Clustering
Lecture 14

David Sontag
New York University

Slides adapted from Luke Zettlemoyer, Vibhav Gogate, Carlos Guestrin, Andrew Moore, Dan Klein

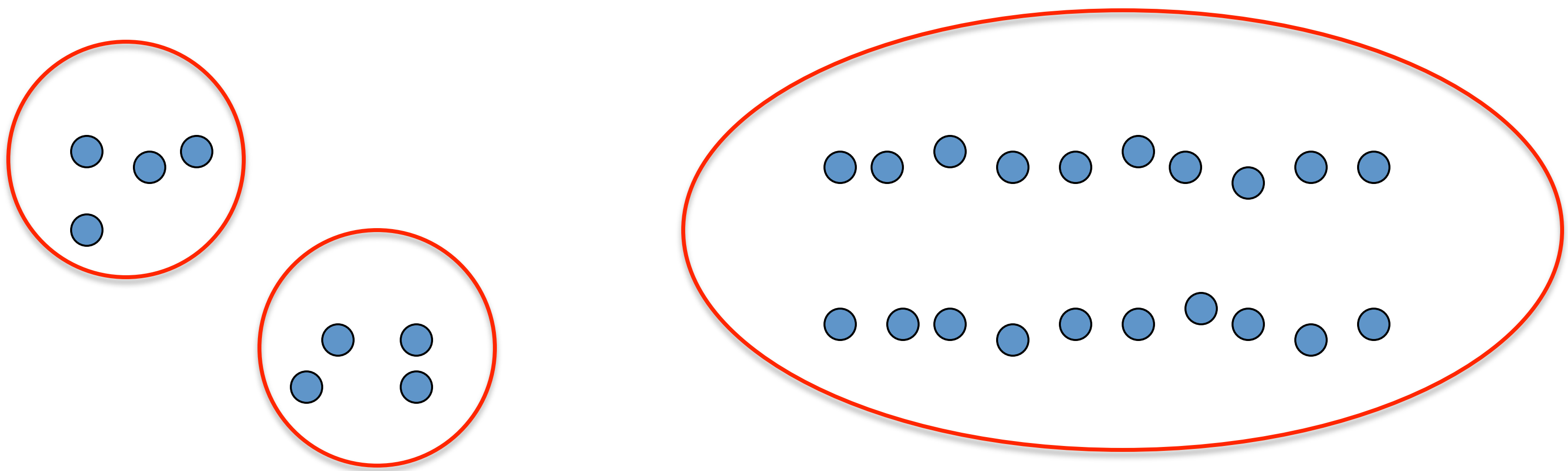
Clustering

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

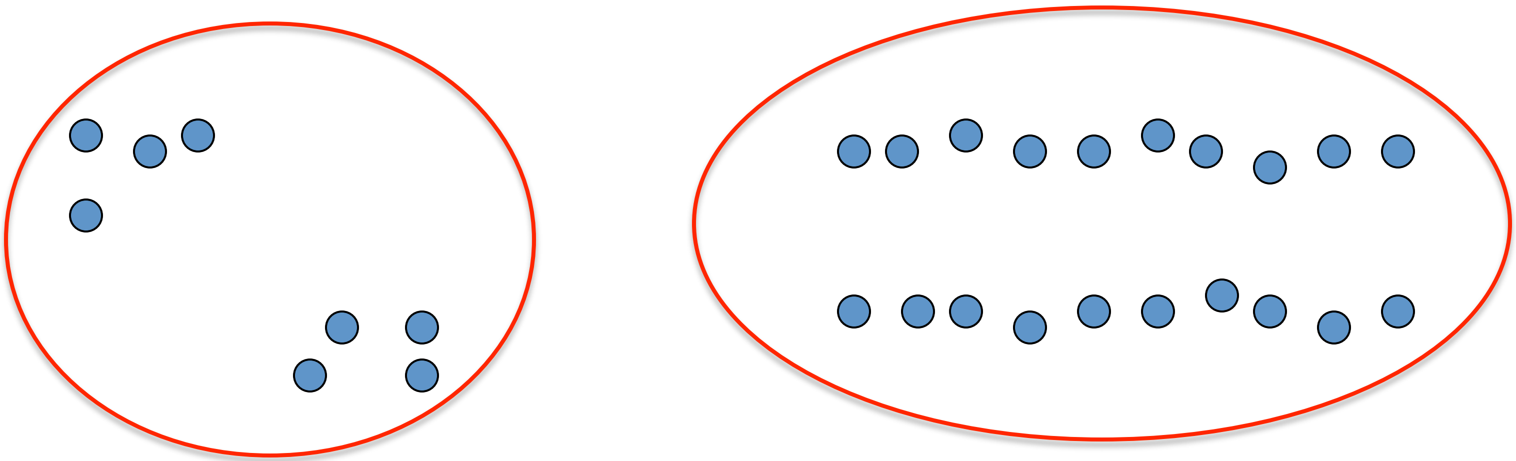
Clustering

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



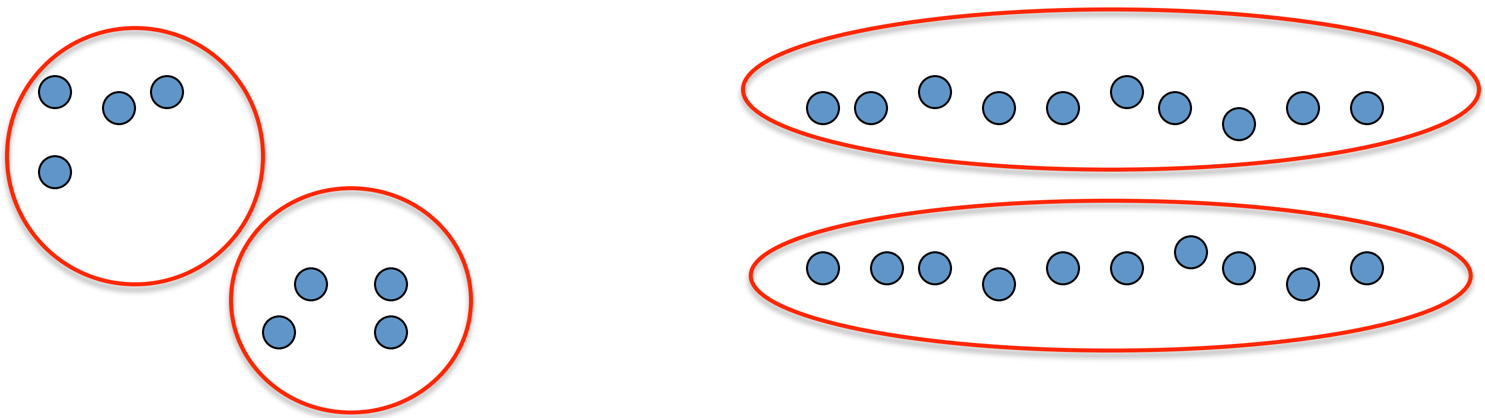
Clustering

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



Clustering

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



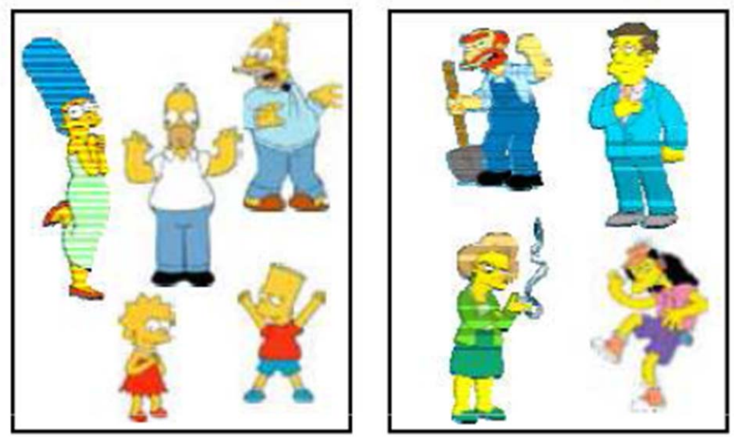
- What could "similar" mean?
  - One option: small Euclidean distance (squared)

