Clustering

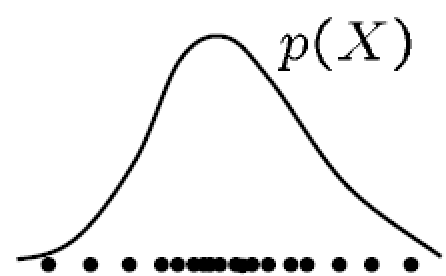
Unsupervised Learning

"Learning from unlabeled/unannotated data" (without supervision)

Training data $\{X_i\}_{i=1}^n$ → **Learning algorithm** → Prediction rule $\widehat{f}_n$

What can we predict from unlabeled data?

- Density estimation



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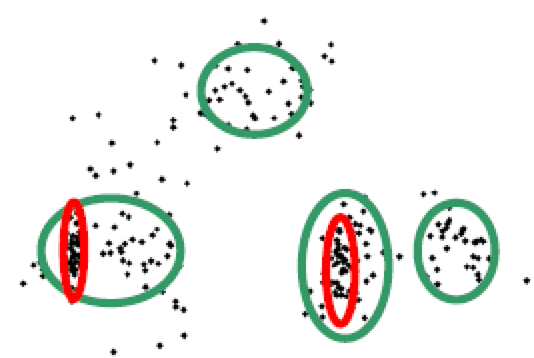

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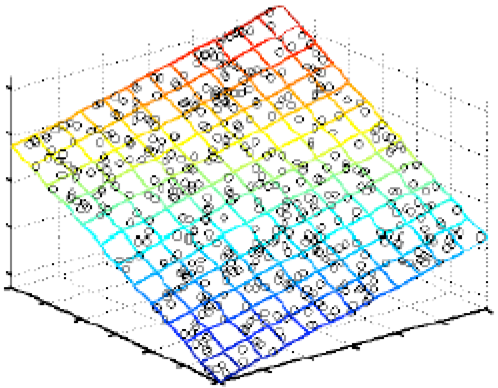
What can we predict from unlabeled data?

- Density estimation
- Groups or clusters in the data
- Low-dimensional structure
    - Principal Component Analysis (PCA) (linear)



Unsupervised Learning

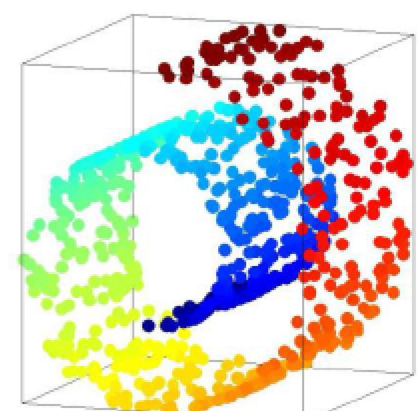
"Learning from unlabeled/unannotated data" (without supervision)

Training data $\{X_i\}_{i=1}^n$ ⇒

⇒ Prediction rule $\widehat{f}_n$

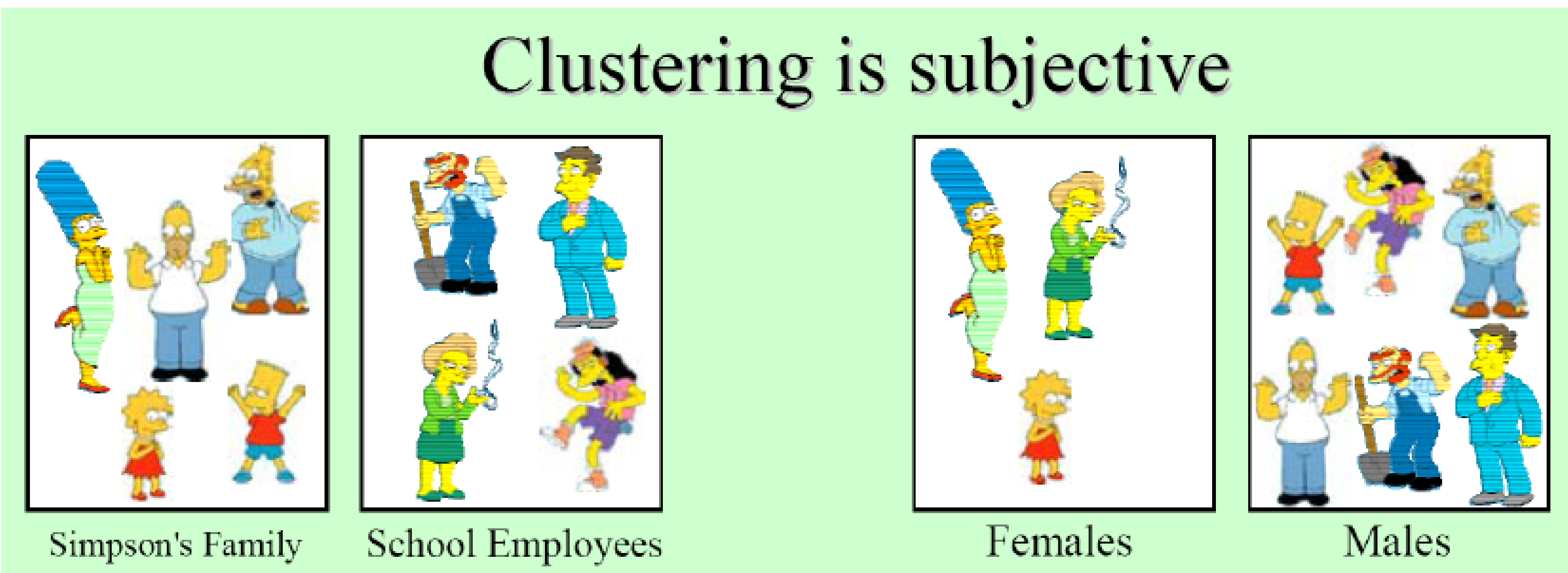
What can we predict from unlabeled data?

- Density estimation
- Groups or clusters in the data
- Low-dimensional structure
  - Principal Component Analysis (PCA) (linear)
  - Manifold learning (non-linear)



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 commonest form of unsupervised learning



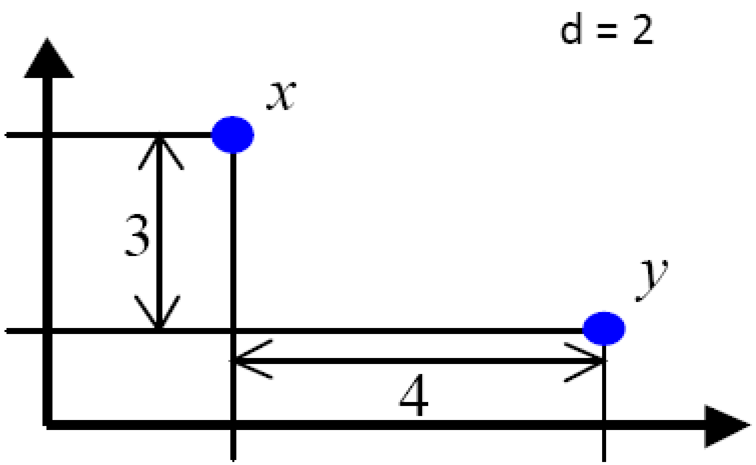
What is similarity?

