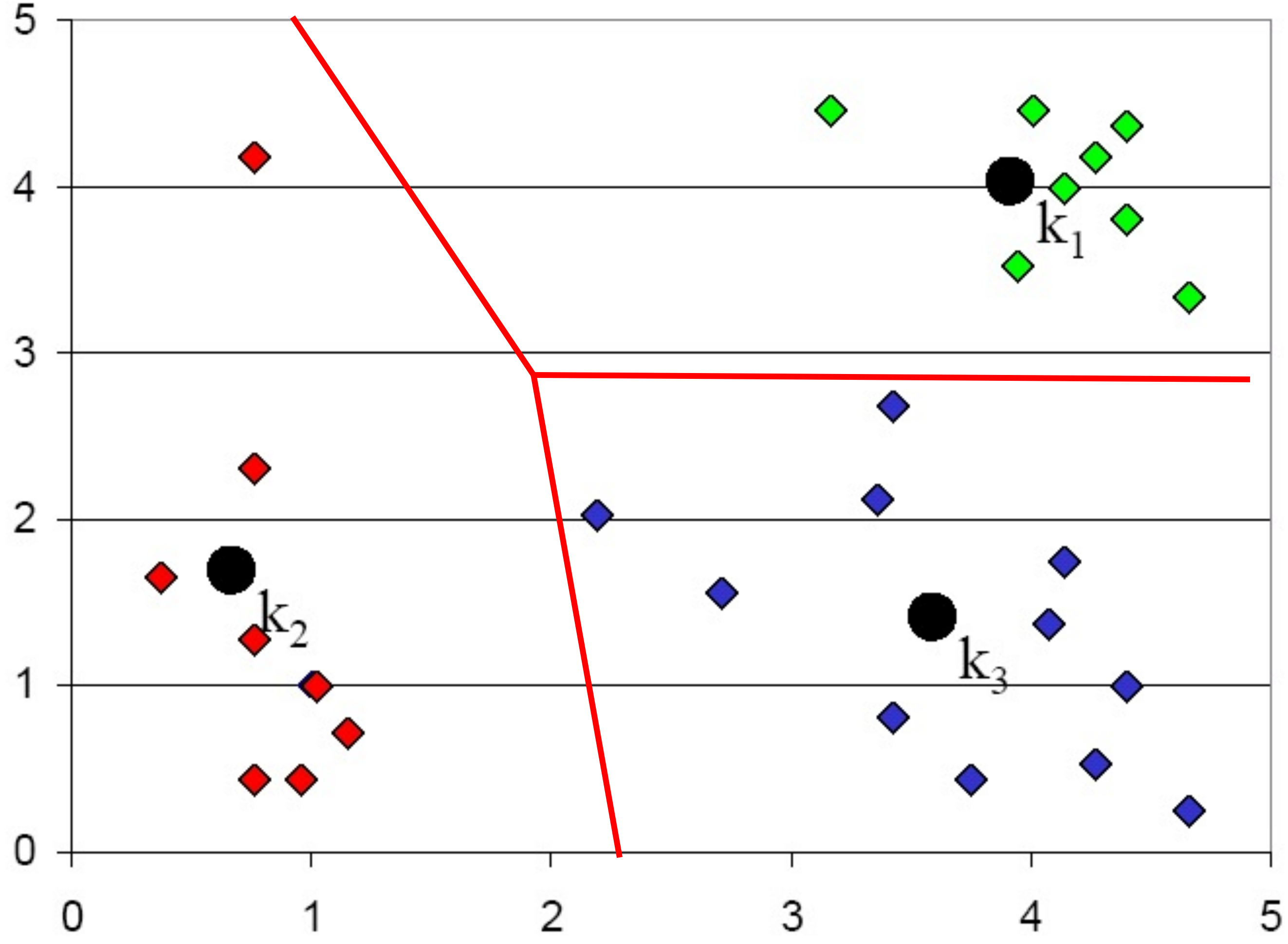
K-means Clustering: Step 3



K-means Clustering: Step 4



K-means Clustering: Step 5



K-means Recap …

- Randomly initialize *k* centers
  - $\mu^{(0)} = \mu_1^{(0)}, \ldots, \mu_k^{(0)}$

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Iterate t = 0, 1, 2, …

- **Classify**: Assign each point $j \in \{1, \ldots m\}$ to nearest center:
  - $C^{(t)}(j) \leftarrow \arg \min_{i=1,\ldots,k} \|\mu_i^{(t)} - x_j\|^2$

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  - $$C^{(t)}(j) \leftarrow \arg \min_{i=1,\ldots,k} \|\mu_i^{(t)} - x_j\|^2$$
- **Recenter**: μ_i becomes centroid of its points:
  - $$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C^{(t)}(j)=i} \|\mu - x_j\|^2 \qquad i \in \{1, \ldots, k\}$$
  - Equivalent to $\mu_i \leftarrow$ average of its points!