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

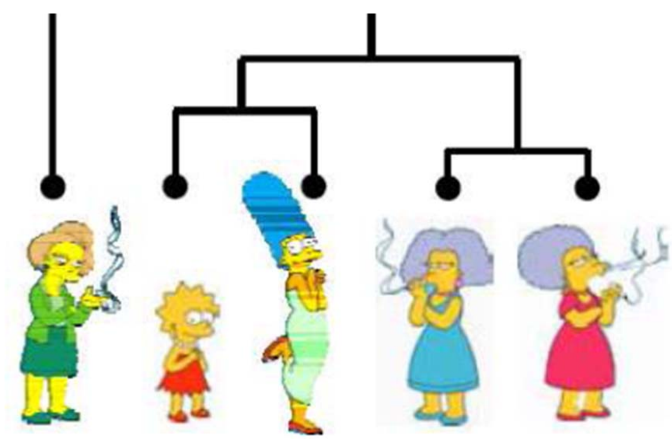
  - Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered

Clustering algorithms

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



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



Clustering examples

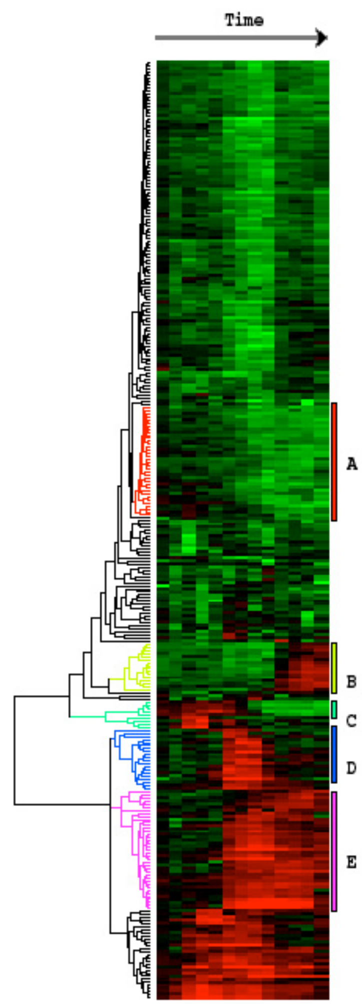
Image segmentation

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

[Slide from James Hayes]

