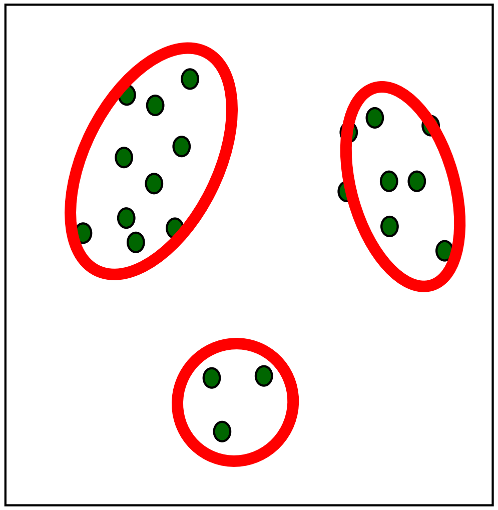
Unsupervised learning

Supervised learning
- Predict target value (“y”) given features (“x”)

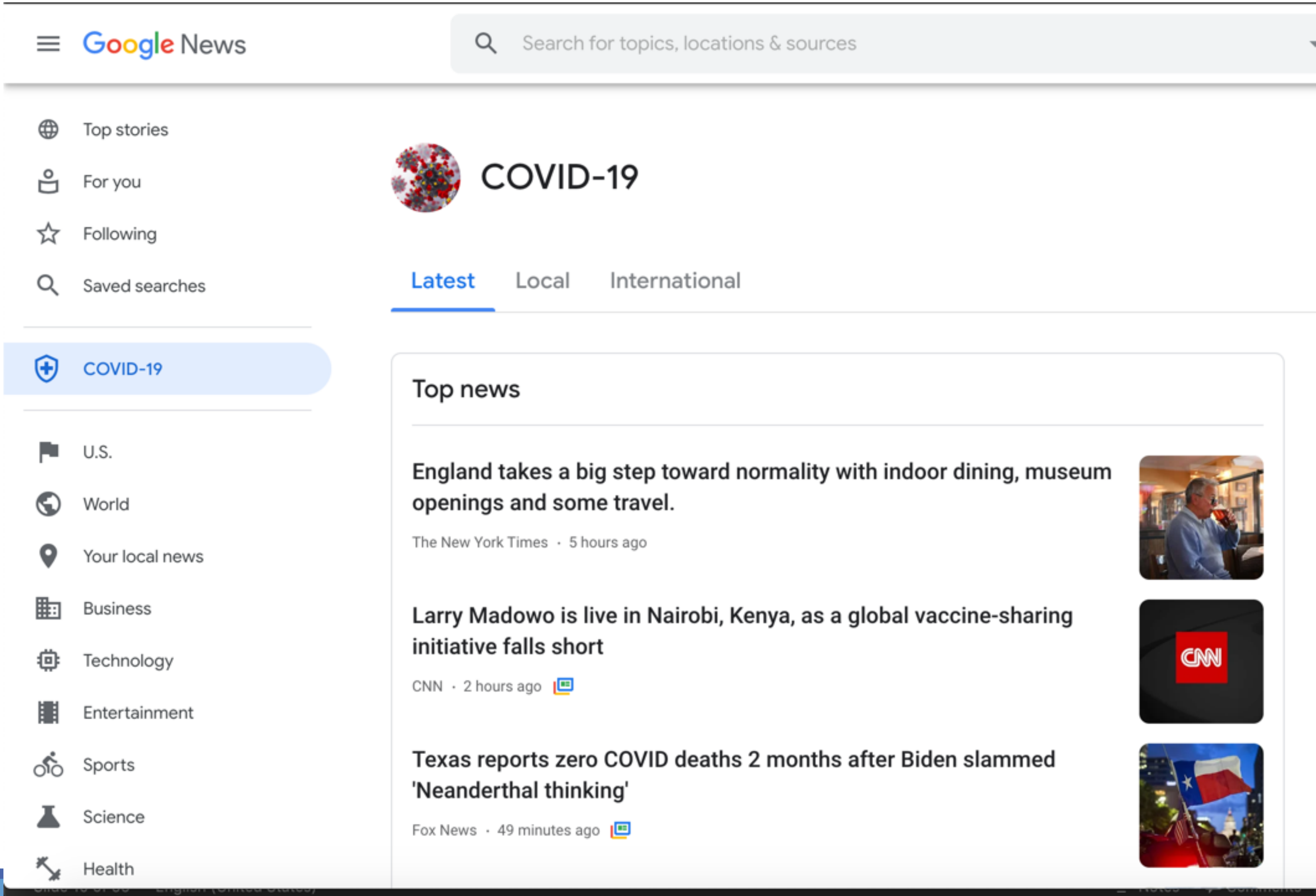


Unsupervised learning
- Understand patterns of data (just “x”)
- Useful for many reasons
  - Data mining (“explain”)
  - Missing data values (“impute”)
  - Representation (feature generation or selection)