What is K-means optimizing?

- Potential function F(μ,C) of centers **μ** and point allocations C:

$$F(\mu, C) = \sum_{j=1}^{m} ||\mu_{C(j)} - x_j||^2$$

$$= \sum_{i=1}^{k} \sum_{j:C(j)=i} ||\mu_i - x_j||^2$$

- Optimal K-means:
  - $\min_{\mu} \min_{C} F(\mu, C)$

➢ Is the K-means objective convex?

K-means algorithm

- Optimize potential function:

$$\min_{\mu} \min_{C} F(\mu, C) = \min_{\mu} \min_{C} \sum_{i=1}^{k} \sum_{j:C(j)=i} ||\mu_i - x_j||^2$$

- **K-means algorithm:** (coordinate descent on F)

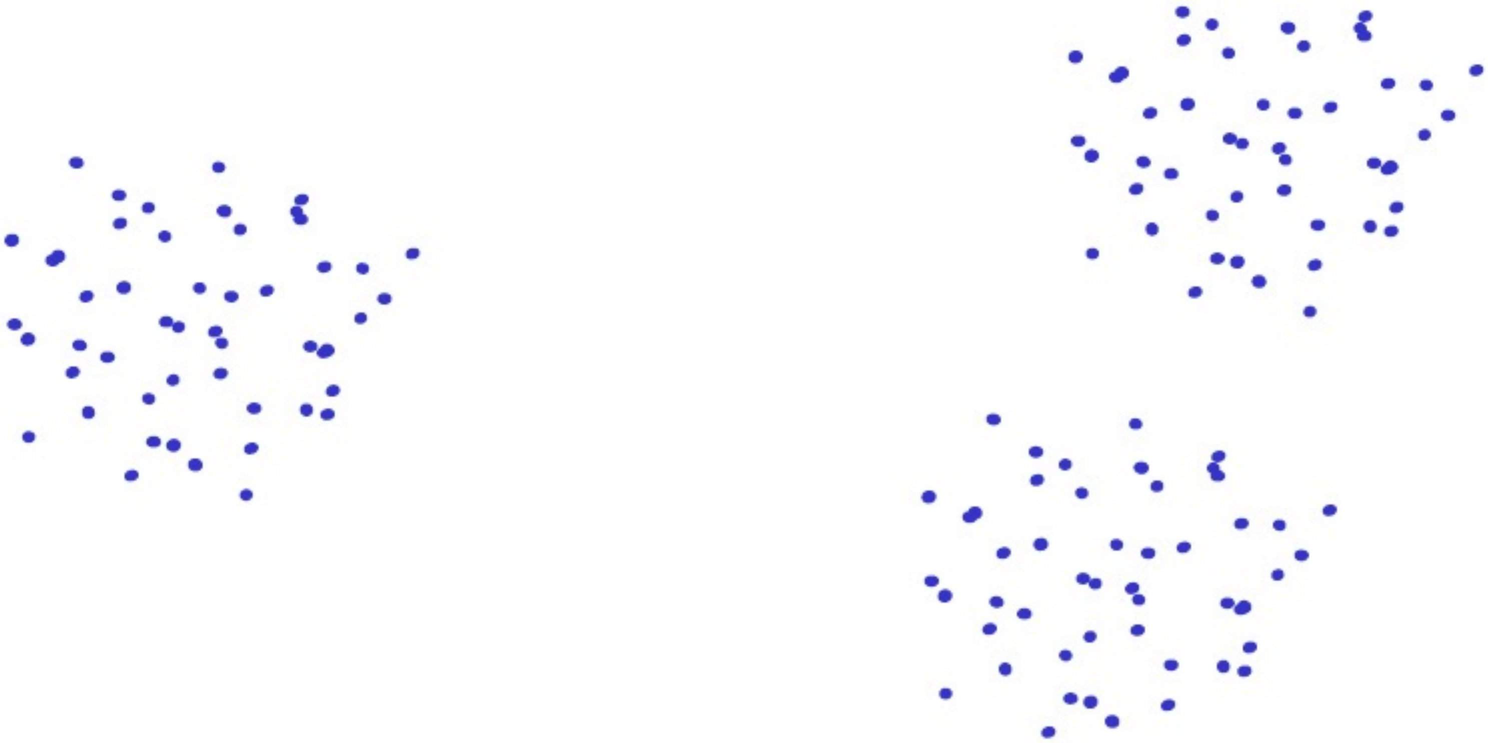
(1) Fix μ, optimize C — **Expected** cluster assignment

(2) Fix C, optimize μ — **Maximum** likelihood for center

Generalization: EM (Expectation-Maximization) algorithm

Seed Choice

- Results are quite sensitive to seed selection.