Clustering examples

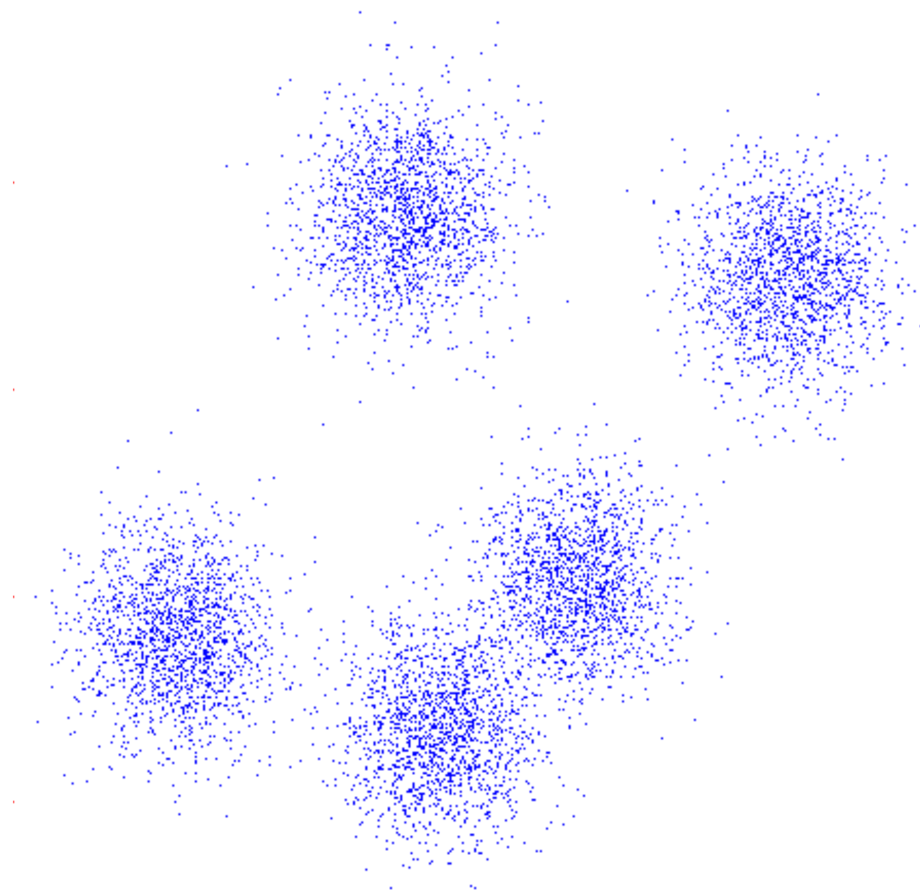
Clustering gene expression data



Eisen et al, PNAS 1998

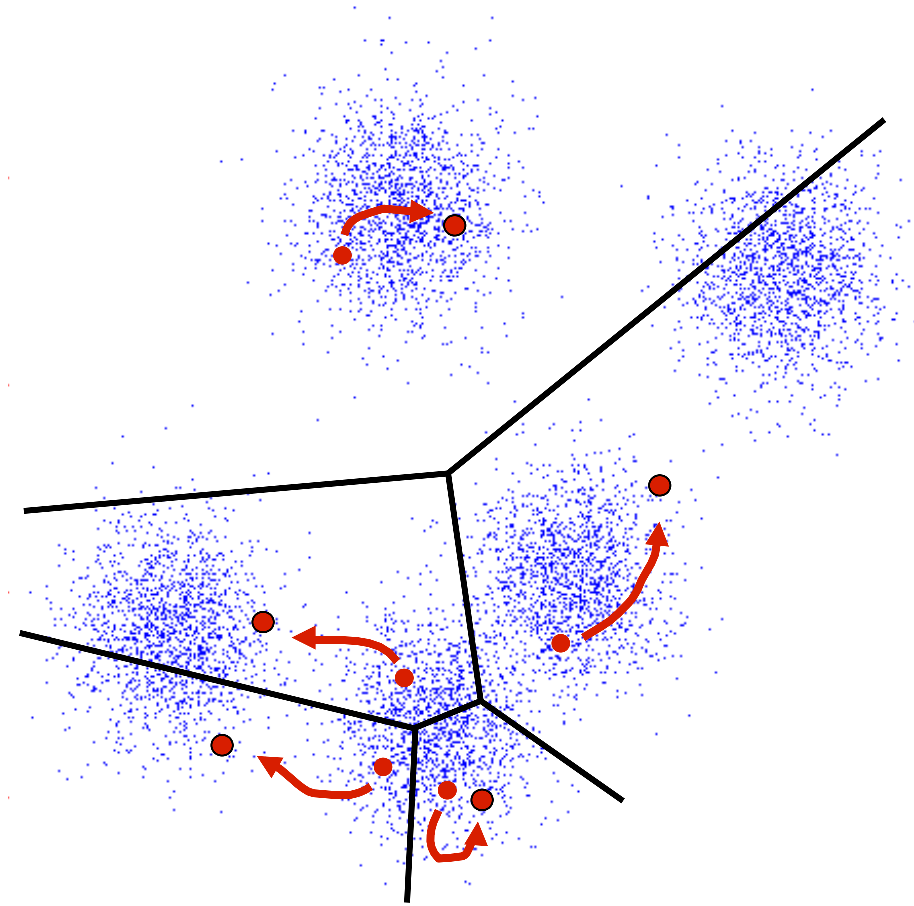
K-Means

- 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

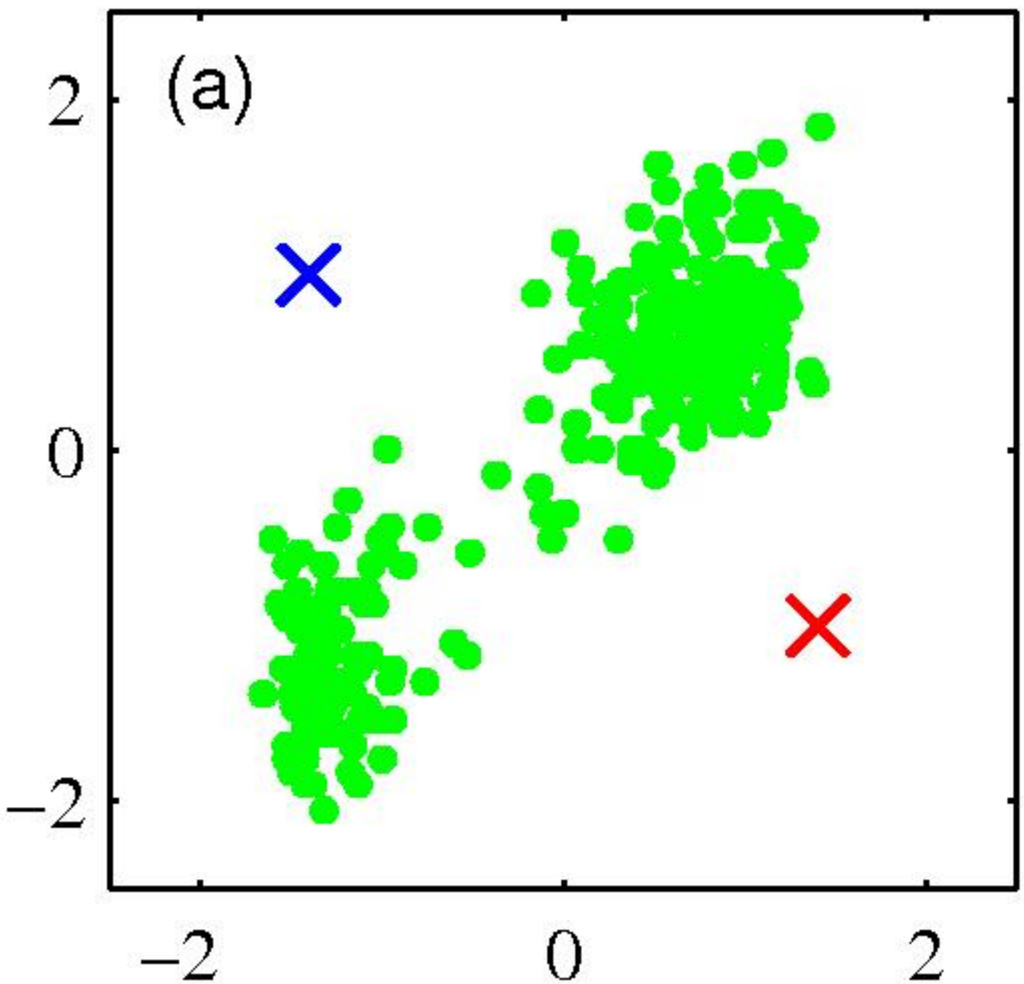


K-Means

- 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



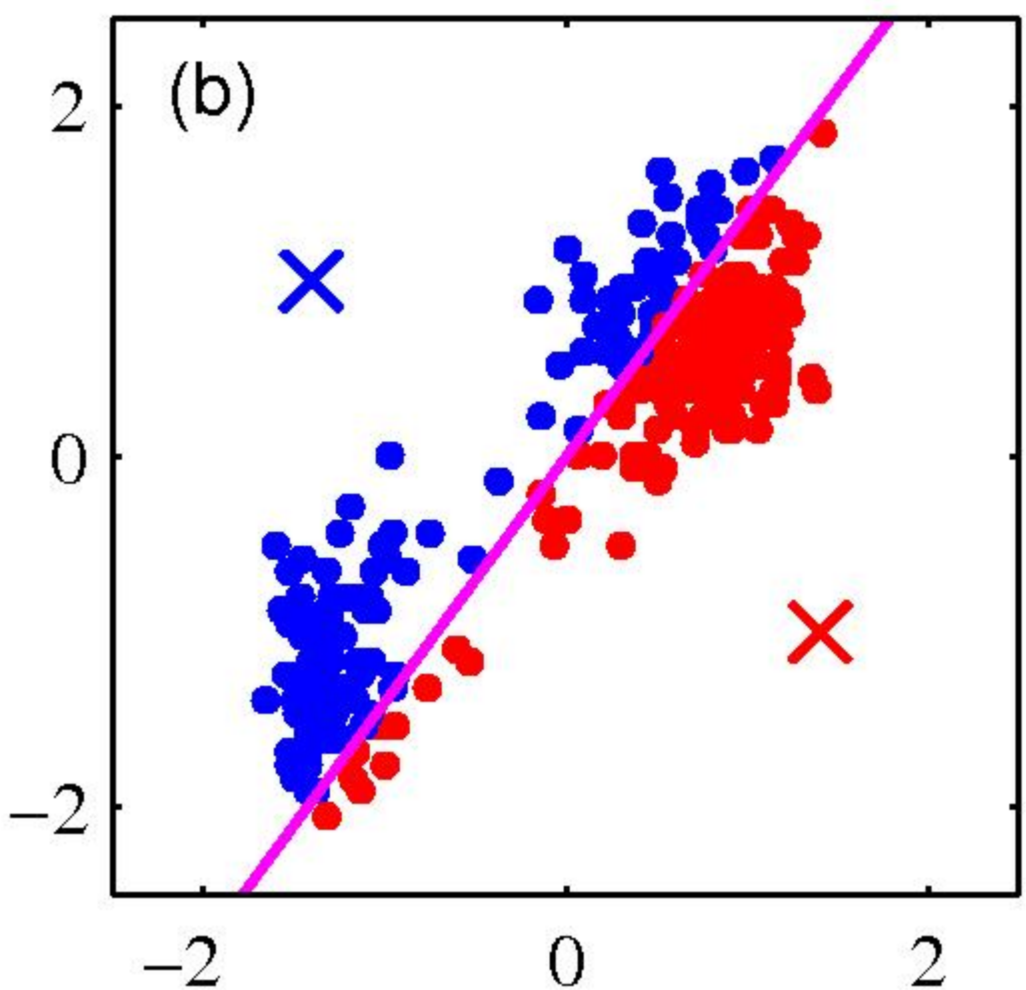
K-means clustering: Example



- Pick K random points as cluster centers (means)