  - Density estimation (outlier detection)

One example: *clustering*
- Describe data by discrete “groups” with some characteristics

Source: Pixabay

Clustering News by Search Engines

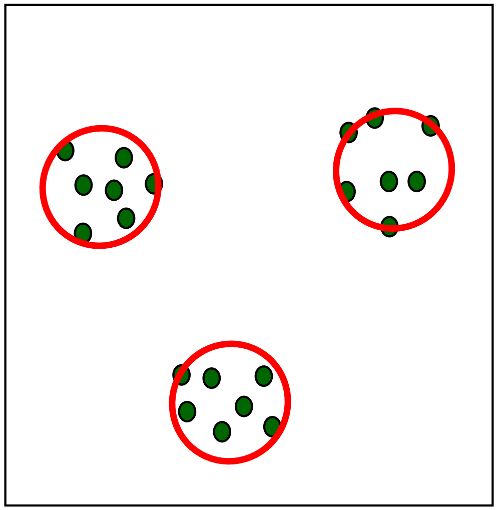


Clustering

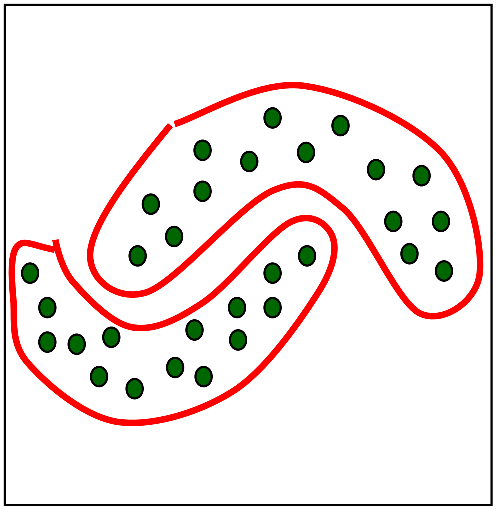
Clustering describes data by “groups”

The meaning of “groups” may vary by data!

