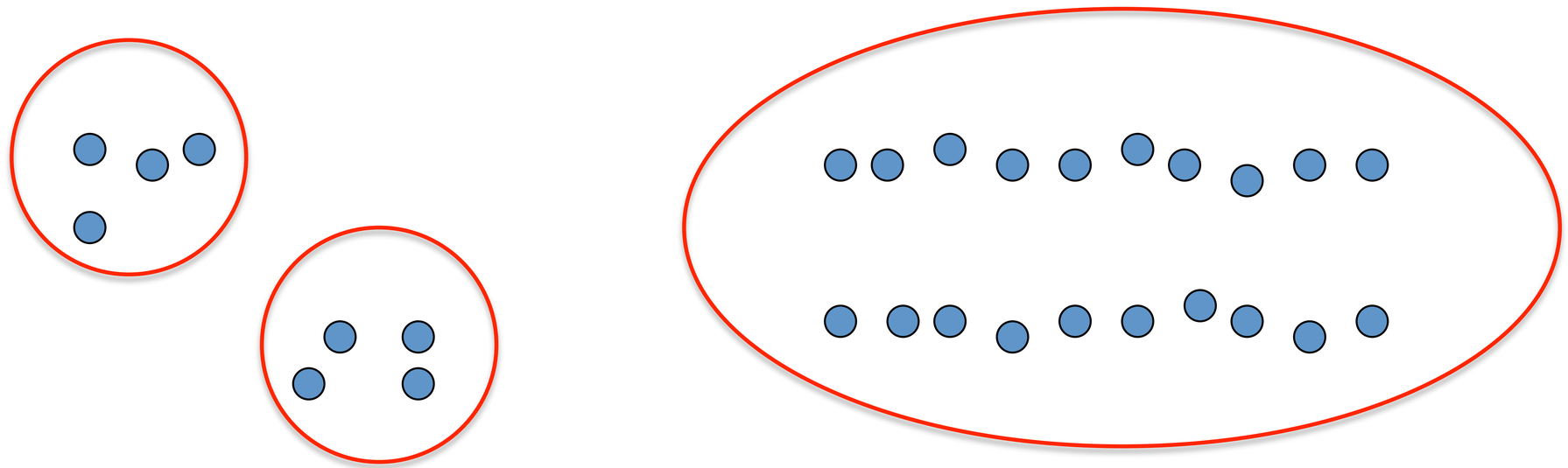
Clustering

Clustering:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns e.g. in
  - Group emails or search results
  - Customer shopping patterns
  - Regions of images
- Useful when don't know what you're looking for
- But: can get gibberish

Clustering

- Basic idea: group together similar instances
- Example: 2D point patterns



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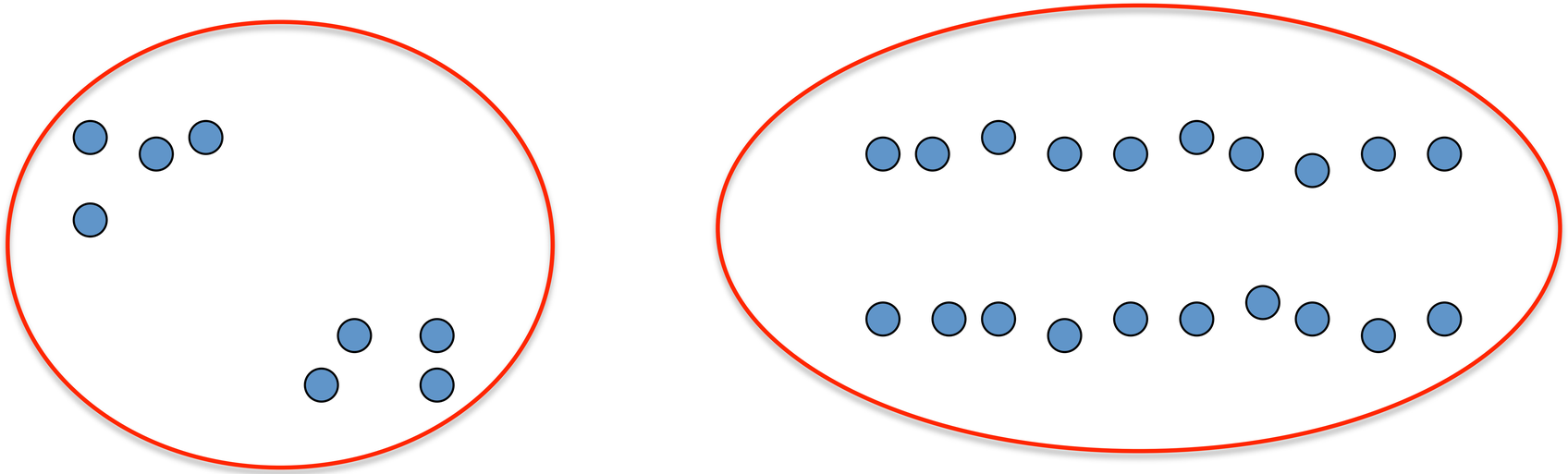

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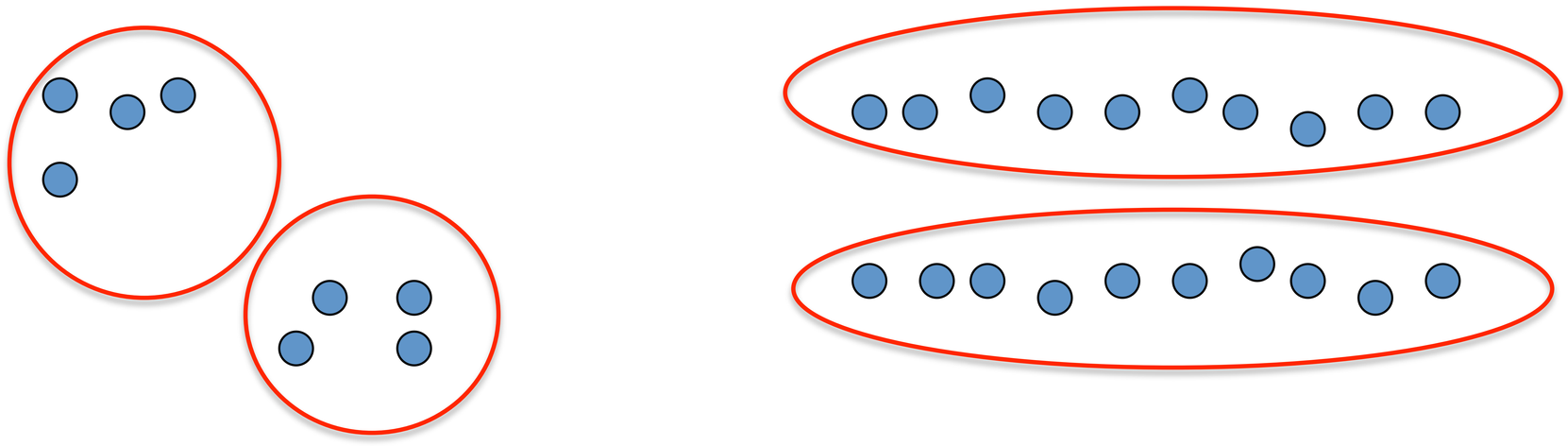