Shown here for K=2

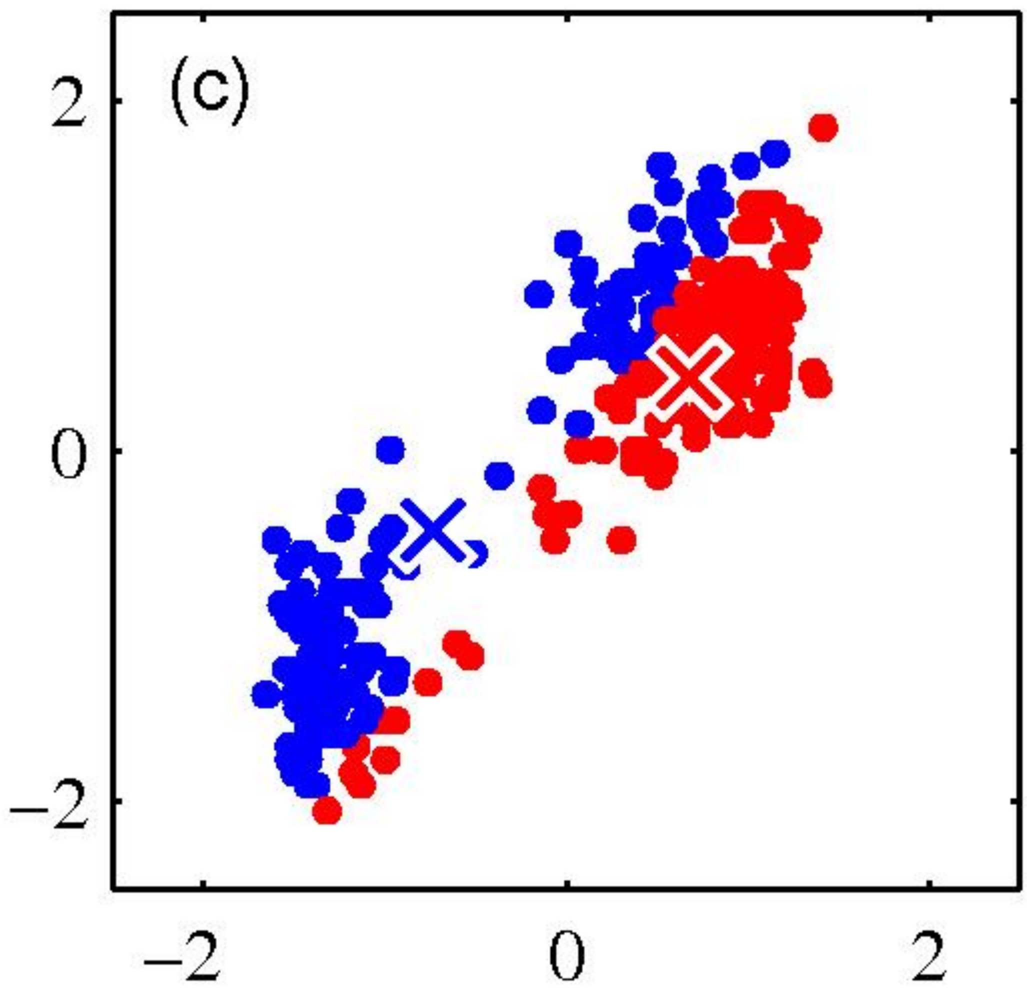
K-means clustering: Example



Iterative Step 1

- Assign data points to closest cluster center

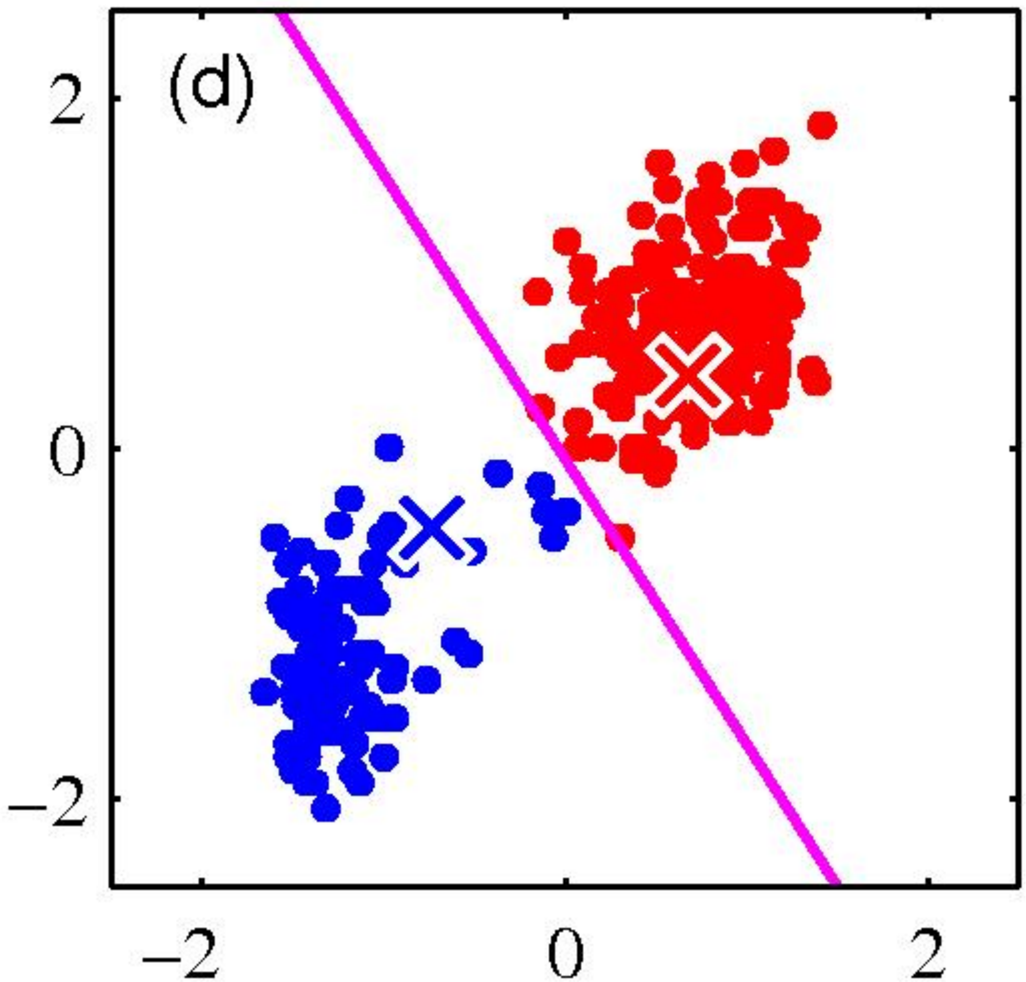
K-means clustering: Example



Iterative Step 2

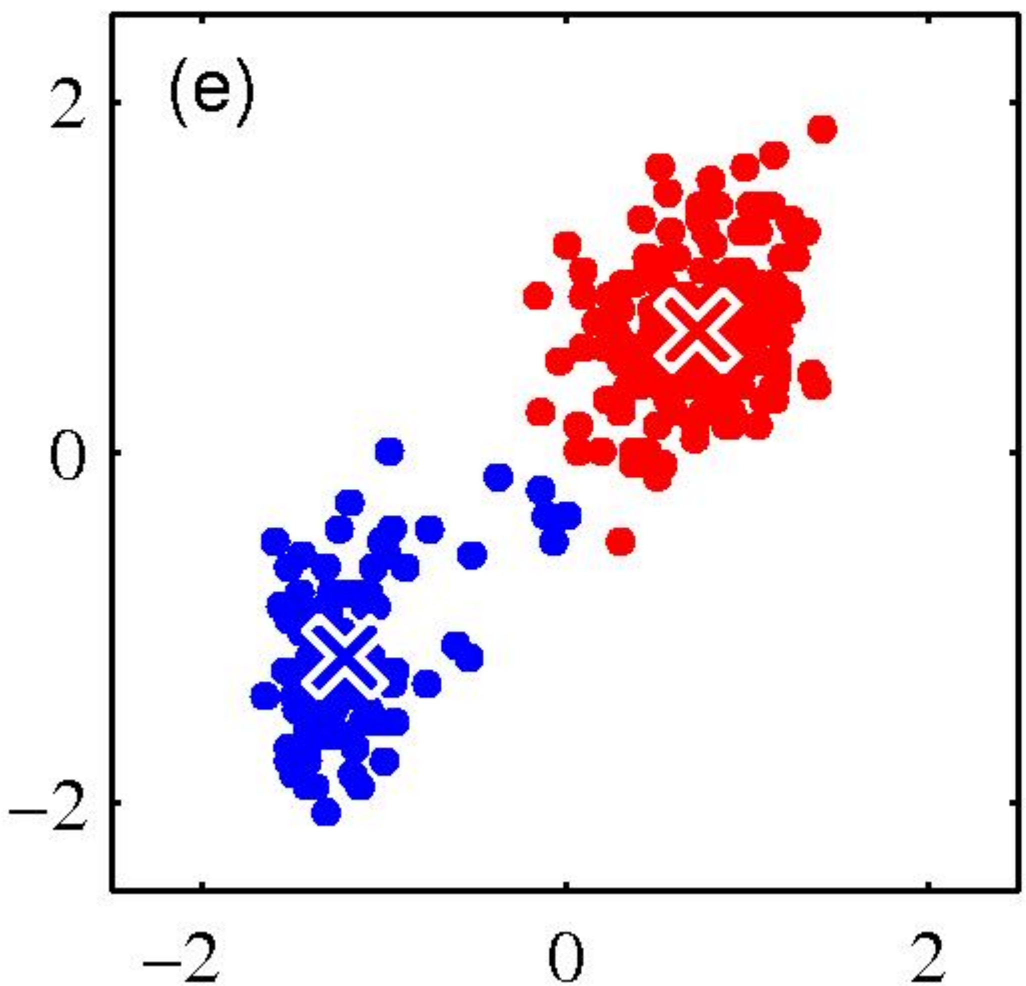
- Change the cluster center to the average of the assigned points