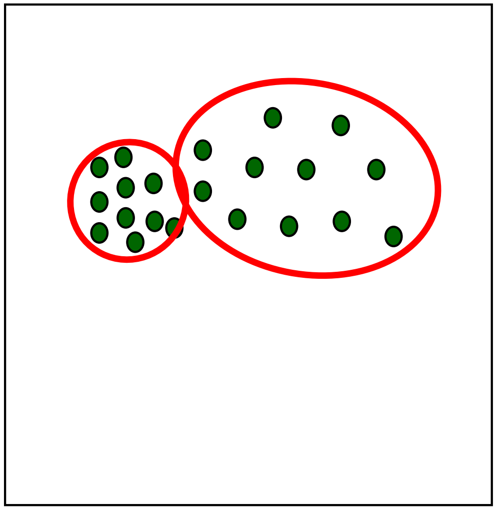
Examples



Location



Shape

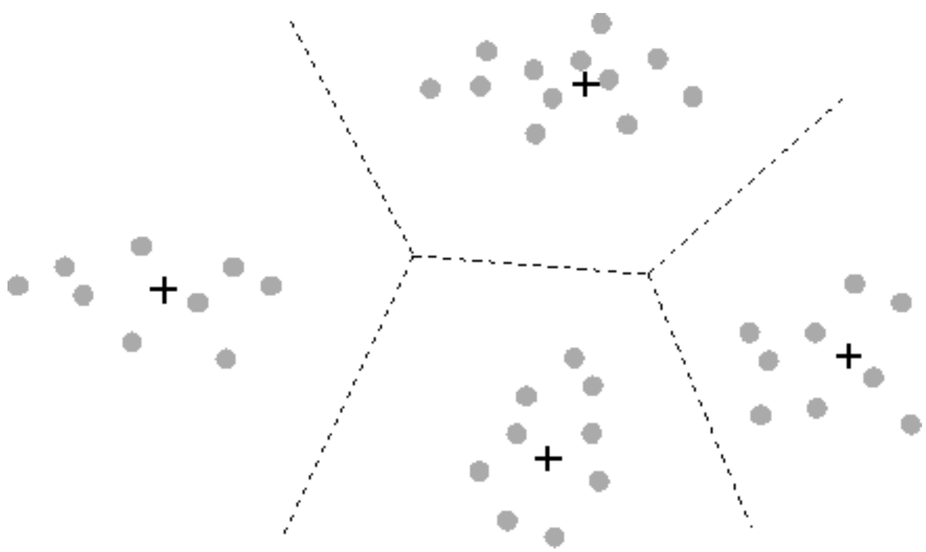


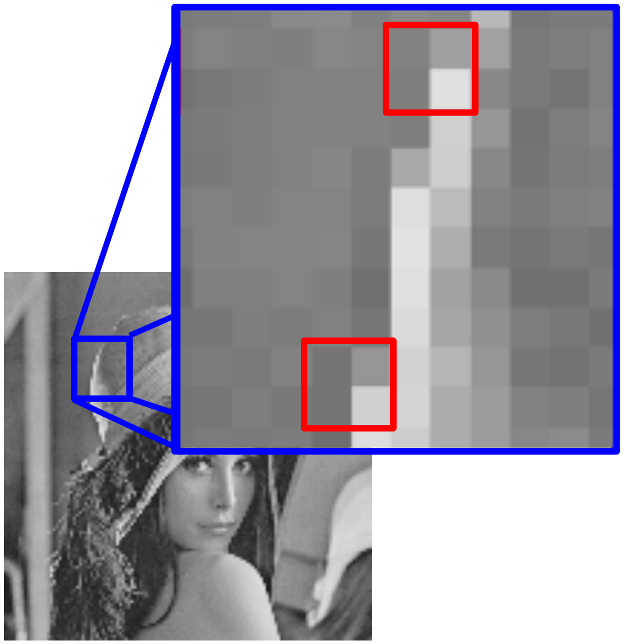
Density

Clustering & Data Compression

Clustering is related to vector quantization

- Dictionary of vectors (the cluster centers)
- Each original value represented using a dictionary index
- Each center "claims" a nearby region (Voronoi region)