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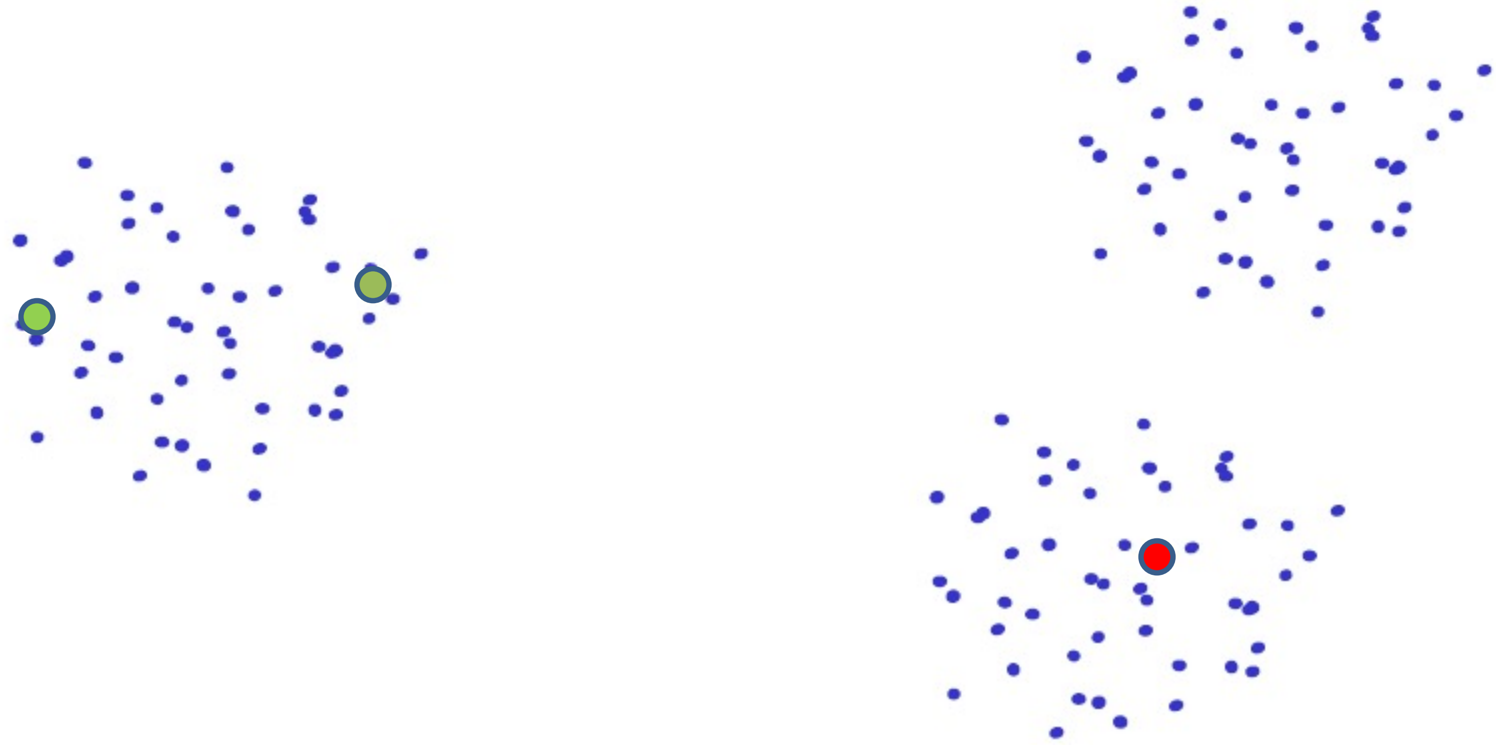