K-means clustering: Example

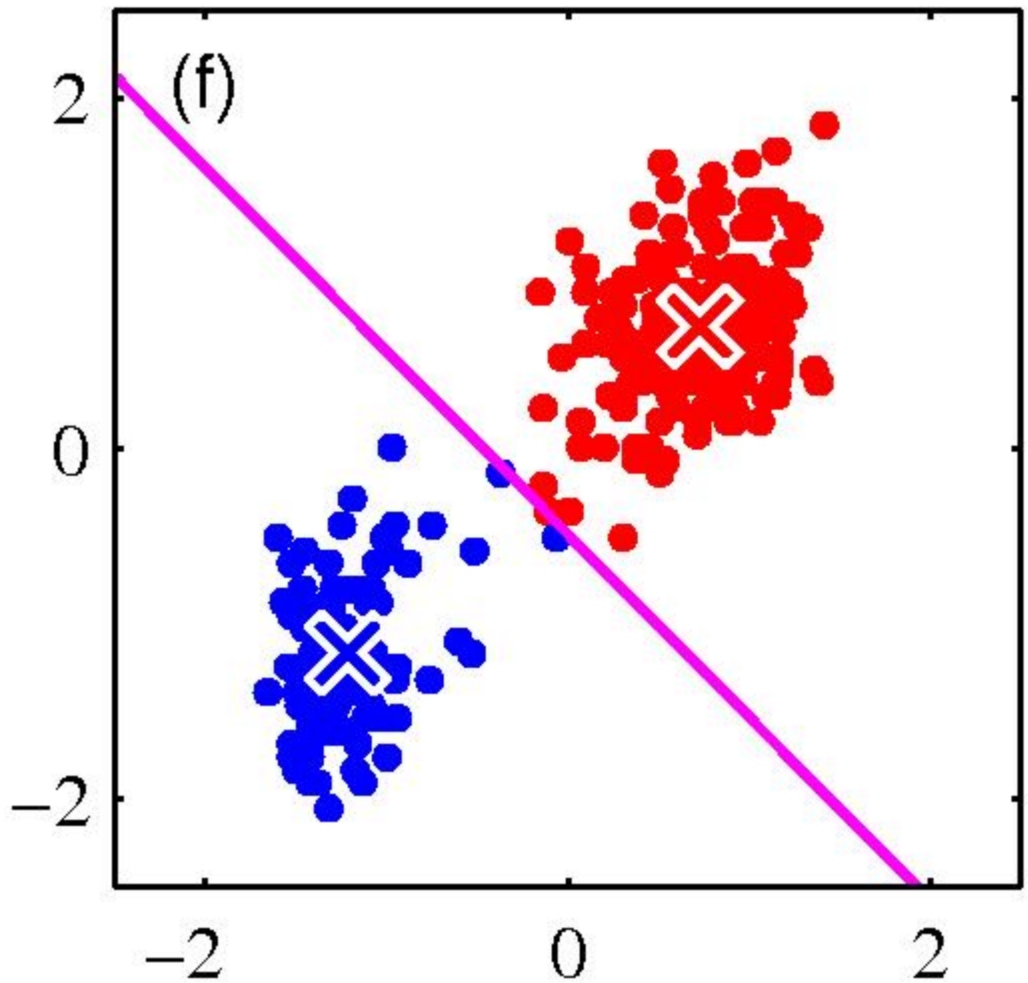


- Repeat until convergence

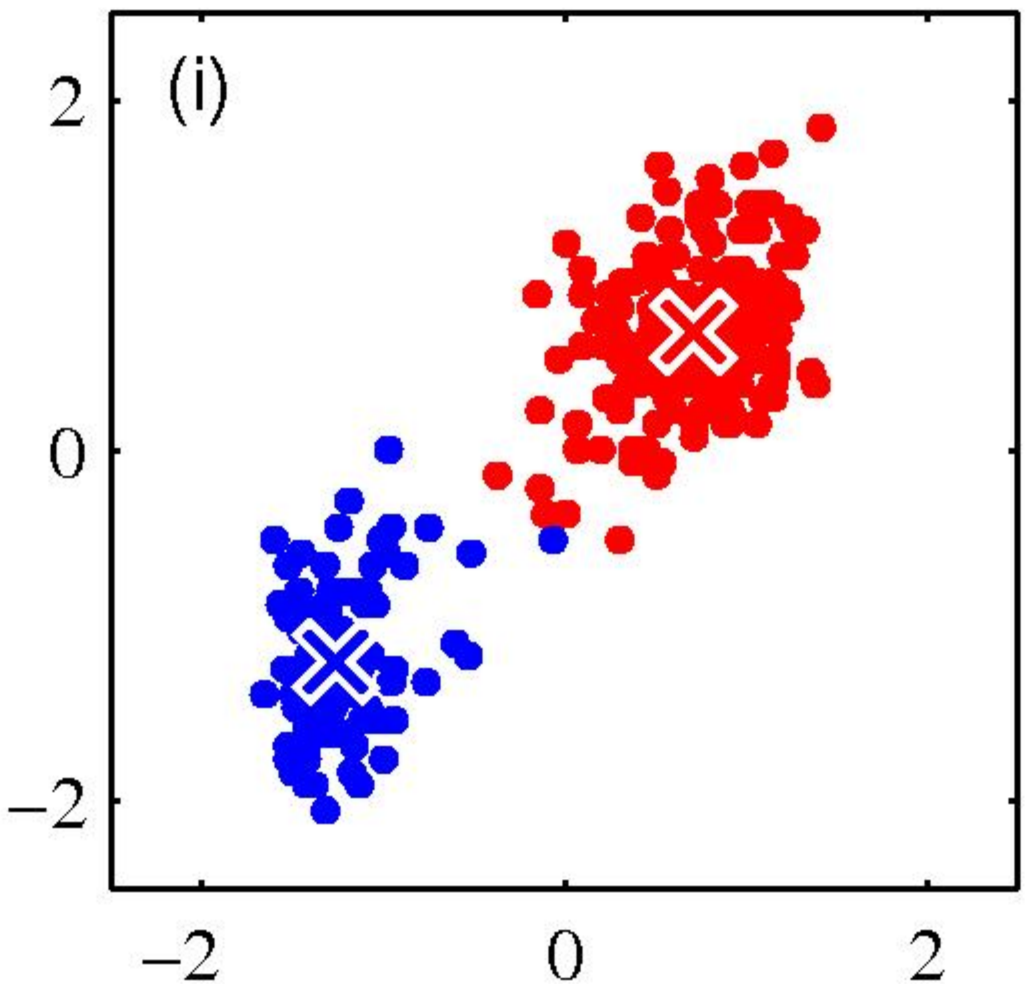
K-means clustering: Example



K-means clustering: Example



K-means clustering: Example



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

[Slide from Alan Fern]

Kmeans Convergence

Objective

$$\min_{\mu}\min_{C} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2$$

1. Fix μ, optimize *C:*

Step 1 of kmeans

$$\min_{C} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2 = \min_{c} \sum_{i}^{n} \left|x_i - \mu_{x_i}\right|^2$$

2. Fix *C,* optimize μ:

$$\min_{\mu} \sum_{i=1}^{k} \sum_{x \in C_i} |x - \mu_i|^2$$

   – Take partial derivative of μ_i and set to zero, we have

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

Step 2 of kmeans

Kmeans takes an alternating optimization approach, each step is guaranteed to decrease the objective – thus guaranteed to converge

[Slide from Alan Fern]

Example: K-Means for Segmentation

K=2

Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.