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

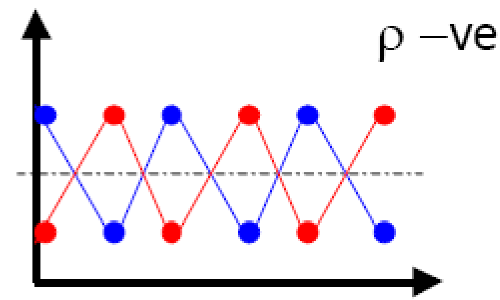
$x = (x_1, x_2, \ldots, x_p)$
$y = (y_1, y_2, \ldots, y_p)$

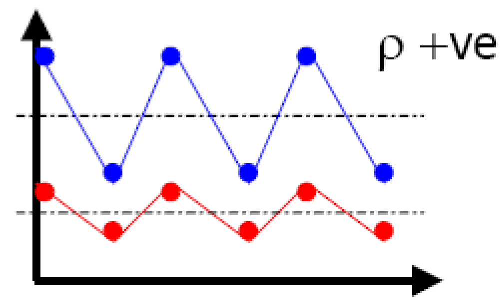
Random vectors (e.g. expression levels of two genes under various drugs)

Pearson correlation coefficient

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

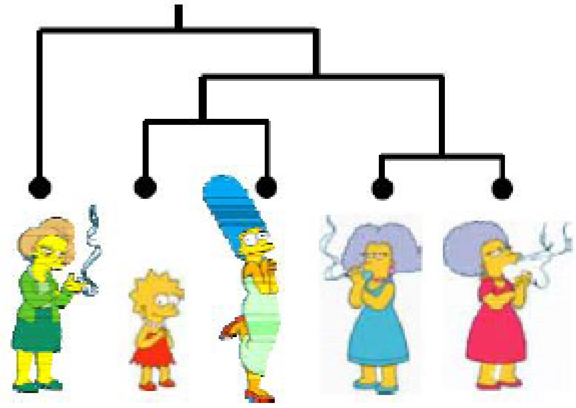
$$\text{where } \bar{x} = \frac{1}{p}\sum_{i=1}^{p} x_i \text{ and } \bar{y} = \frac{1}{p}\sum_{i=1}^{p} y_i.$$



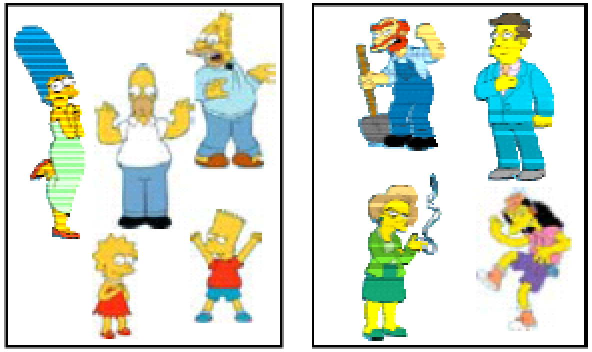


Clustering Algorithms

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



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



Hierarchical Clustering

- Bottom-Up Agglomerative Clustering

  Starts with each object in a separate cluster, and repeat:

  – Joins the most similar pair of clusters,

  – Update the similarity of the new cluster to other clusters

  until there is only one cluster.

  Greedy - less accurate but simple, typically computationally expensive

- Top-Down divisive

  Starts with all the data in a single cluster, and repeat:

  – Split each cluster into two using a partition based algorithm

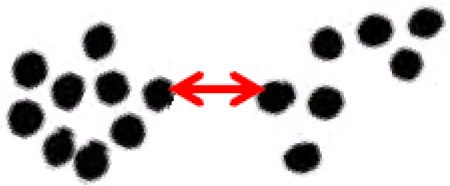
  Until each object is a separate cluster.

  More accurate but complex, can be computationally cheaper

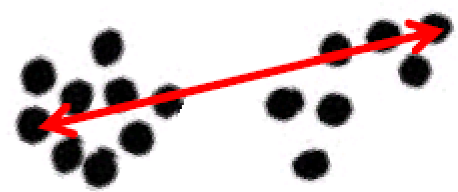
Bottom-up Agglomerative Clustering

Different algorithms differ in how the similarities are defined (and hence updated) between two clusters

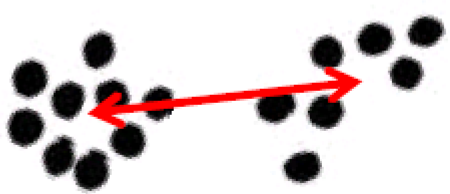
- Single-Link
  - Nearest Neighbor: similarity between their closest members.



- Complete-Link
  - Furthest Neighbor: similarity between their furthest members.



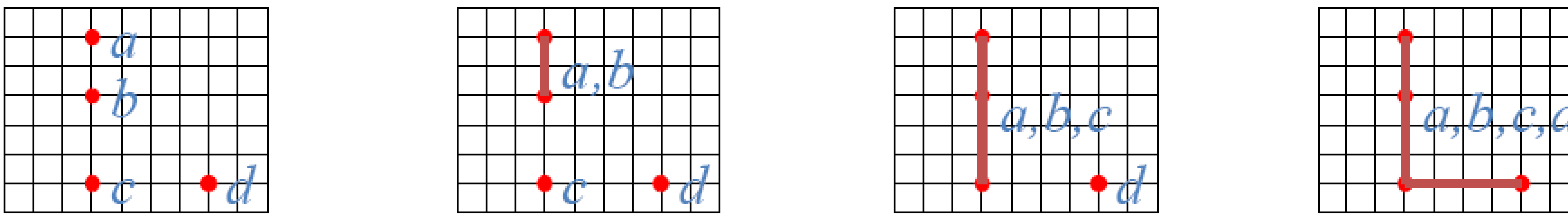
- Centroid
  - Similarity between the centers of gravity



- Average-Link
  - Average similarity of all cross-cluster pairs.

Single-Link Method

Euclidean Distance



(1) (2) (3)