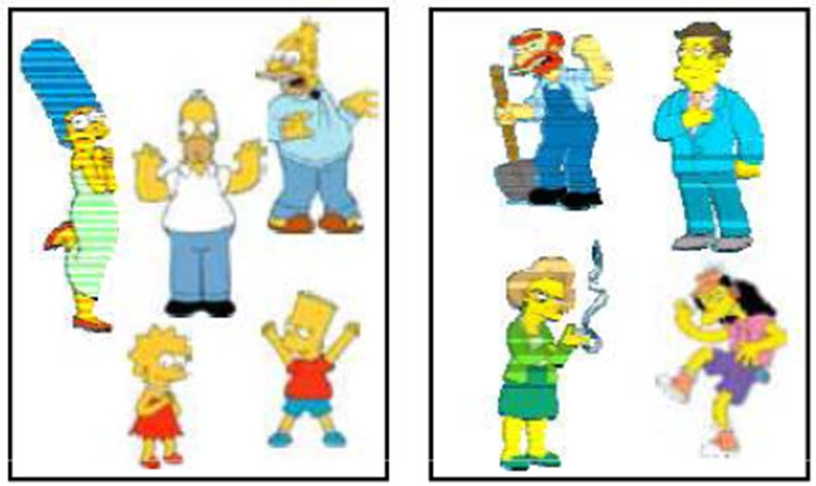
- What could "similar" mean?
  - One option: small Euclidean distance (squared)

$$\text{dist}(\vec{x}, \vec{y}) = ||\vec{x} - \vec{y}||_2^2$$

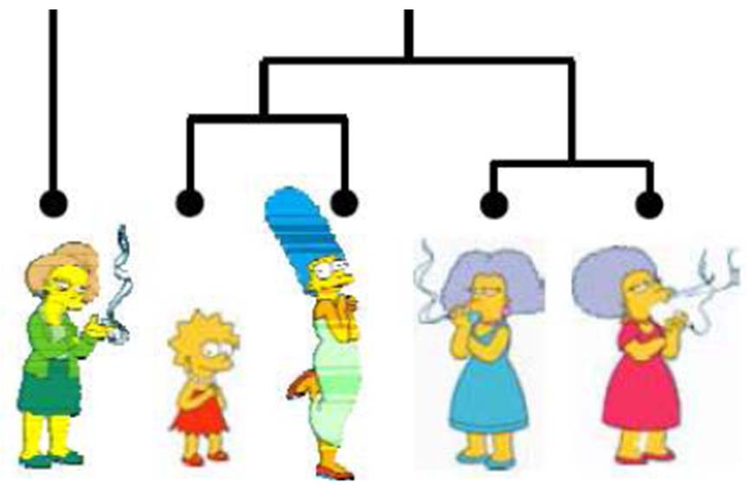
  - Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered

Clustering algorithms

- Partition algorithms (Flat)
  - K-means
  - Mixture of Gaussian
  - Spectral Clustering



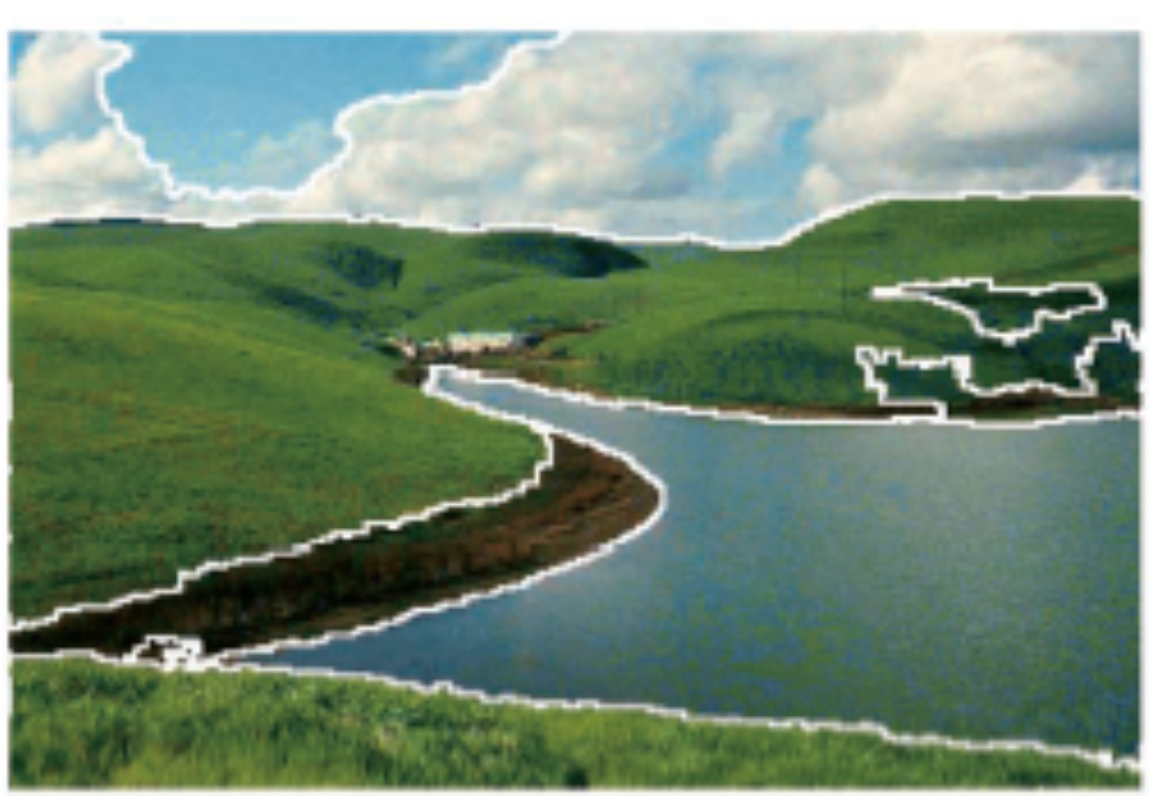
- Hierarchical algorithms
  - Bottom up – agglomerative
  - Top down – divisive