Machine Learning

Clustering

K-Means Clustering

Agglomerative Clustering

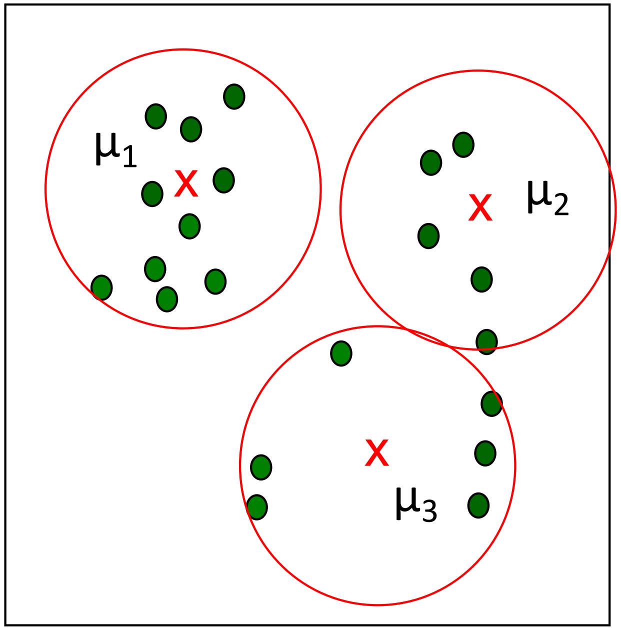
Gaussian Mixtures and EM

K-Means Clustering

A simple clustering algorithm

Iterate between

- Updating the assignment of data to clusters
- Updating the cluster's summarization



Notation:

Data example i has features x_i

Assume K clusters, e.g. K=3

Each cluster c "described" by a center μ_c

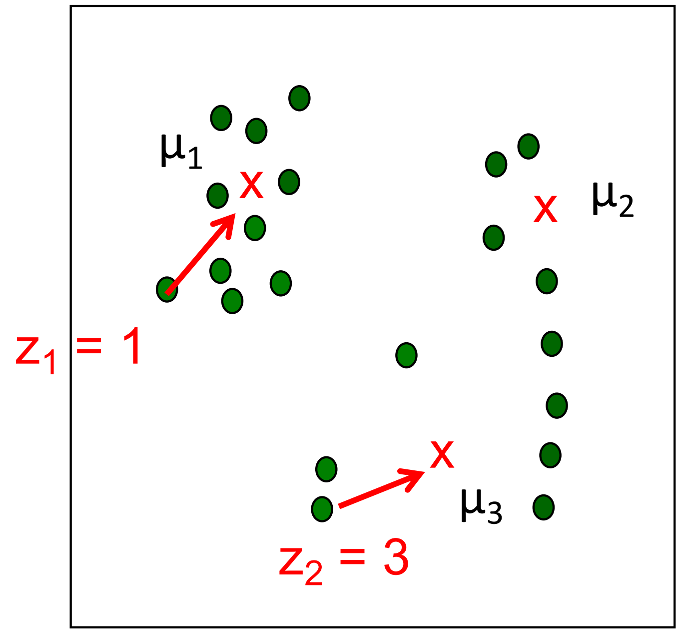
Each cluster will "claim" a set of nearby points

K-Means Clustering

A simple clustering algorithm

Iterate between

- Updating the assignment of data to clusters (z-step)
- Updating the cluster's summarization (μ-step)



Notation:

- Data example i has features x_i
- Assume K clusters
- Each cluster c "described" by a center μ_c
- Each cluster will "claim" a set of nearby points
- "Assignment" of i^{th} example: $z_i \in 1..K$

K-Means Clustering

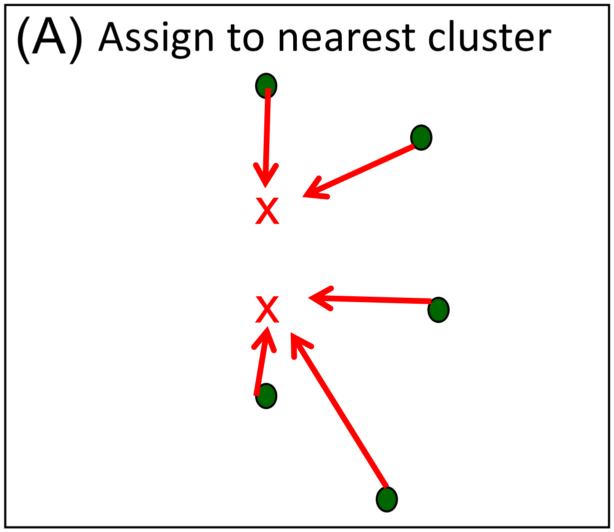
Iterate until convergence:

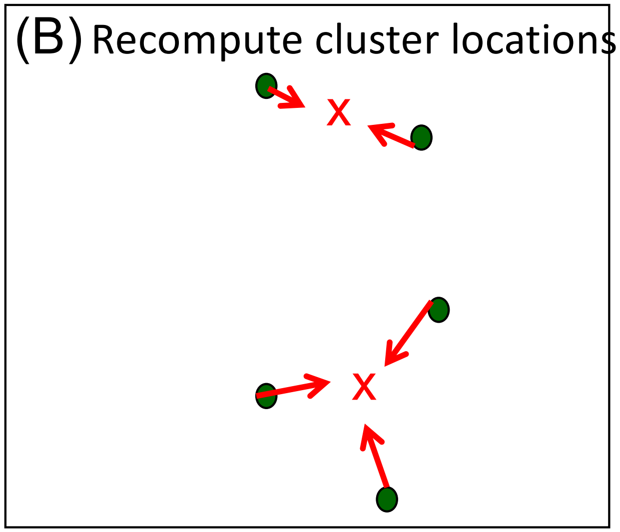
- (A) For each datum, find the closest cluster

$$z_i = \arg\min_c \|x_i - \mu_c\|^2 \qquad \forall i$$

- (B) Set each cluster to the mean of all assigned data:

$$\forall c, \qquad \mu_c = \frac{1}{m_c} \sum_{i \in S_c} x_i \qquad\qquad S_c = \{i : z_i = c\}, \; m_c = |S_c|$$





K-Means Clustering

Optimizing the cost function:

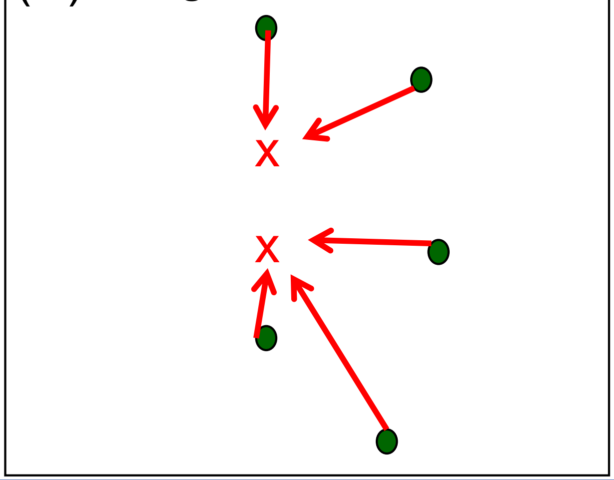
$$C(\underline{z}, \underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$$

Coordinate descent:

Q: does this procedure converge?
hint: monotonicity and boundedness…
A: **Yes**!:
1. the cost function is bounded by 0
2. every update lowers the cost

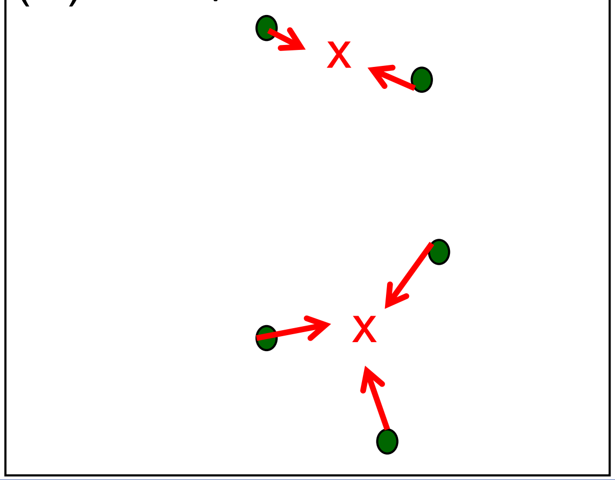
Over the cluster assignments (fixed μ):
Only one term in sum depends on z_i
Minimized by selecting closest μ_c

(A) Assign to nearest cluster



Over the cluster centers (fixed z):
Cluster c only depends on x_i with z_i=c
Minimized by selecting the mean