	b	c	d
a	2	5	6
b		3	5
c			4

	b	c	d
a	2	5	6
b		3	5
c			4

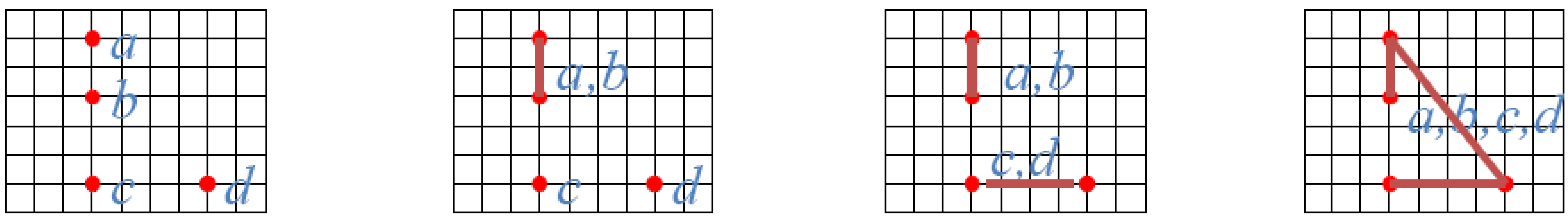
	c	d
a,b	3	5
c		4

	d
a,b,c	4

Distance Matrix

Complete-Link Method

Euclidean Distance



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	b	c	d
a	2	5	6
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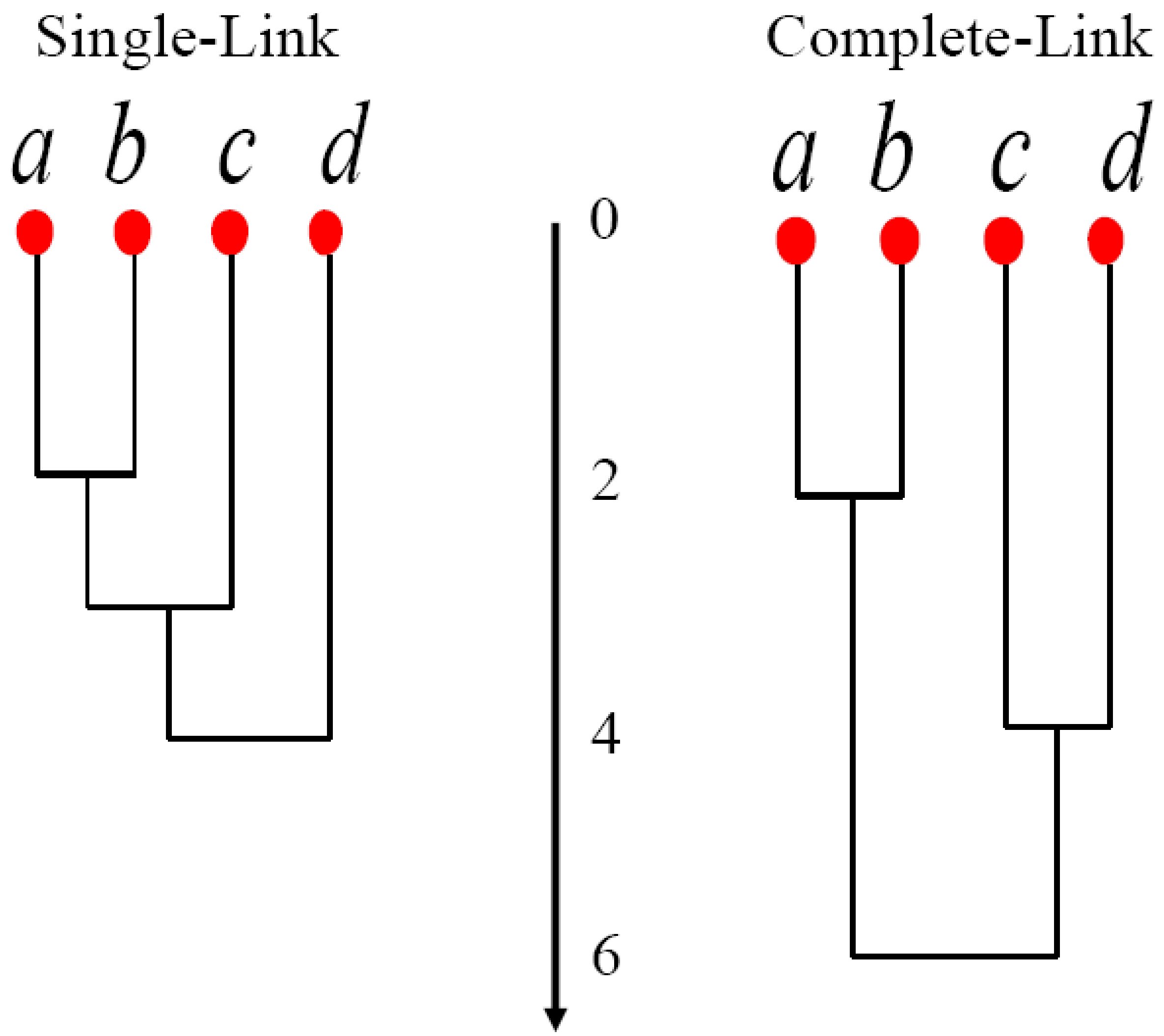
c			4

	c	d
a, b	5	6
c		4

	c, d
a, b	6

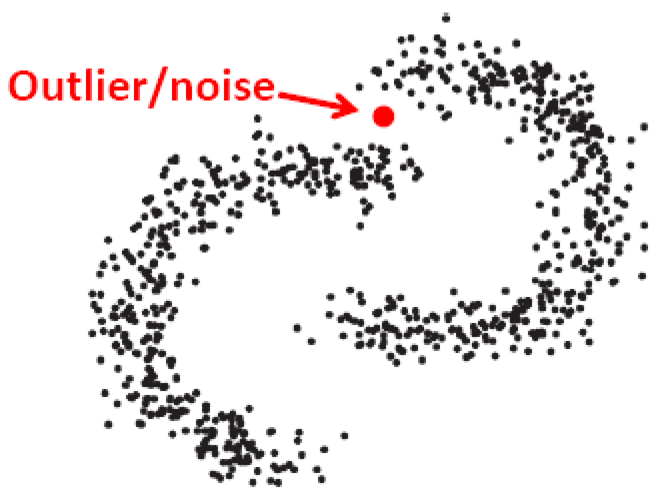
Distance Matrix

Dendrograms



Single vs. Complete Linkage

	Shape of clusters	Outliers
Single-linkage	allows anisotropic and non-convex shapes	sensitive to outliers
Complete-linkage	assumes isotopic, convex shapes	robust to outliers



Computational Complexity

- All hierarchical clustering methods need to compute similarity of all pairs of *n* individual instances which is $O(n^2)$.
- At each iteration,
  - Sort similarities to find largest one $O(n^2 \log n)$.
  - Update similarity between merged cluster and other clusters.
- In order to maintain an overall $O(n^2)$ performance, computing similarity to each other cluster must be done in constant time.
- So we get $O(n^2 \log n)$ or $O(n^3)$