Clustering examples

Image segmentation

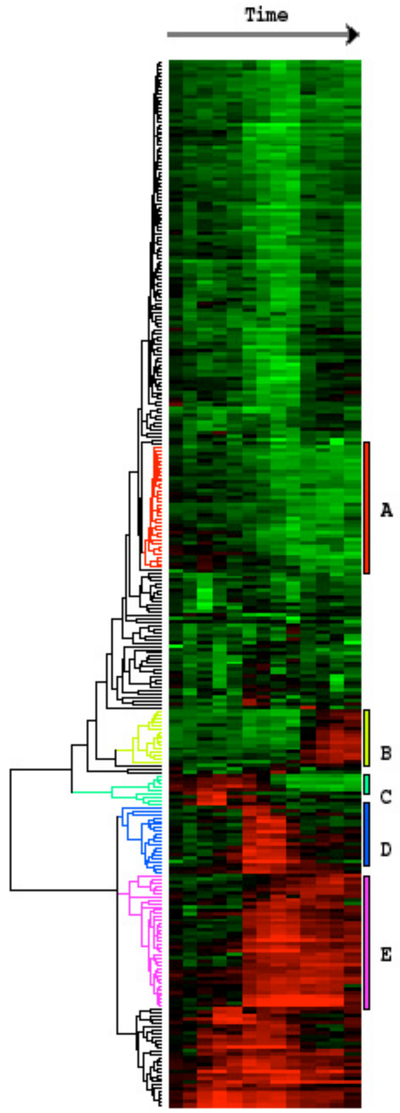
Goal: Break up the image into meaningful or perceptually similar regions



[Slide from James Hayes]

Clustering examples

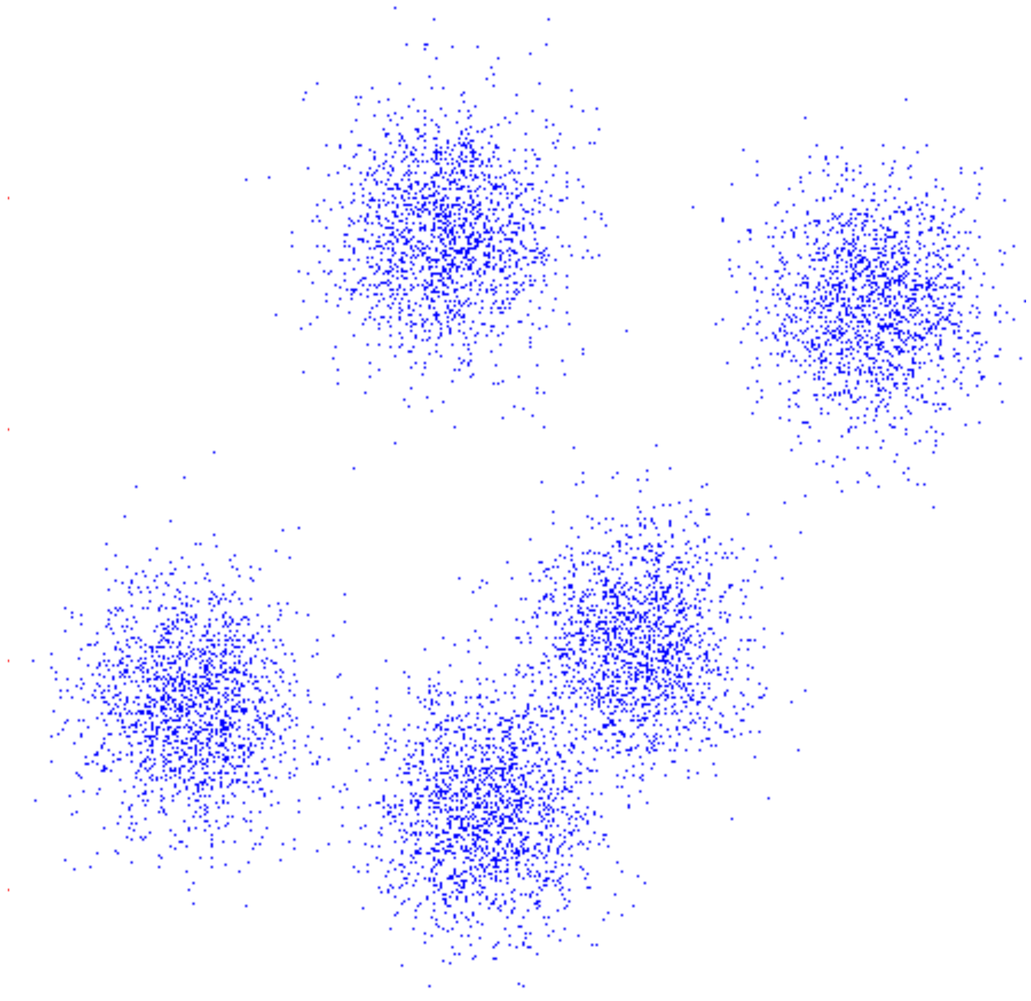
Clustering gene expression data



Eisen et al, PNAS 1998

K-Means

- An iterative clustering algorithm
  - Initialize: Pick *K* random points as cluster centers
  - Alternate:
    1. Assign data points to closest cluster center
    2. Change the cluster center to the average of its assigned points
  - Stop when no points' assignments change