(B)Recompute cluster locations

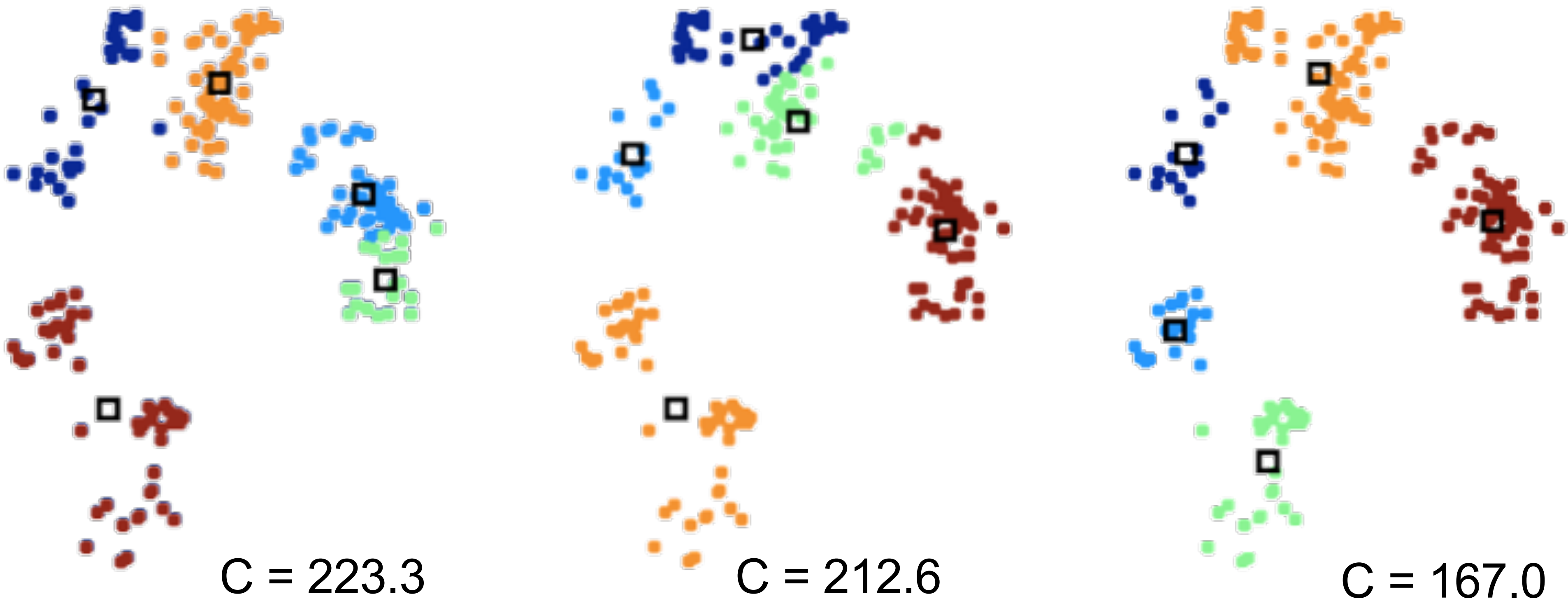


Sensitivity to Initialization

Multiple local optima, depending on initialization

Try different (randomized) initializations

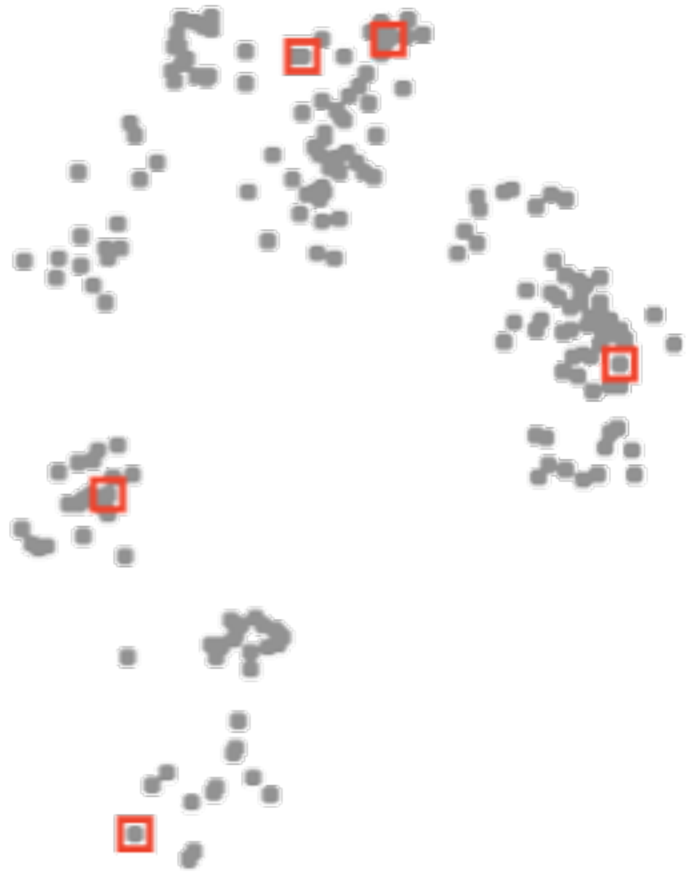
Can use cost C to decide which we prefer



Initialization methods

Random

- Usually, choose random data index
- Ensures centers are near some data