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 Clustering

Algorithm

Input – Desired number of clusters, *k*

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

Iterate –

1. Decide the class memberships of the *N* objects by assigning them to the nearest cluster centers

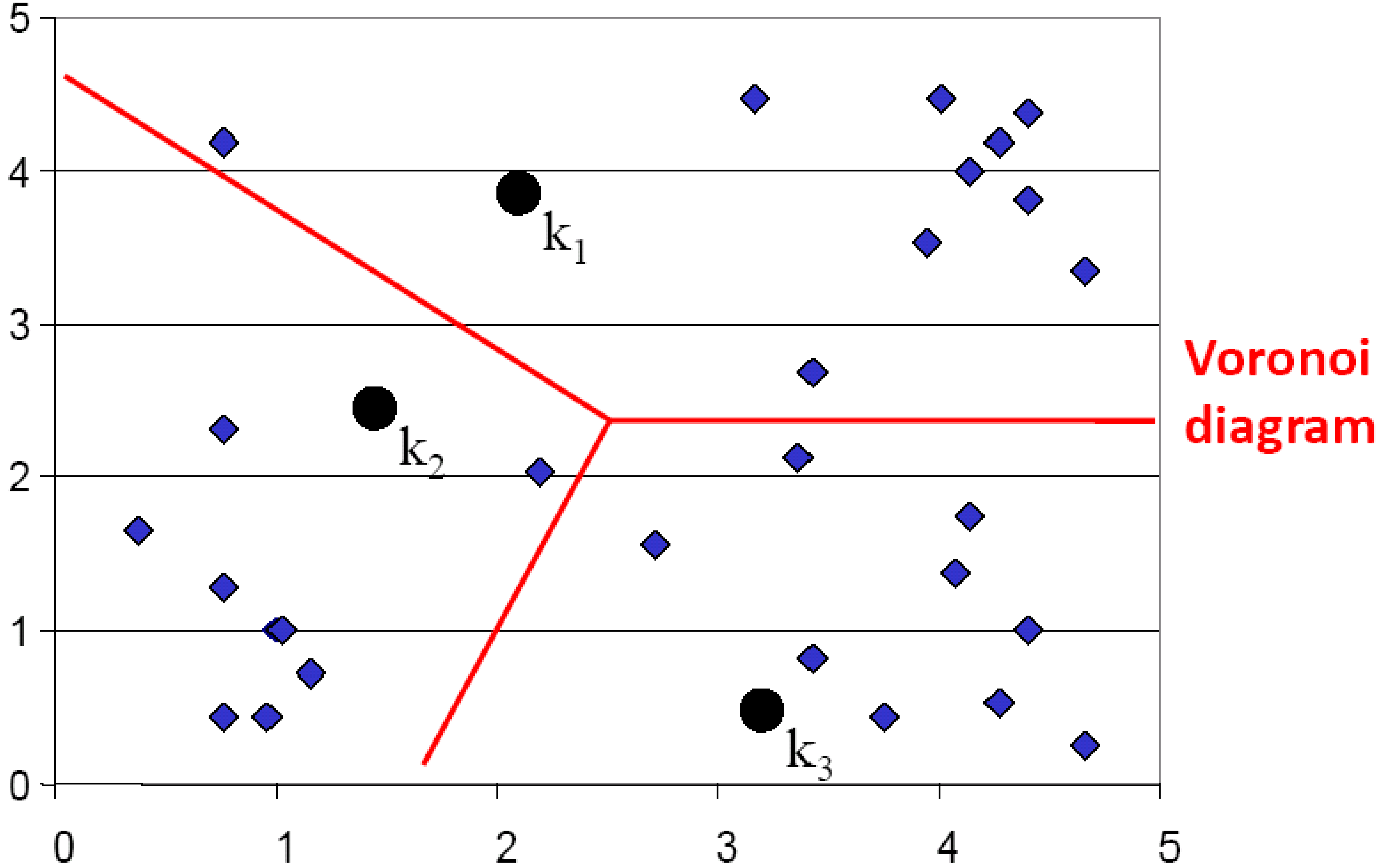
2. Re-estimate the *k* cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