Original

Example: K-Means for Segmentation

K=2 | K=3 | Original

Example: K-Means for Segmentation

K=2 K=3 K=10 Original

4% 8% 17%

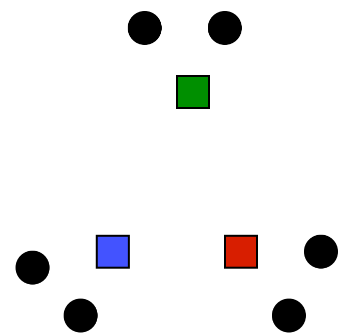
Example: Vector quantization

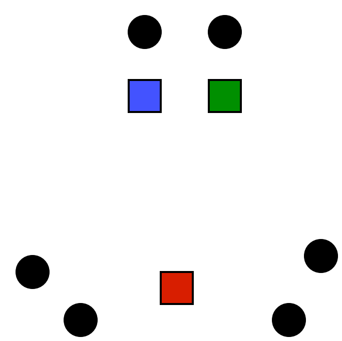
FIGURE 14.9. *Sir Ronald A. Fisher* (1890 − 1962) *was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a* 1024×1024 *grayscale image at* 8 *bits per pixel. The center image is the result of* 2×2 *block VQ, using* 200 *code vectors, with a compression rate of* 1.9 *bits/pixel. The right image uses only four code vectors, with a compression rate of* 0.50 *bits/pixel*

[Figure from Hastie *et al.* book]

Initialization

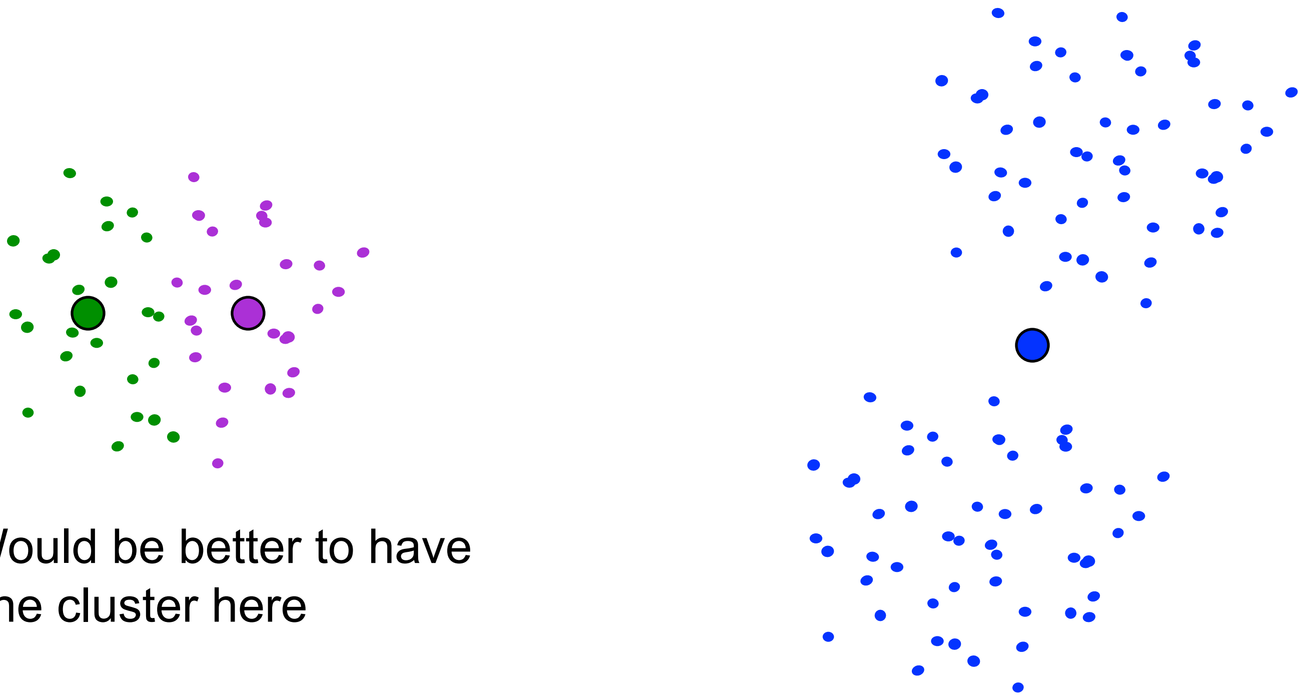
- K-means **algorithm** is a heuristic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics





K-Means Getting Stuck

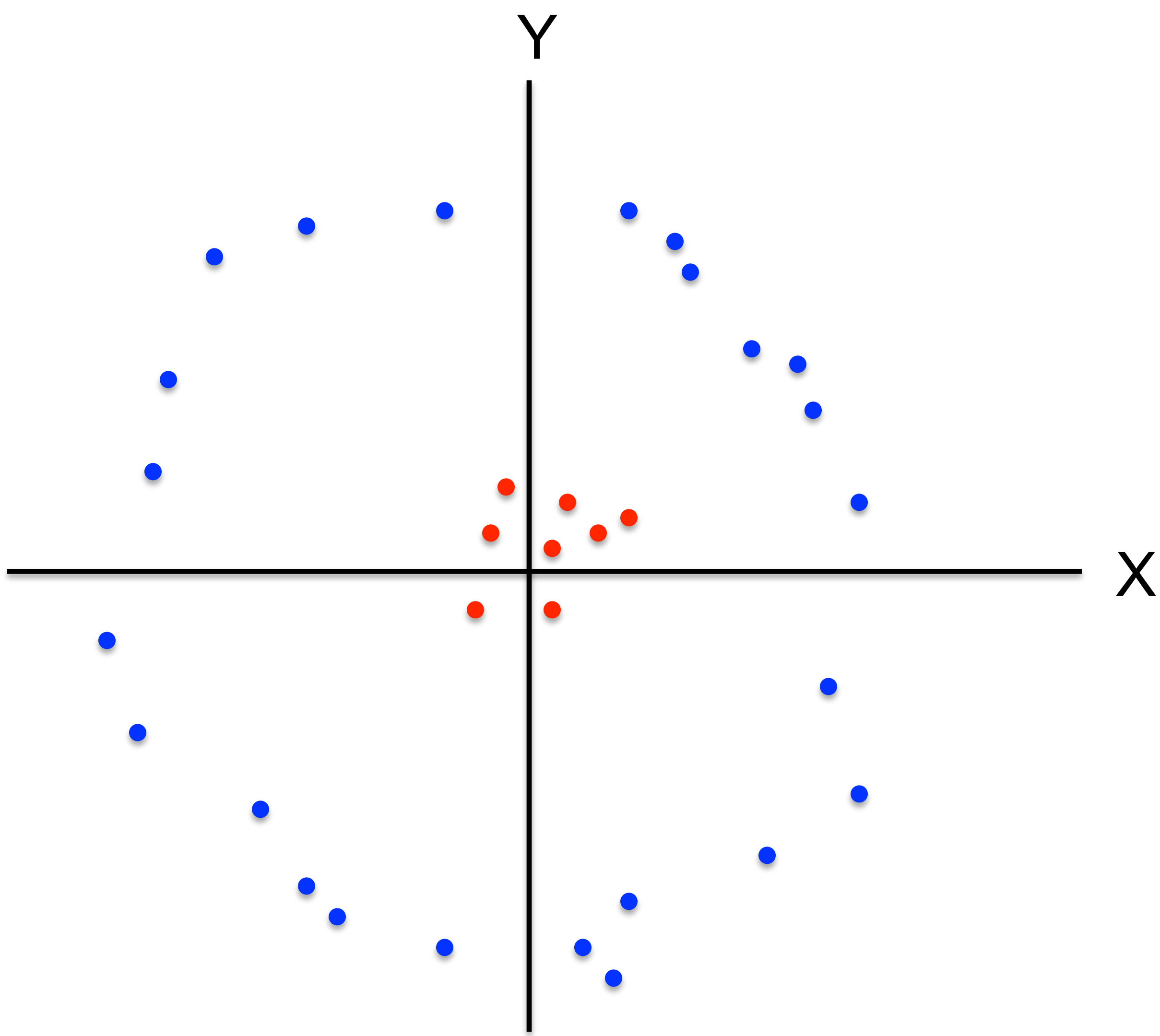
A local optimum:



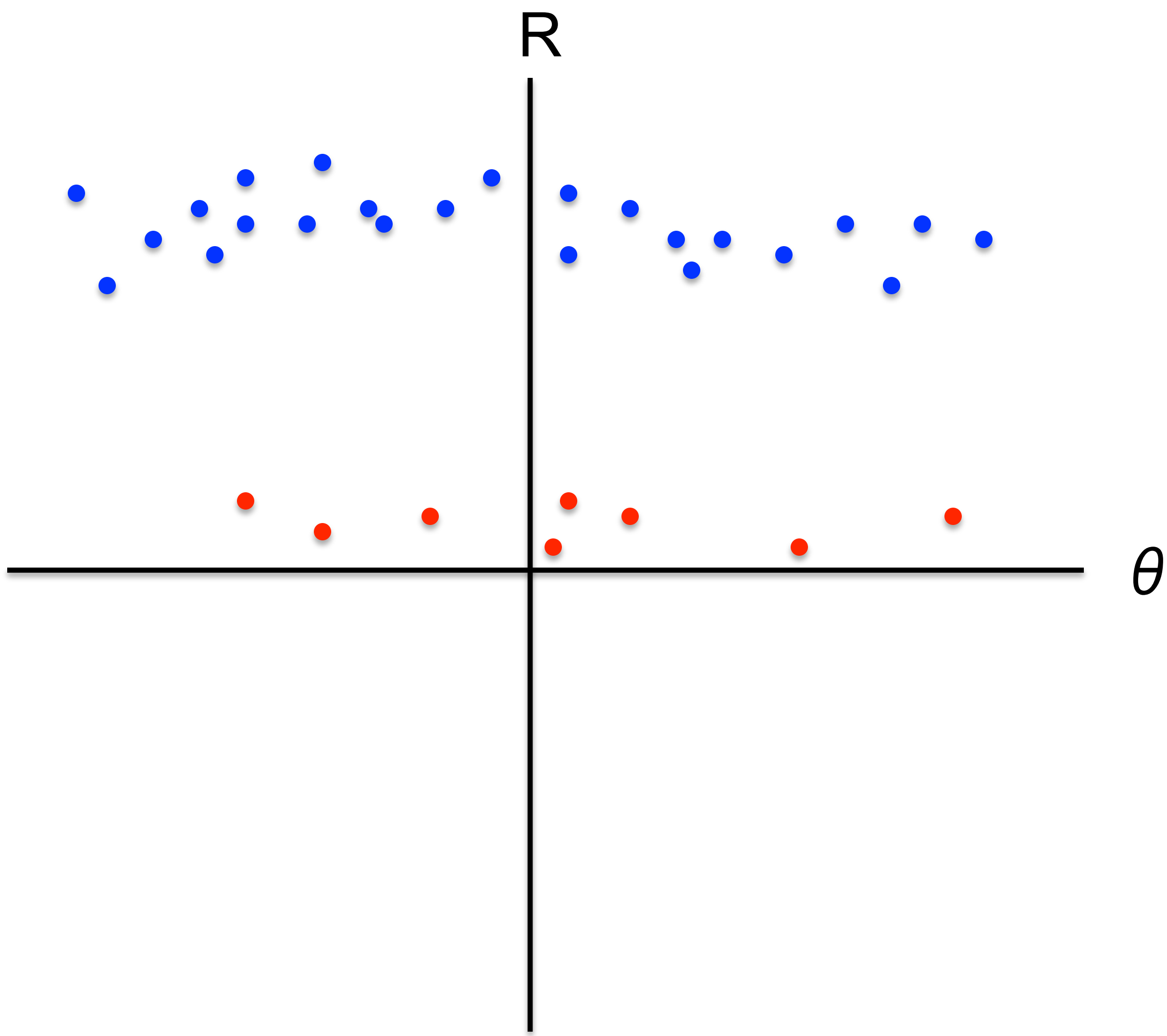
Would be better to have
one cluster here

… and two clusters here

K-means not able to properly cluster

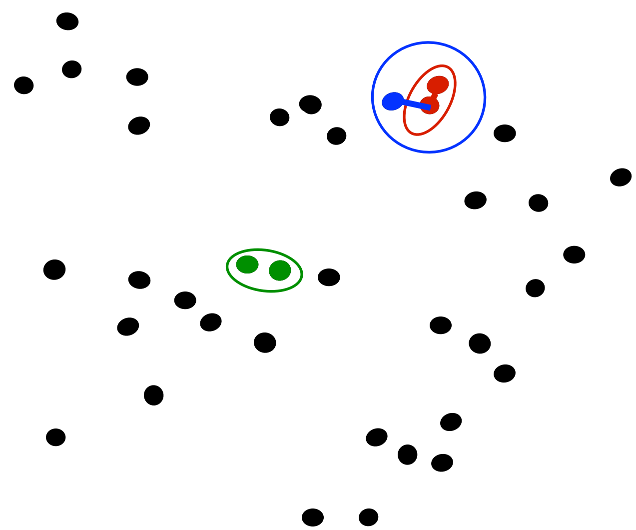


Changing the features (distance function) can help



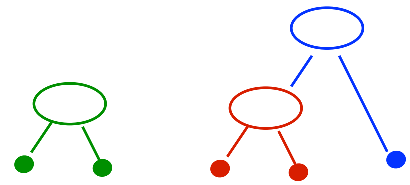
Agglomerative Clustering

- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters



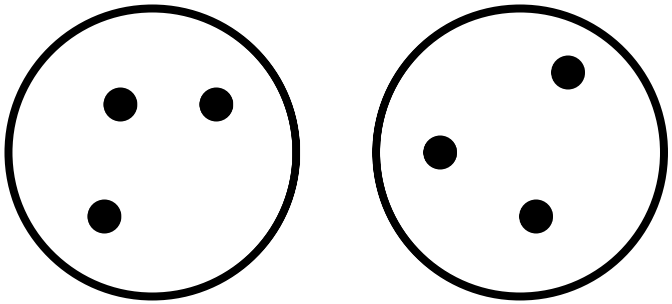
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left

- Produces not one clustering, but a family of clusterings represented by a dendrogram



Agglomerative Clustering

- How should we define “closest” for clusters with multiple elements?

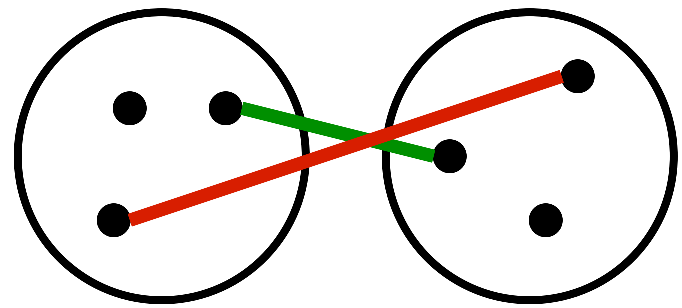


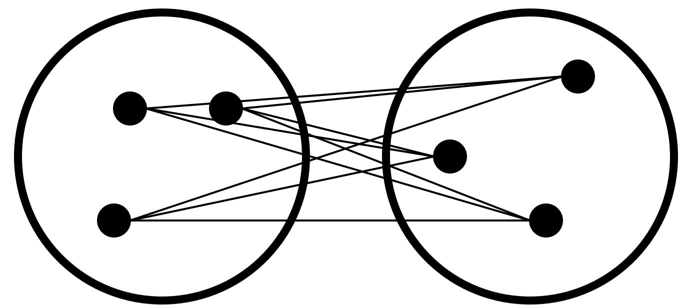
Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?