- Issue: may choose nearby points



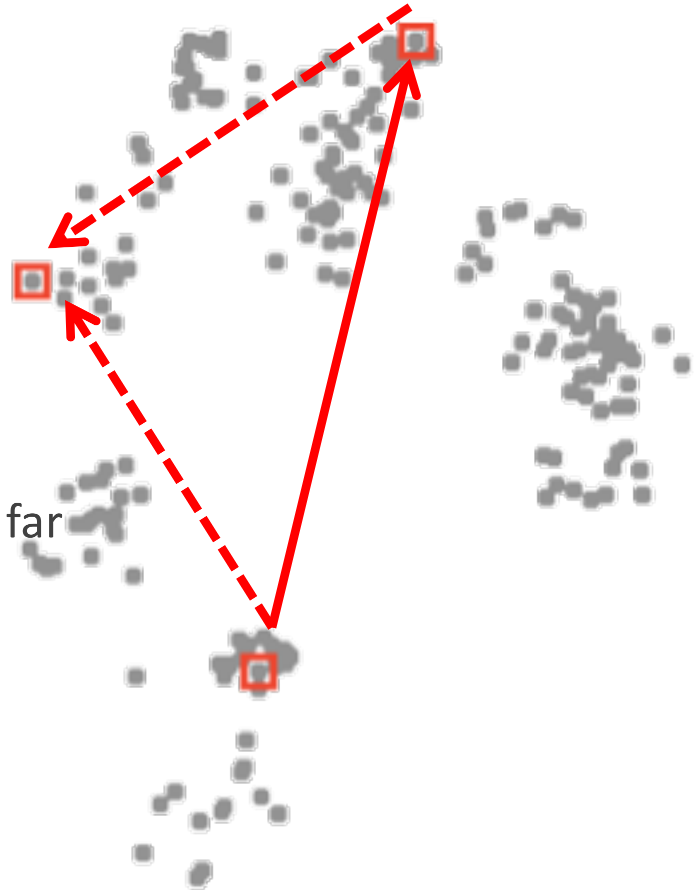
Initialization methods

Random

- Usually, choose random data index
- Ensures centers are near some data
- Issue: may choose nearby points

Distance-based

- Start with one random data point
- Find the point farthest from the clusters chosen so far
- Issue: may choose outliers