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

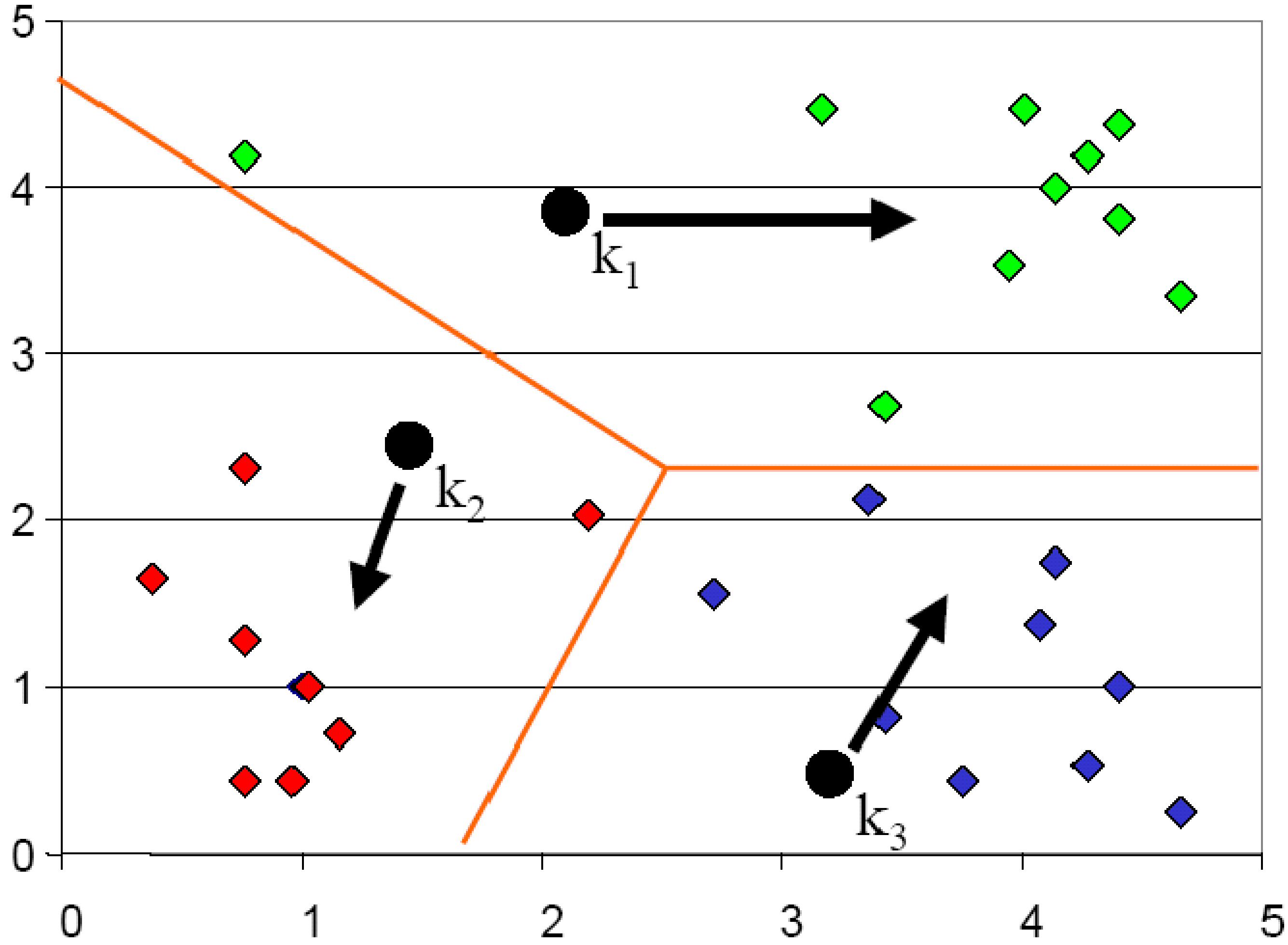
Termination –

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

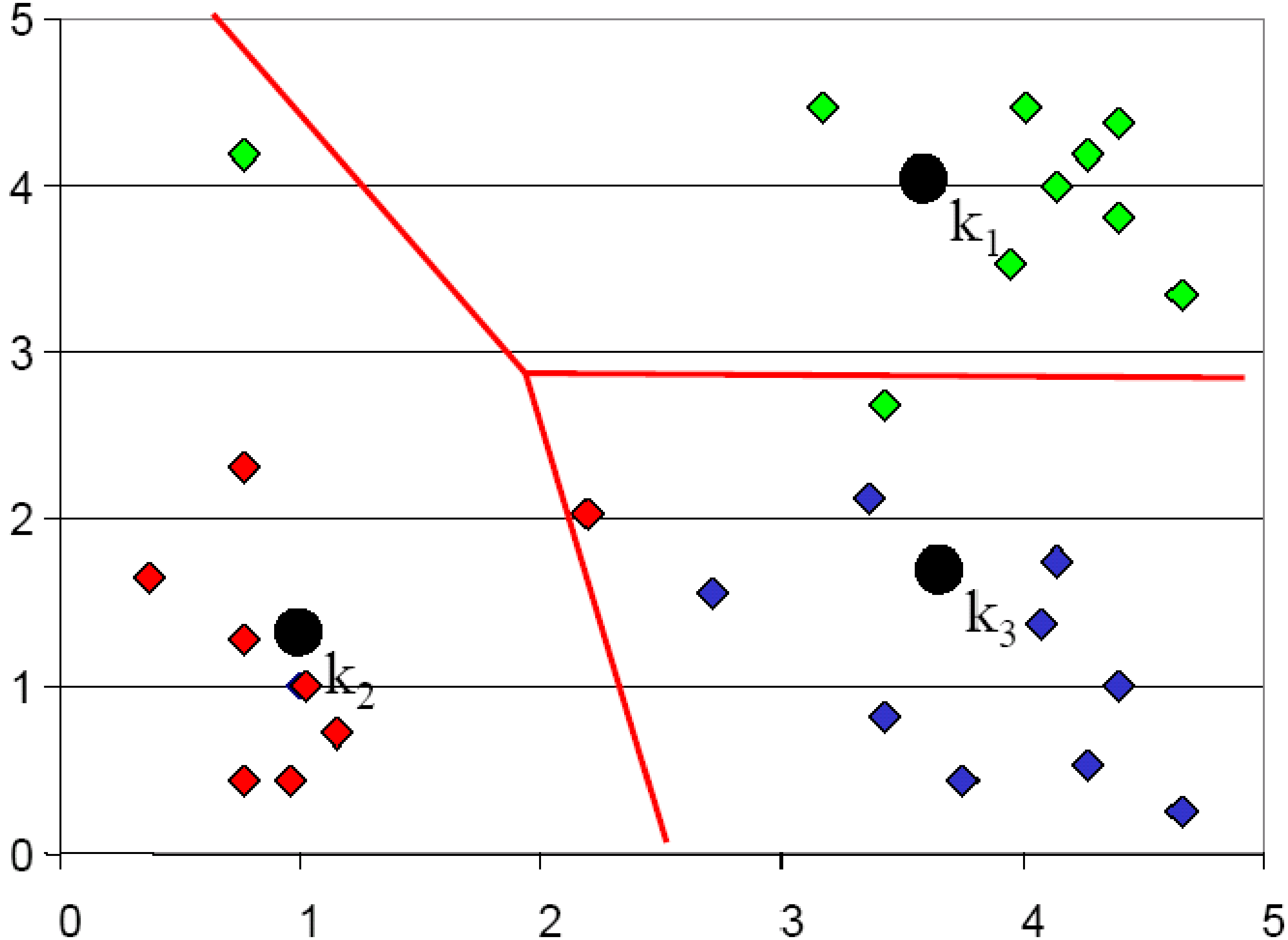
K-means Clustering: Step 1



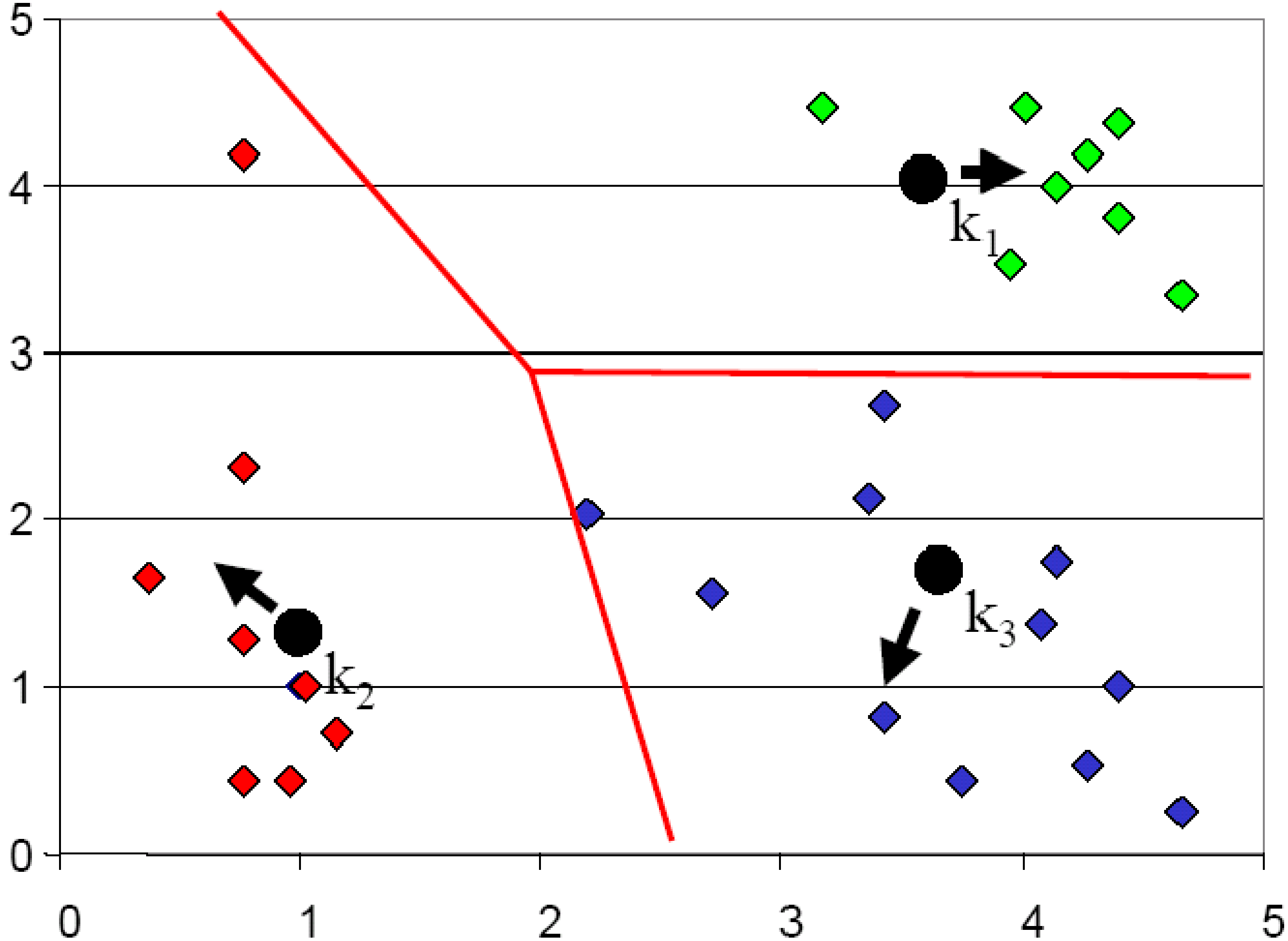
K-means Clustering: Step 2



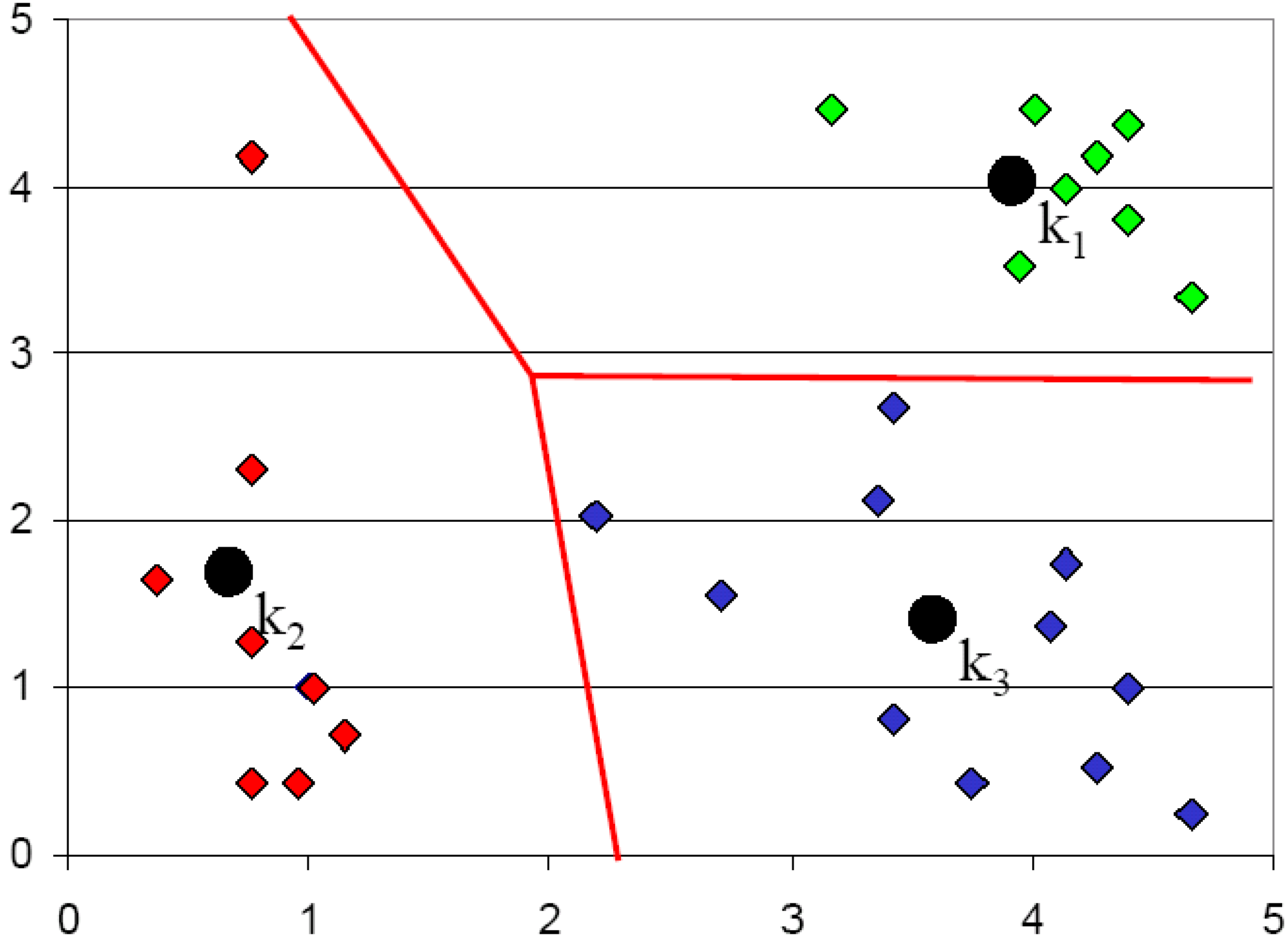