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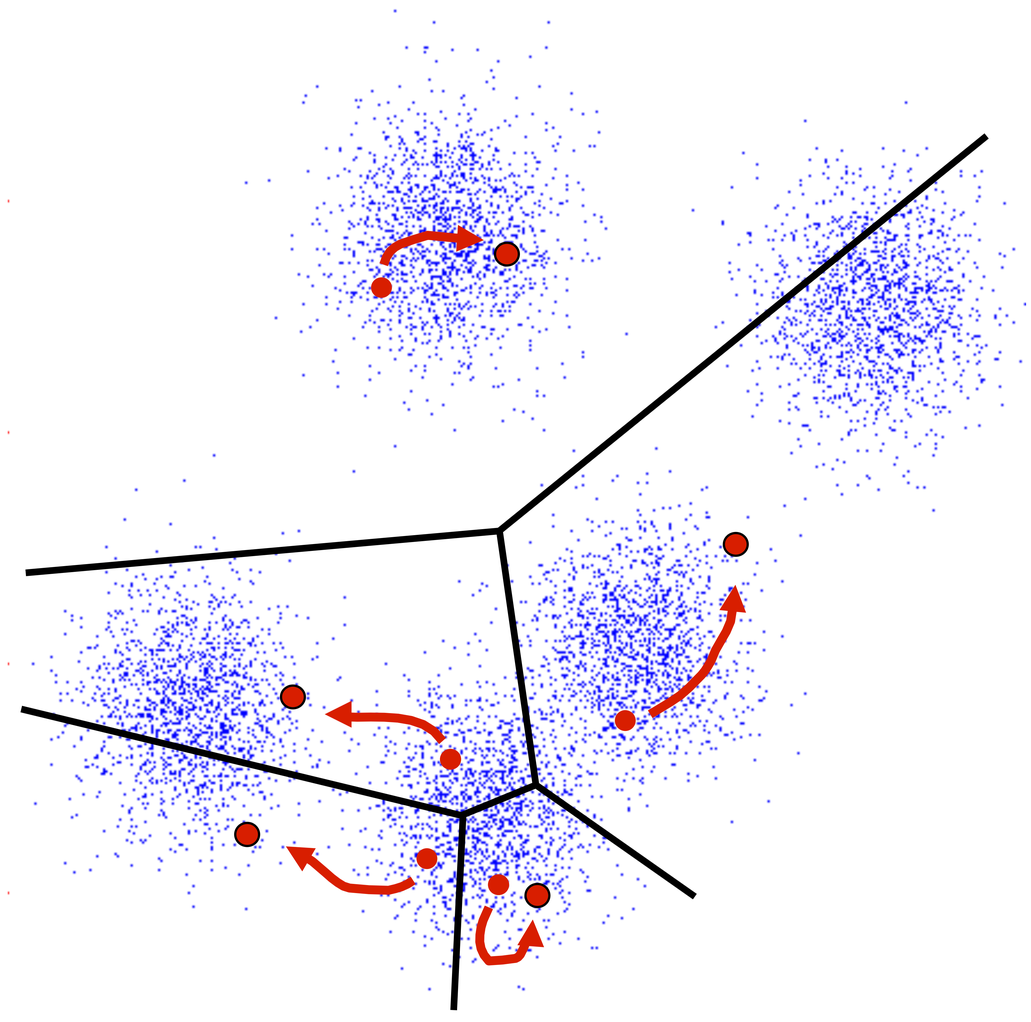
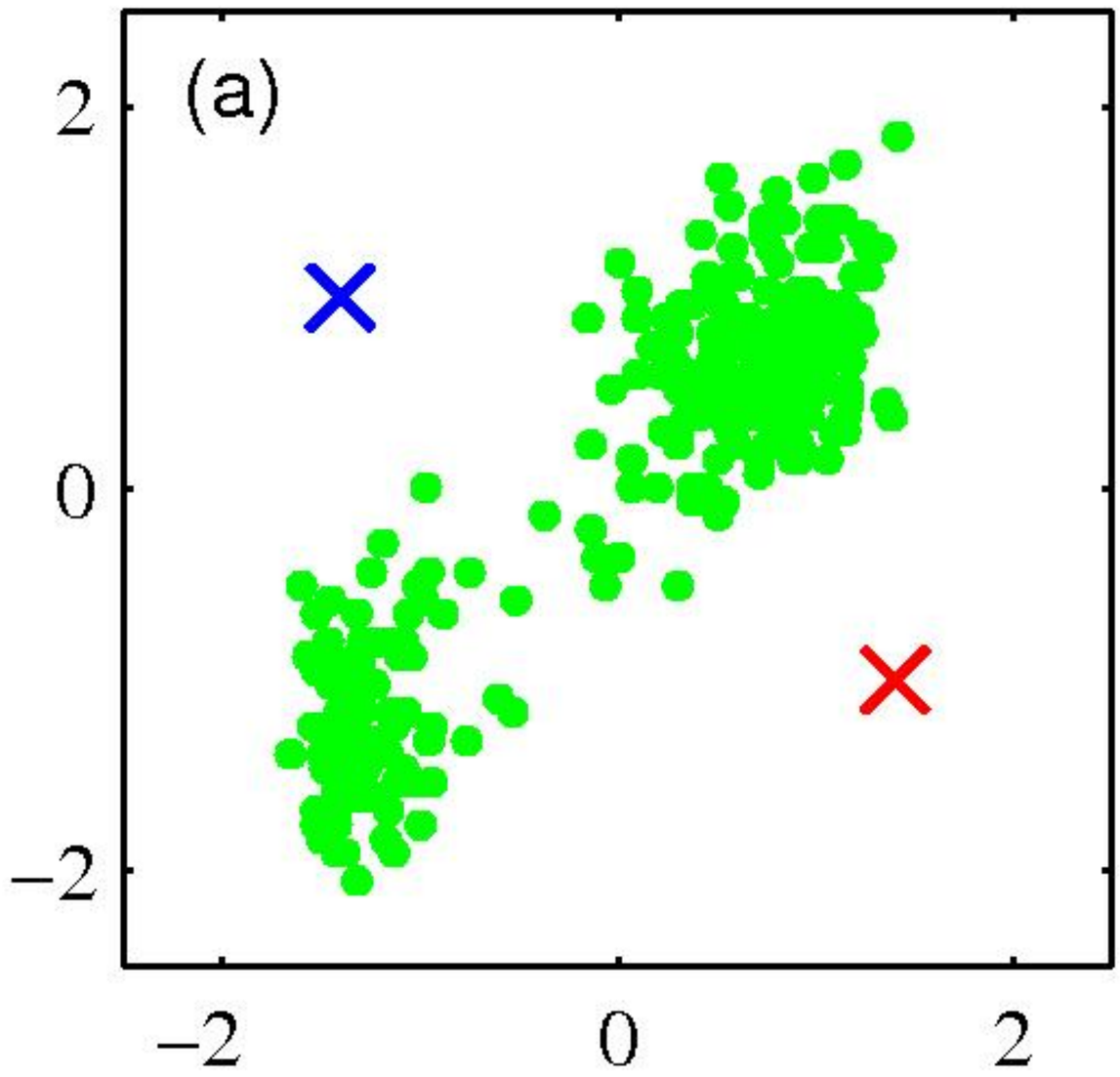