- Many options:
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs

- Different choices create different clustering behaviors

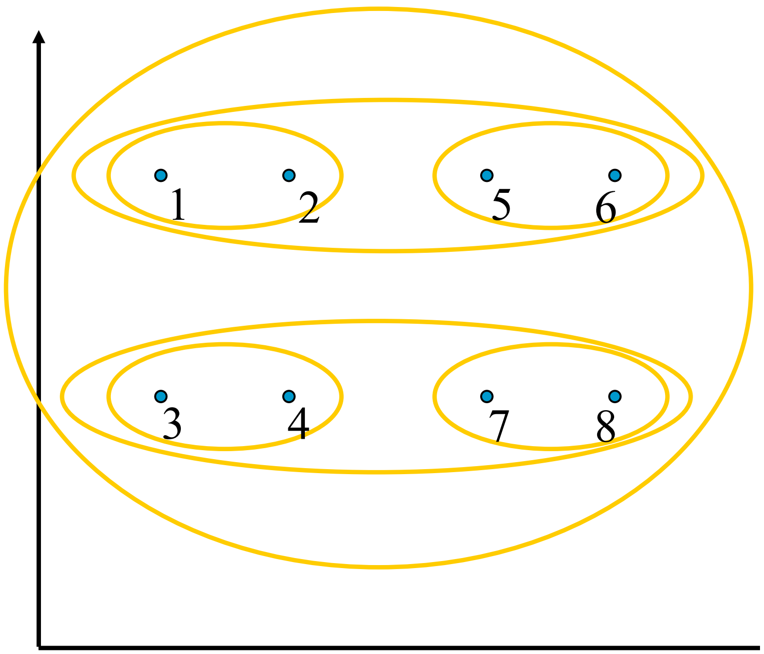




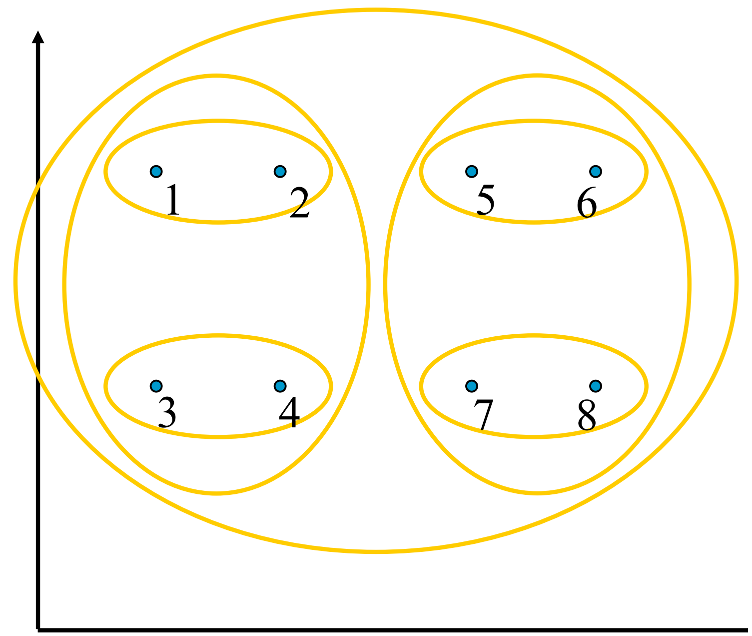
Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?

Closest pair
(single-link clustering)

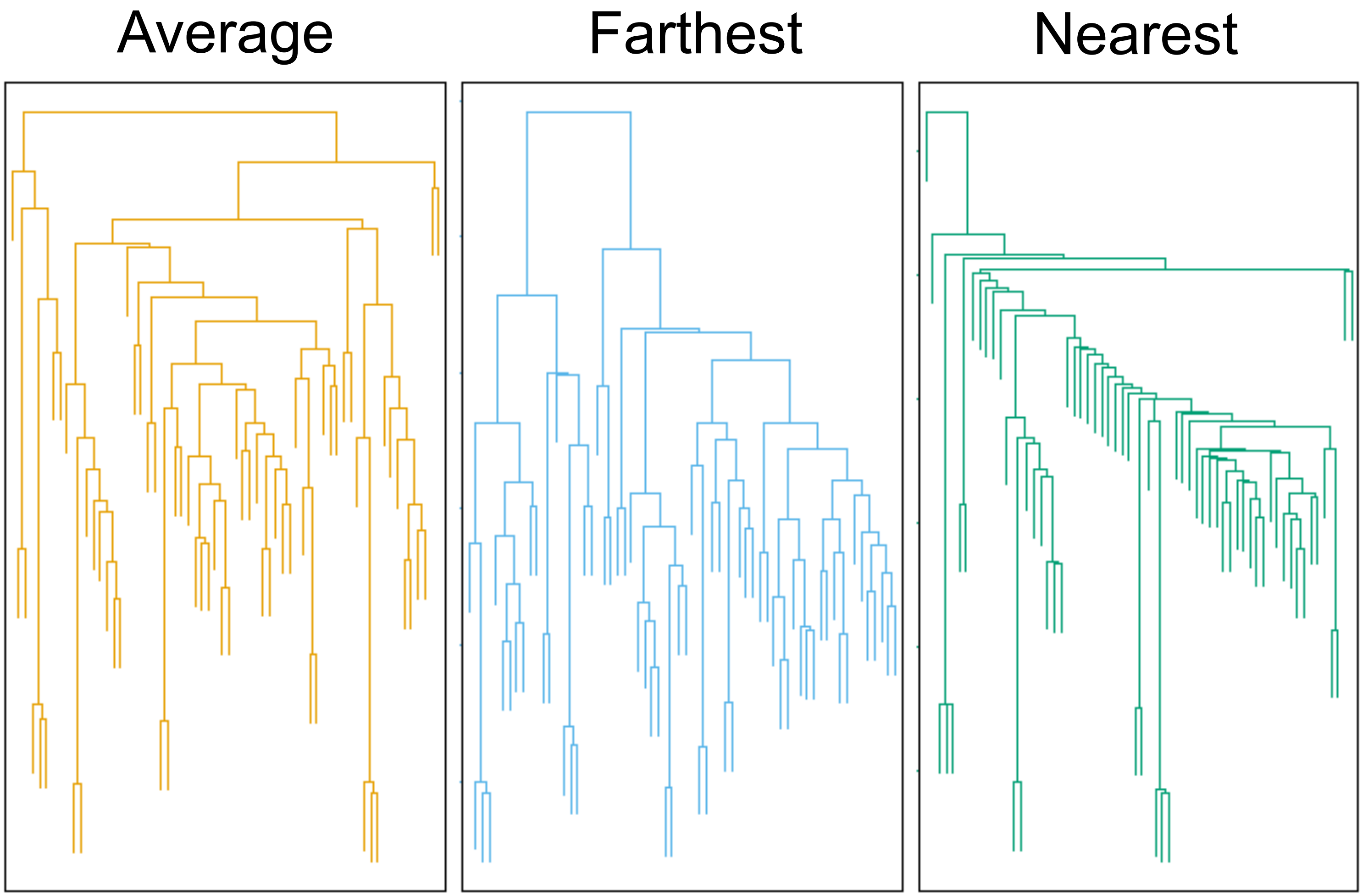


Farthest pair
(complete-link clustering)



[Pictures from Thorsten Joachims]

Clustering Behavior

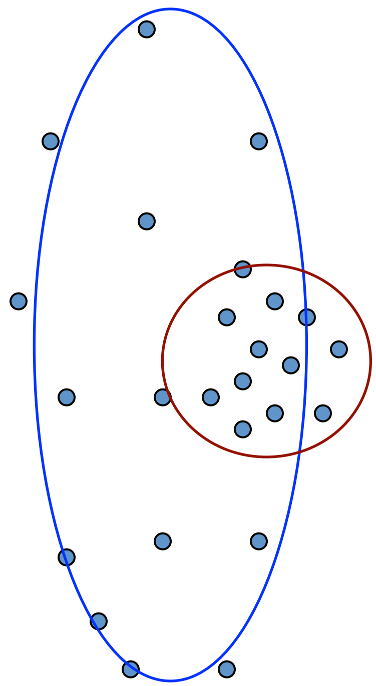


Mouse tumor data from [Hastie *et al.*]

Agglomerative Clustering Questions

- Will agglomerative clustering converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
- Do people ever use it?
- How many clusters to pick?

Reconsidering “**hard assignments**”?



- Clusters may overlap
- Some clusters may be “wider” than others
- Distances can be deceiving!

Extra

- K-means Applets:
  - http://home.dei.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html
  - http://www.cs.washington.edu/research/imagedatabase/demo/kmcluster/