K-means Clustering: Step 3



K-means Clustering: Step 4



K-means Clustering: Step 5



Computational Complexity

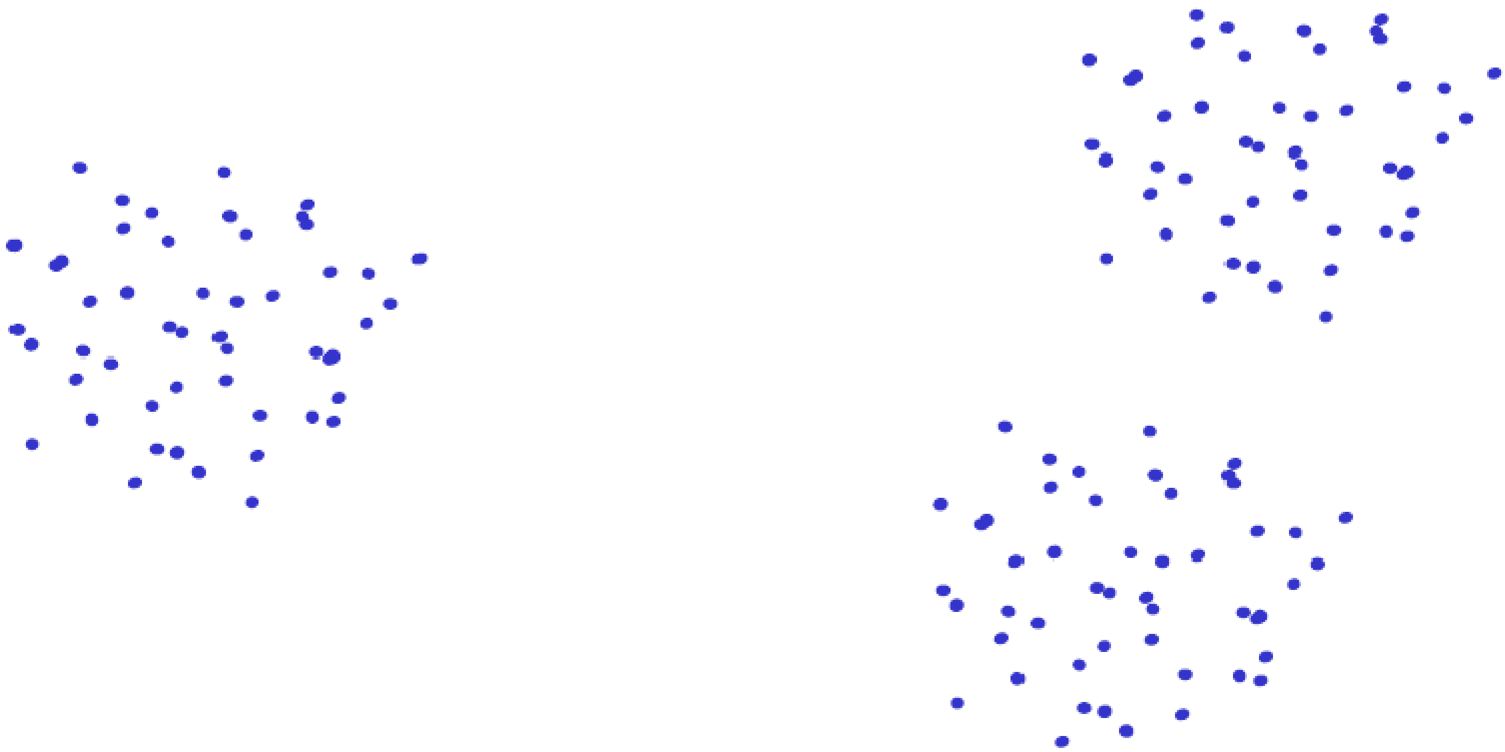
- At each iteration,
  - Computing distance between each of the n objects and the K cluster centers is $O(Kn)$.
  - Computing cluster centers: Each object gets added once to some cluster: $O(n)$.