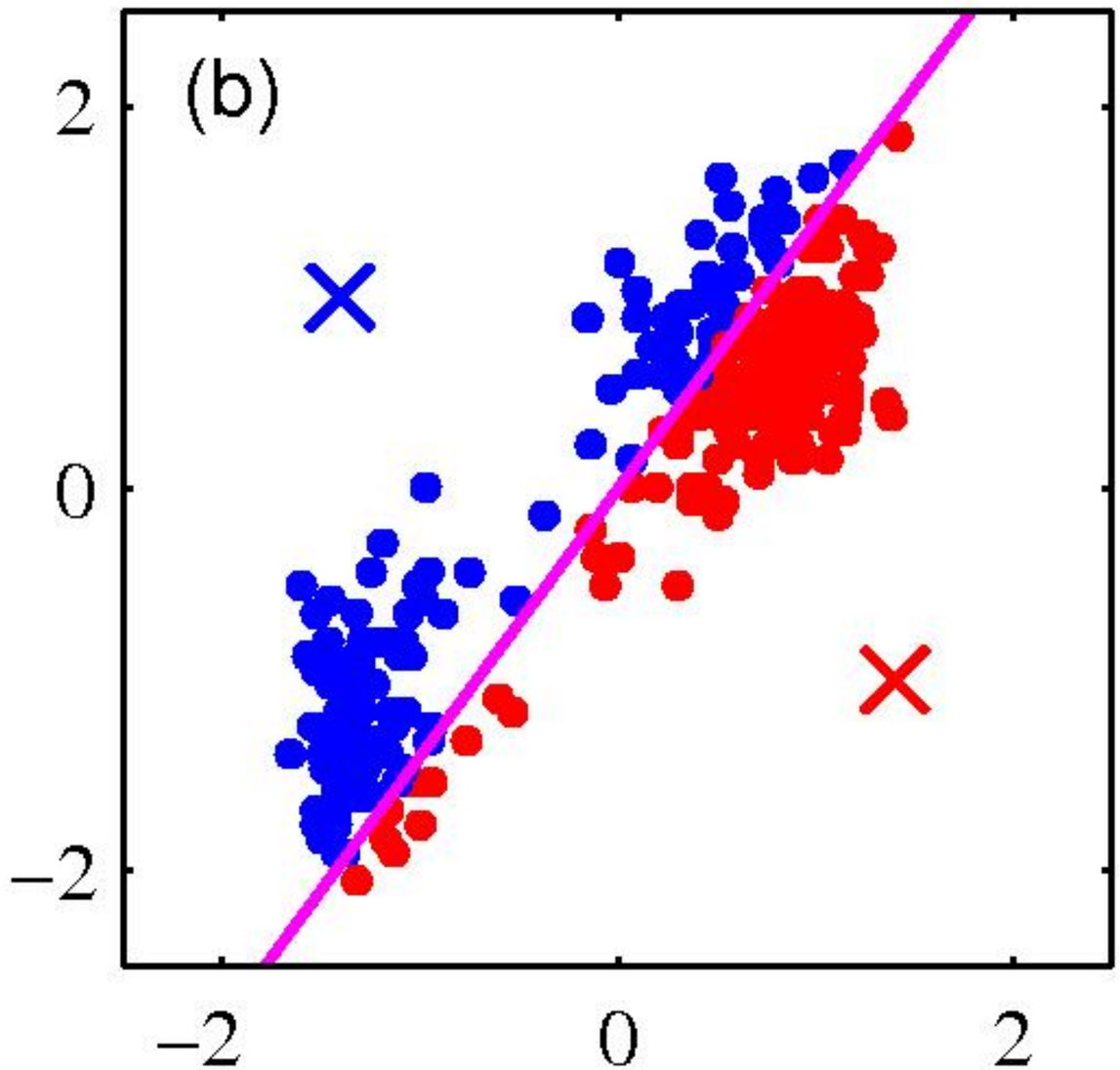
K-means clustering: Example



- Pick *K* random points as cluster centers (means)