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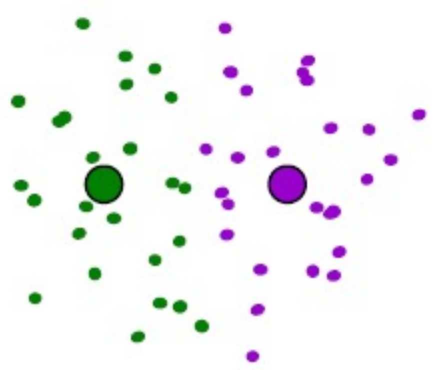
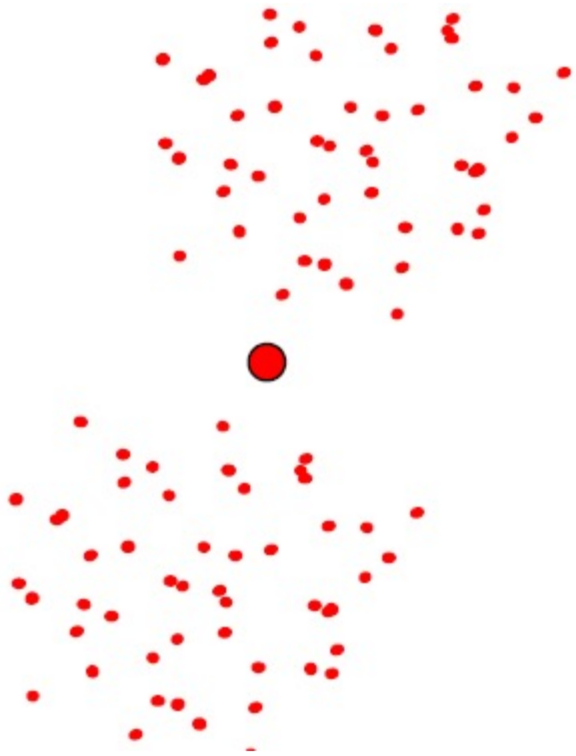




Seed Choice

- Results can vary based on random seed selection.

- Some seeds can result in poor convergence rate, or convergence to sub-optimal clustering.
  - Try out multiple starting points (very important!!!)
  - k-means ++ algorithm of Arthur and Vassilvitskii

    key idea: choose centers that are far apart

    (probability of picking a point as cluster center $\propto$ distance from nearest center picked so far)

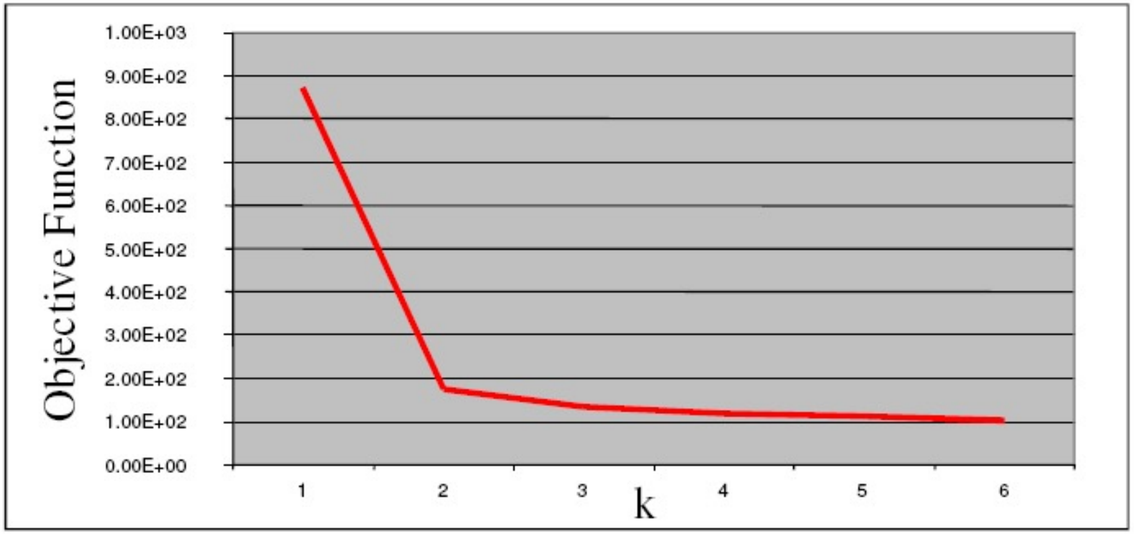
Other Issues

- Number of clusters K
  - Objective function

$$\sum_{j=1}^{m} ||\mu_{C(j)} - x_j||^2$$

➢ Can you pick K by minimizing the objective over K?

  - Look for "Knee" in objective function



Other Issues

- Sensitive to Outliers
  - use K-medoids

- Shape of clusters

  Assumes isotropic, equal variance, convex clusters

Partitioning Algorithms

- K-means
  - **hard assignment**: each object belongs to only one cluster
- Mixture modeling
  - **soft assignment**: probability that an object belongs to a cluster

Generative approach