- Assume these two steps are each done once for l iterations: $O(lKn)$.

- Is K-means guaranteed to converge?

Seed Choice

- Results are quite sensitive to seed selection.



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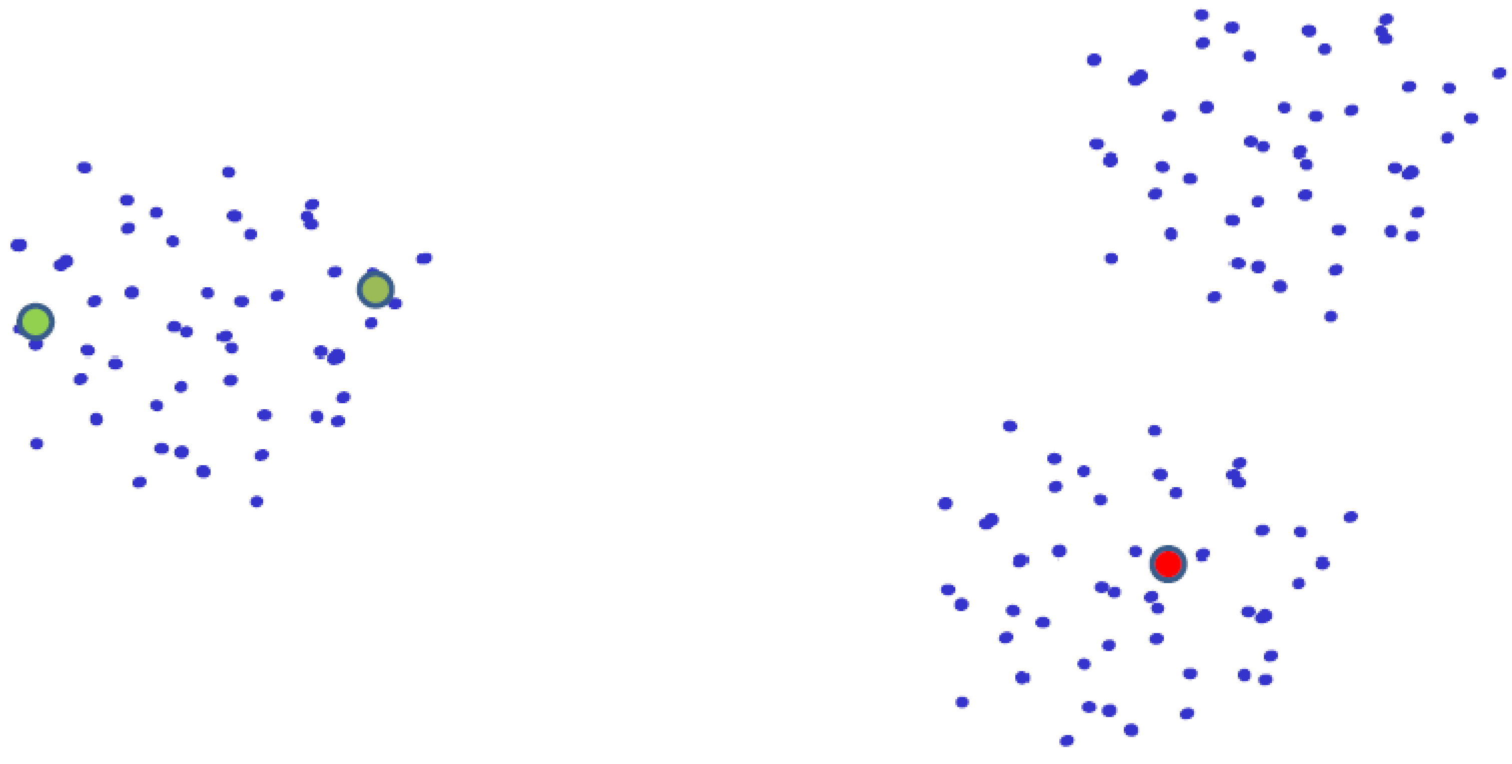

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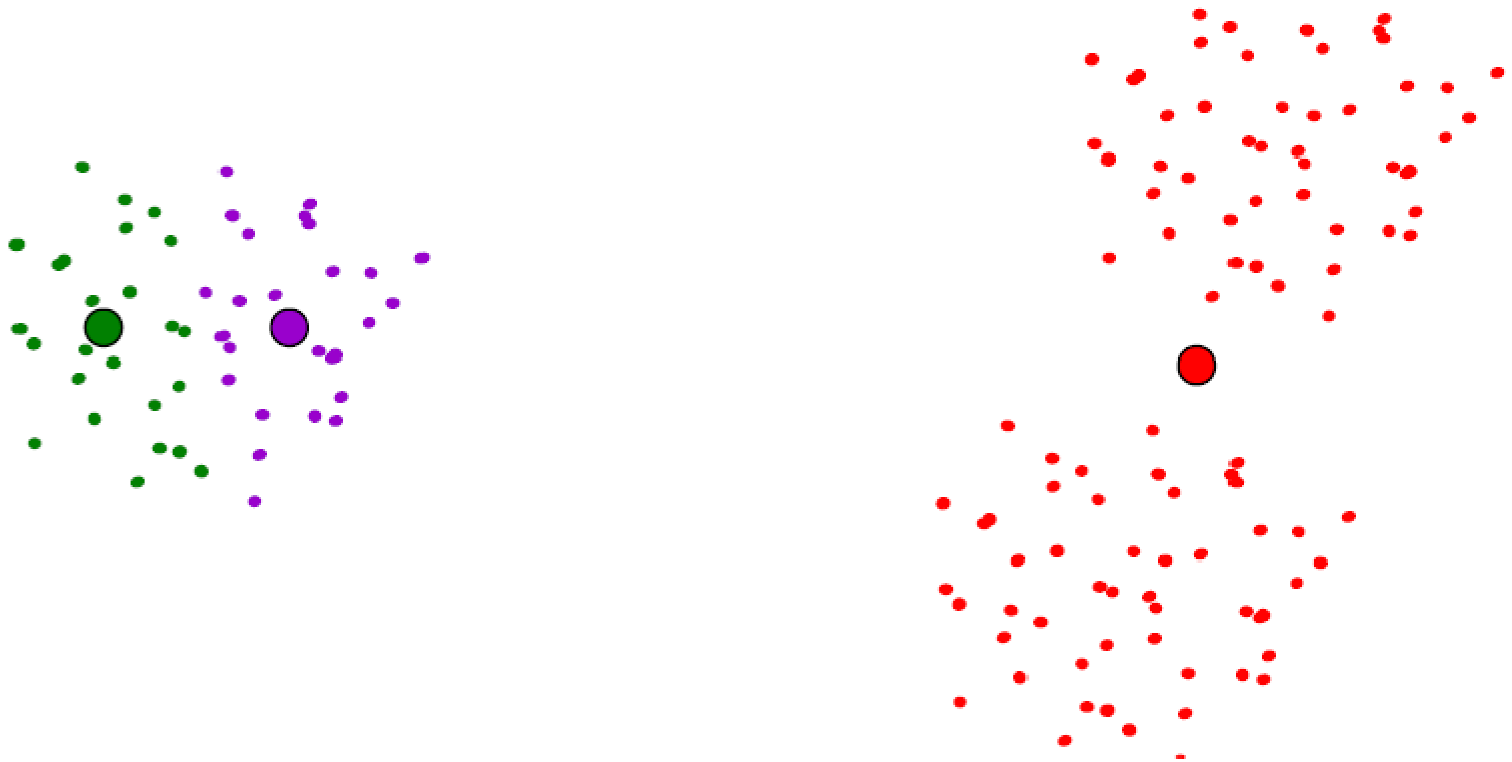
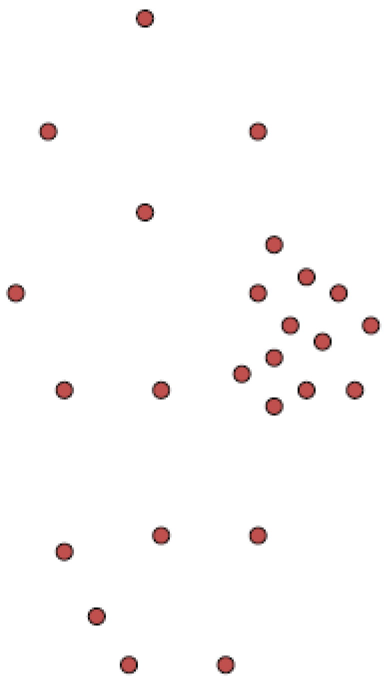