Shown here for *K*=2

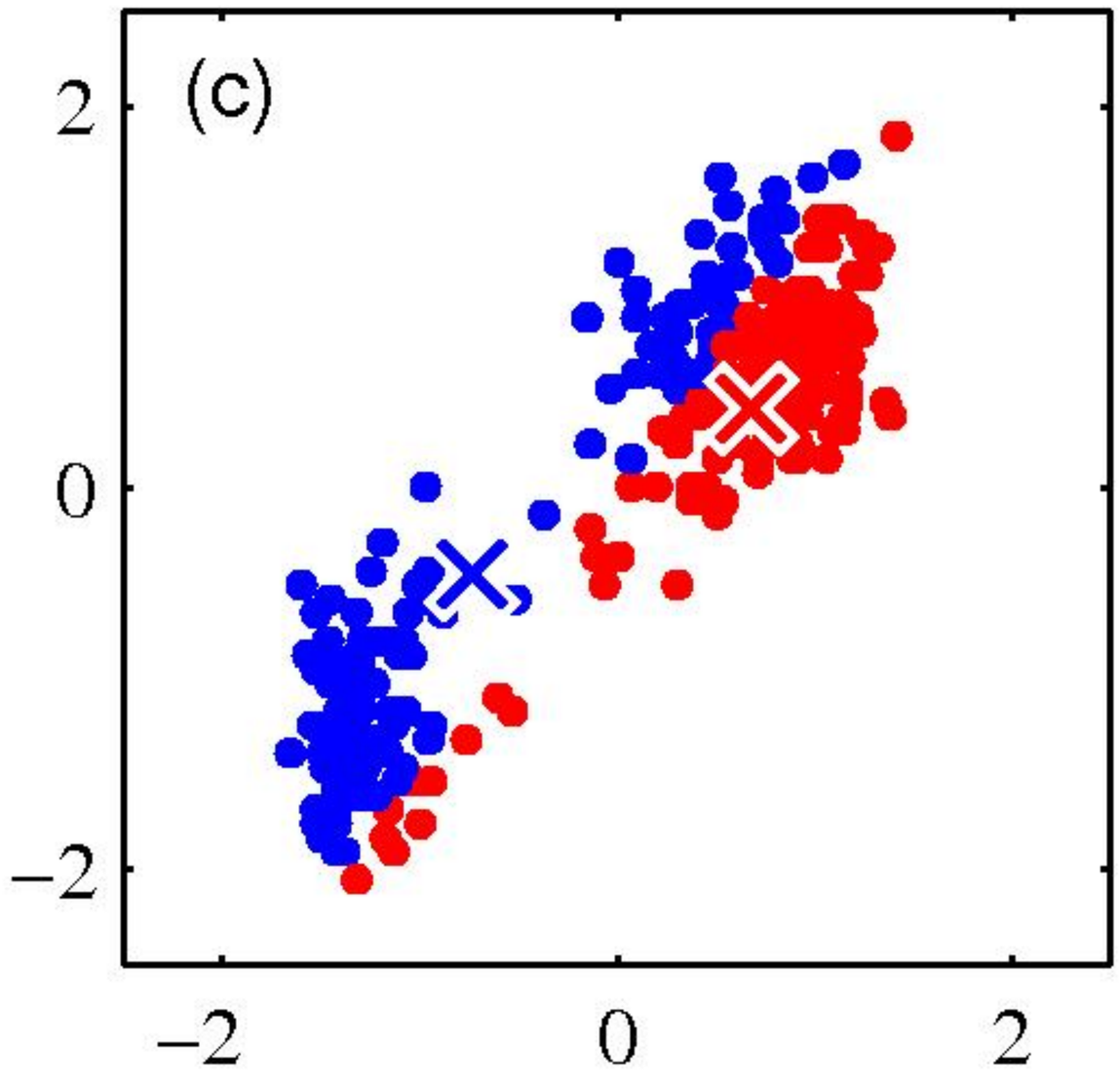
K-means clustering: Example



Iterative Step 1

- Assign data points to closest cluster center