Seed Choice

- Results can vary based on random seed selection.

- Some seeds can result in poor convergence rate, or convergence to sub-optimal clustering.
  - Select good seeds using a heuristic (e.g., object least similar to any existing mean)
  - Try out multiple starting points (very important!!!)
  - Initialize with the results of another method.
  - Further reading: k-means ++ algorithm of Arthur and Vassilvitskii

Bad cases for K-means

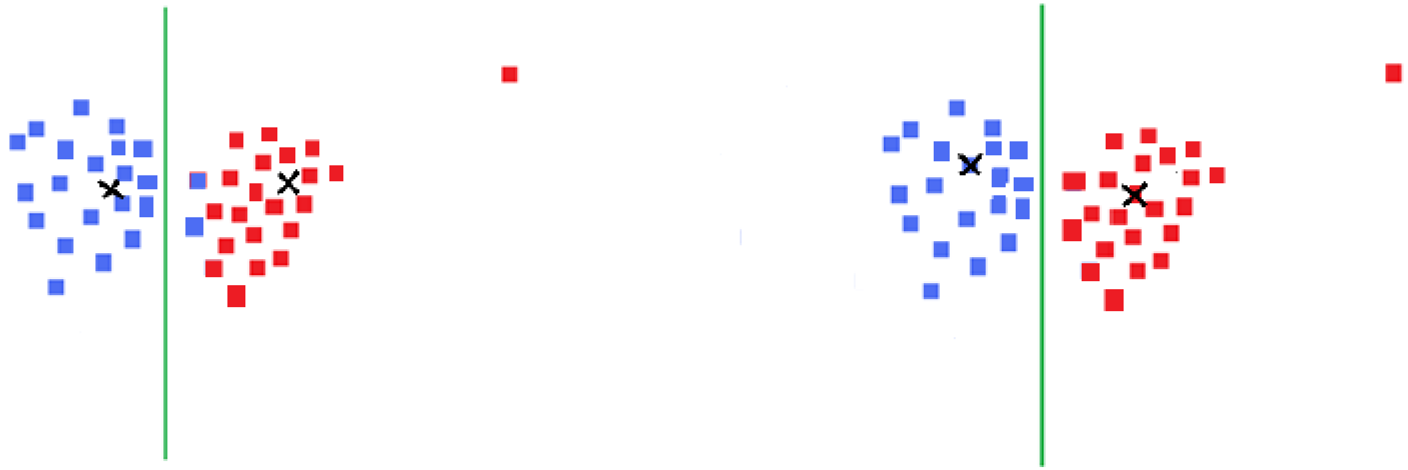


- Clusters may not be linearly separable
- Clusters may overlap
- Some clusters may be “wider” than others

Other Issues

- Shape of clusters
  - Assumes isotopic, convex clusters

- Sensitive to Outliers – use K-medoids

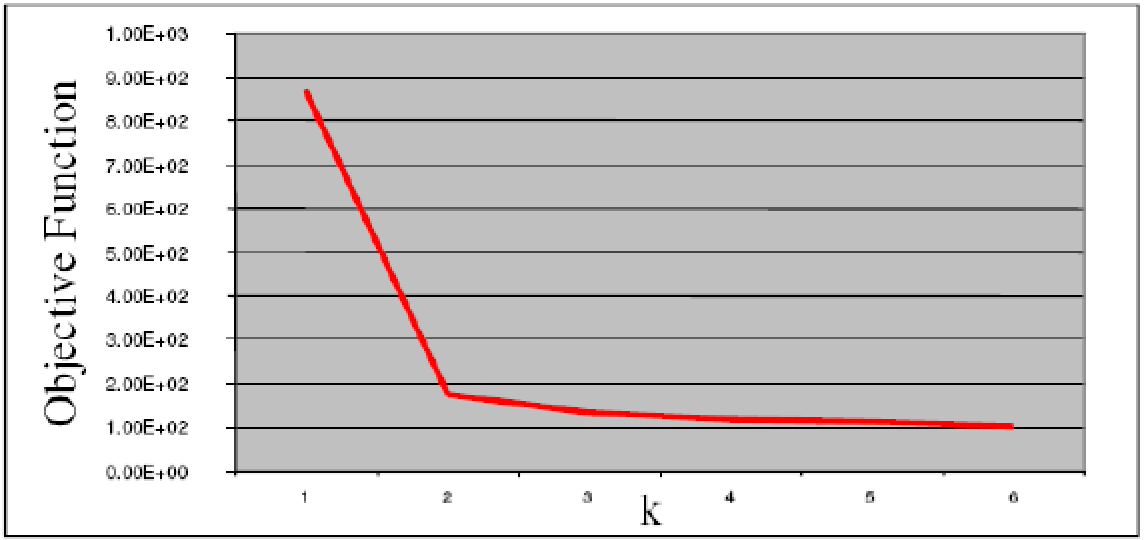


Other Issues

- Number of clusters K
  - Objective function

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

  - Look for "Knee" in objective function



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