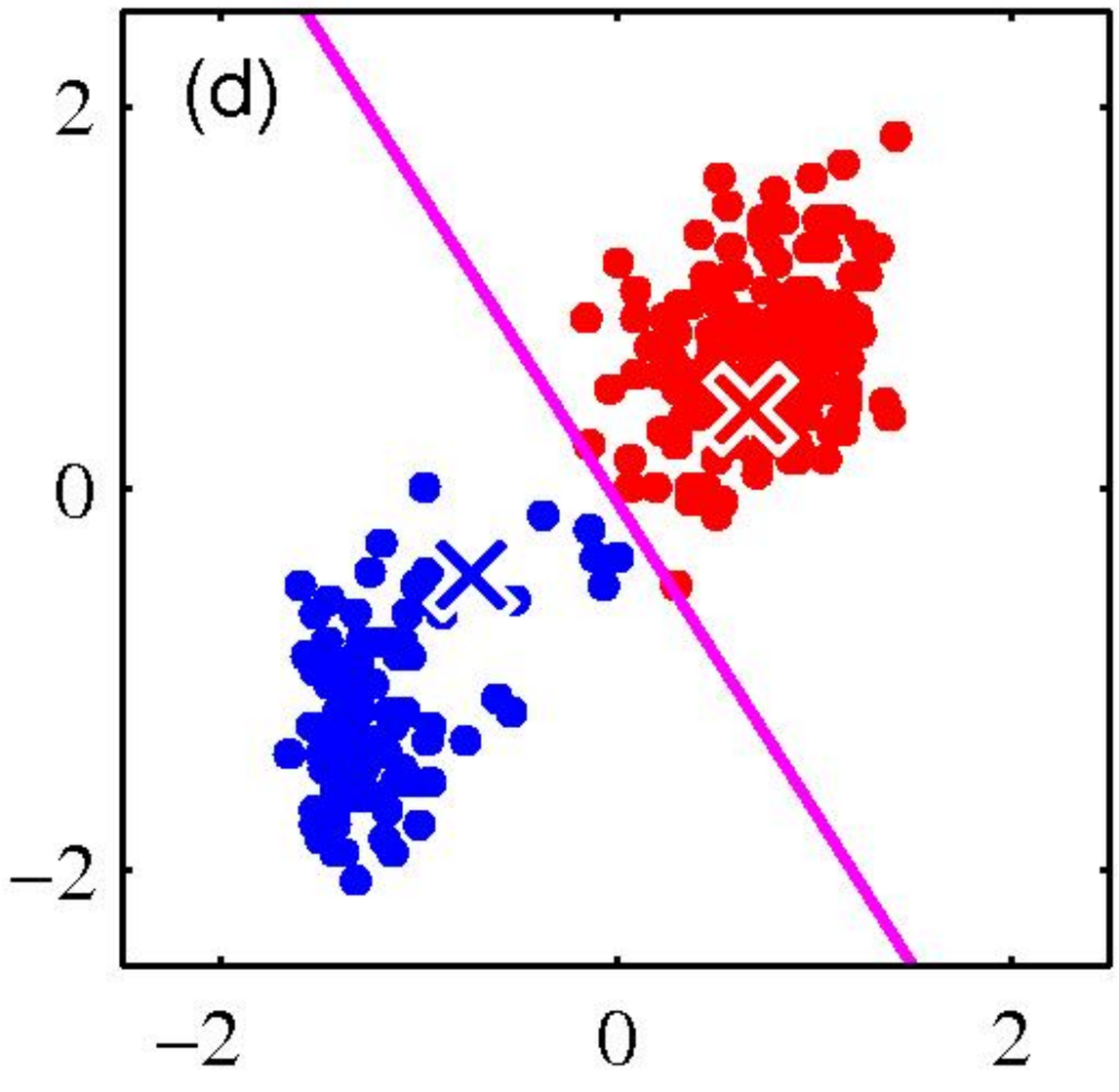
K-means clustering: Example



Iterative Step 2

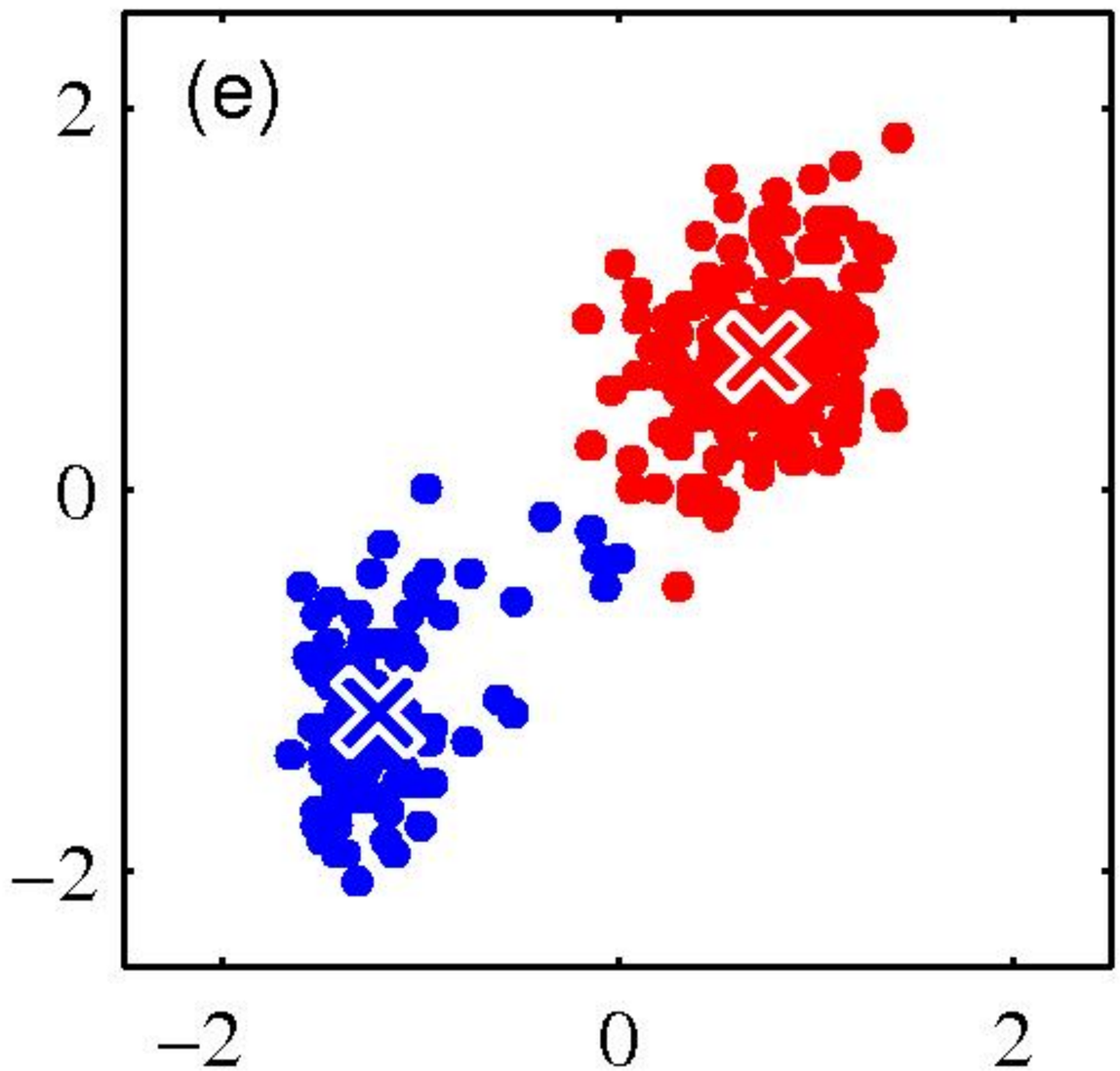
- Change the cluster center to the average of the assigned points

K-means clustering: Example

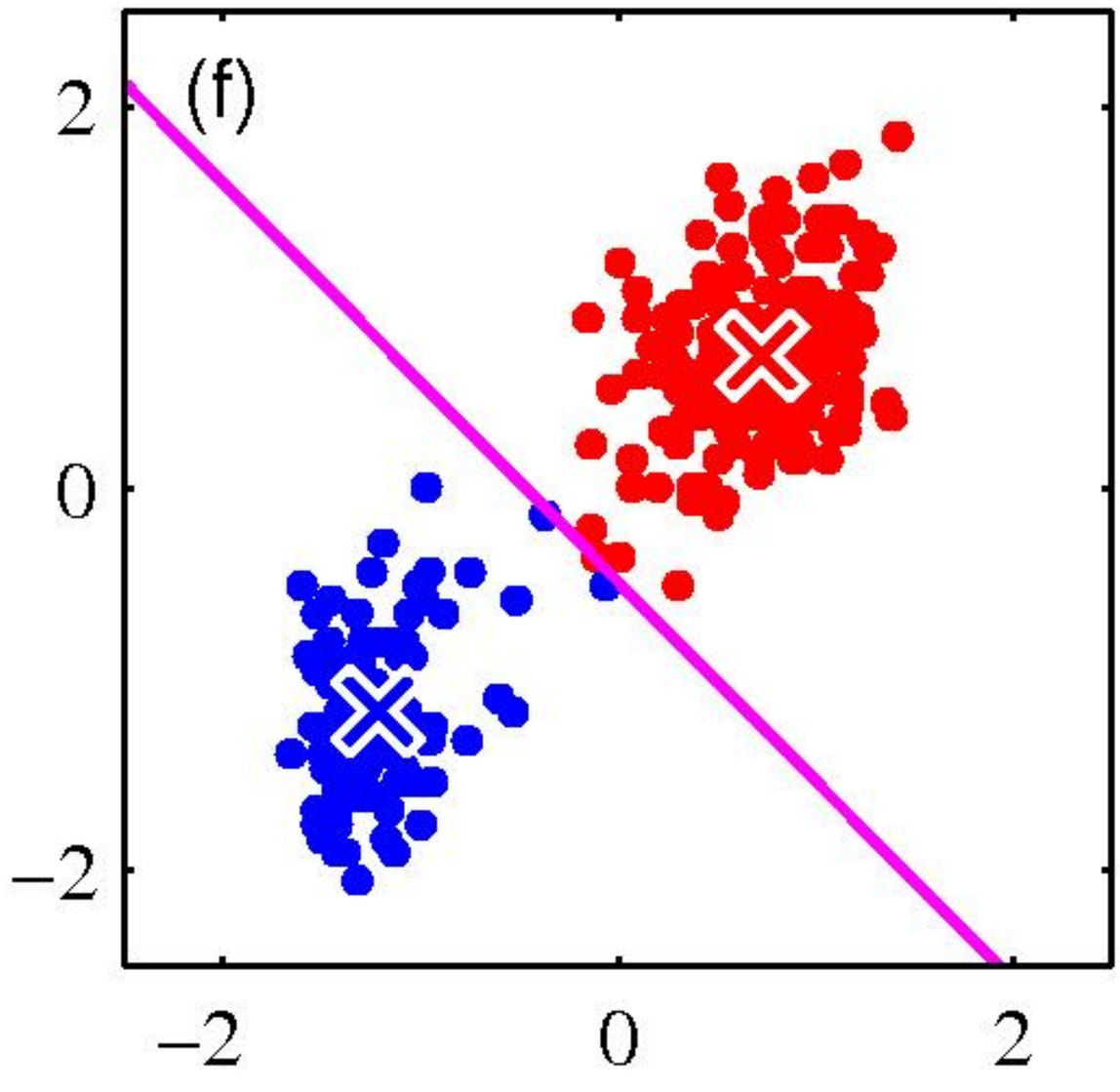


- Repeat until convergence

K-means clustering: Example



K-means clustering: Example



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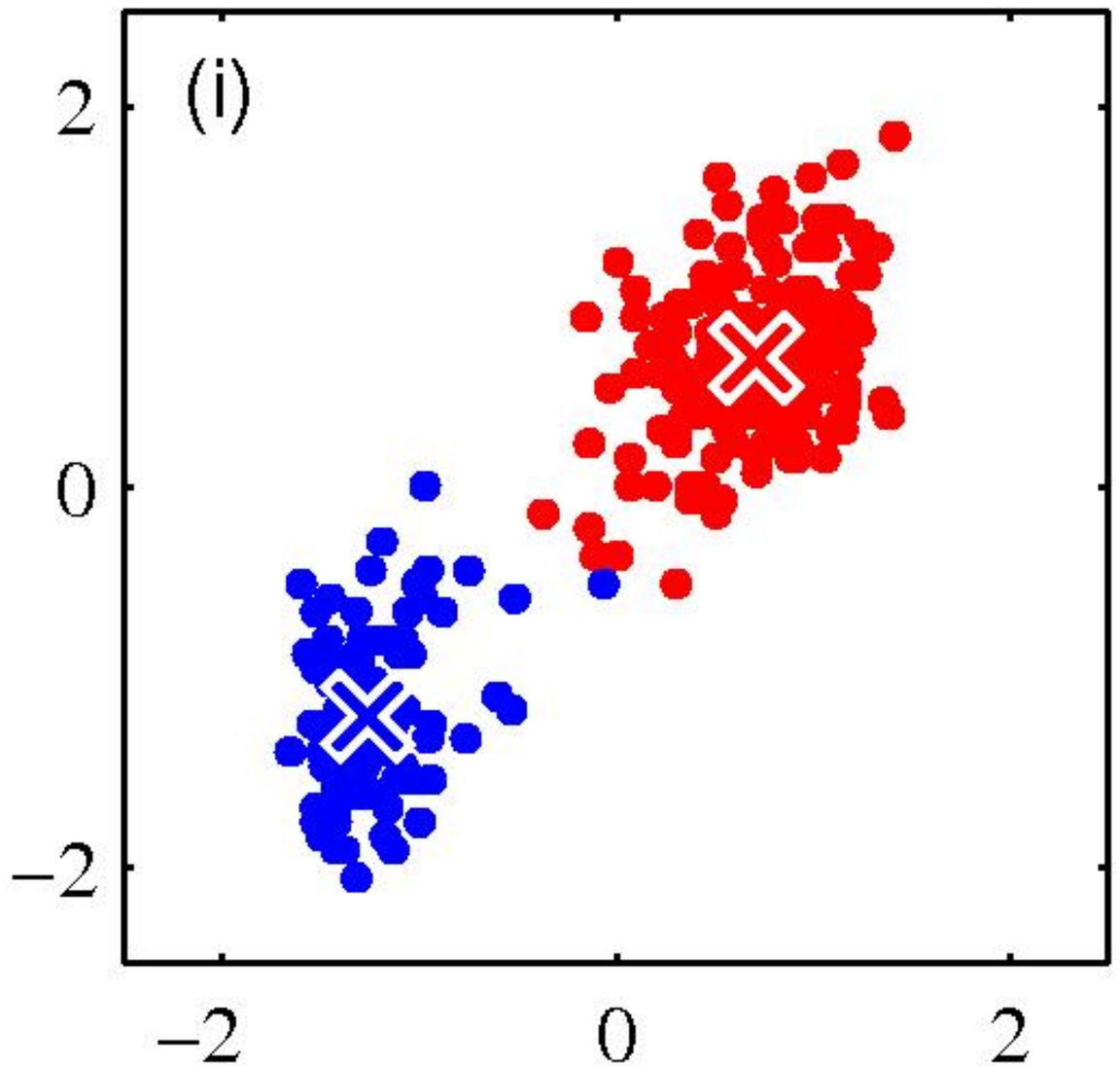

Properties of K-means **algorithm**

- Guaranteed to converge in a finite number of iterations

- Running time per iteration:

  1. Assign data points to closest cluster center

     O(KN) time

  2. Change the cluster center to the average of its assigned points

     O(N)

What properties should a distance measure have?

- 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)≥0, and D(A,B)=0 iff A=B
  - Otherwise there will different objects that we cannot tell apart
- Triangle inequality
  - D(A,B)+D(B,C) ≥ D(A,C)
  - Otherwise one can say “A is like B, B is like C, but A is not like C at all”

[Slide from Alan Fern]