Initialization methods

Random

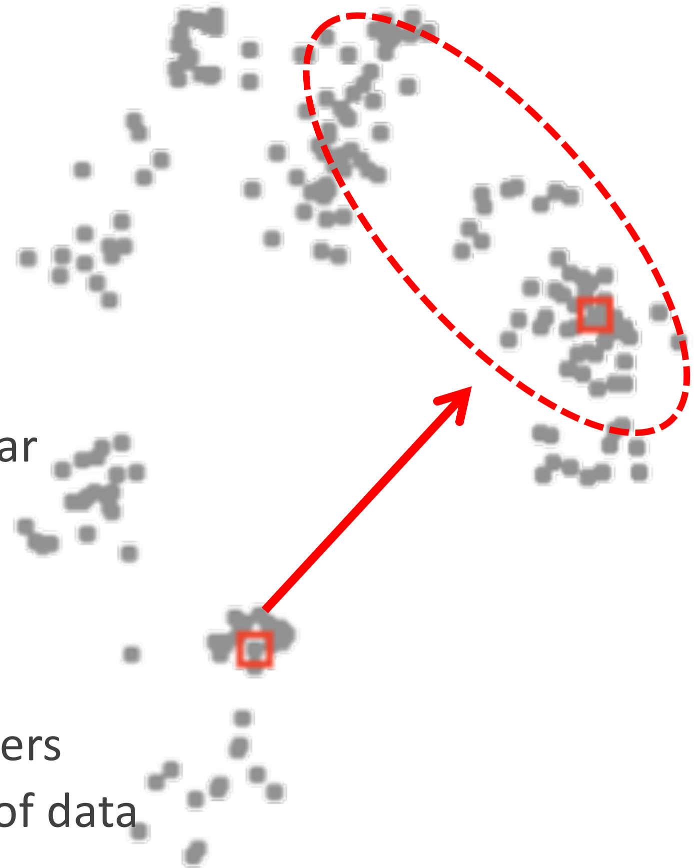
- Usually, choose random data index
- Ensures centers are near some data
- Issue: may choose nearby points

Distance-based

- Start with one random data point
- Find the point farthest from the clusters chosen so far
- Issue: may choose outliers

Random + distance (“k-means++”)

- Choose next points “far but randomly”
- $p(x) \propto$ squared distance from x to current centers
- Likely to put a cluster far away, in a region with lots of data



Out-of-sample points

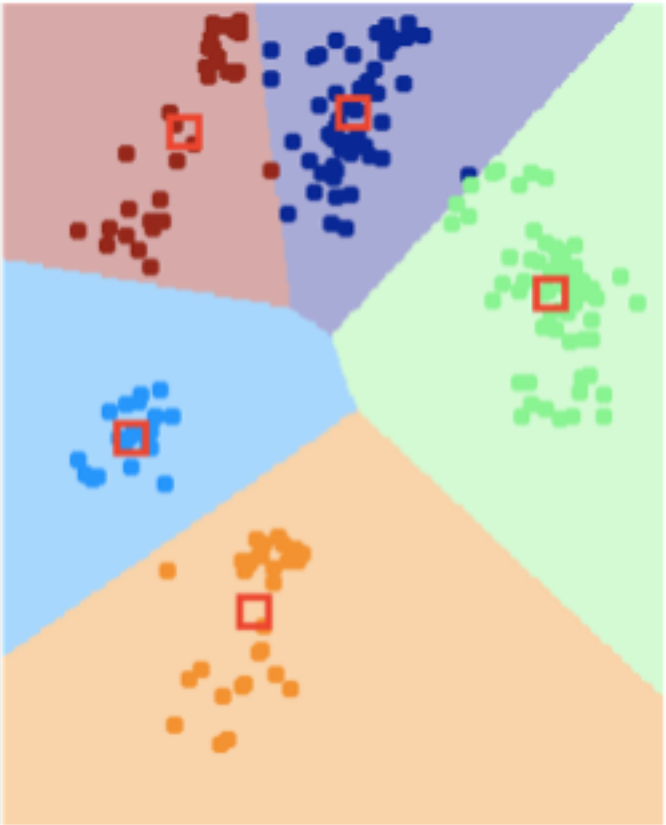
Often want to use clustering on new data

Easy for k-means: choose nearest cluster center

```
# perform clustering
Z , mu , score = kmeans(X, K);

# cluster id = nearest center
L = knnClassify(mu, range(K), 1);

# assign in- or out-of-sample points
Z = L.predict(X);
```

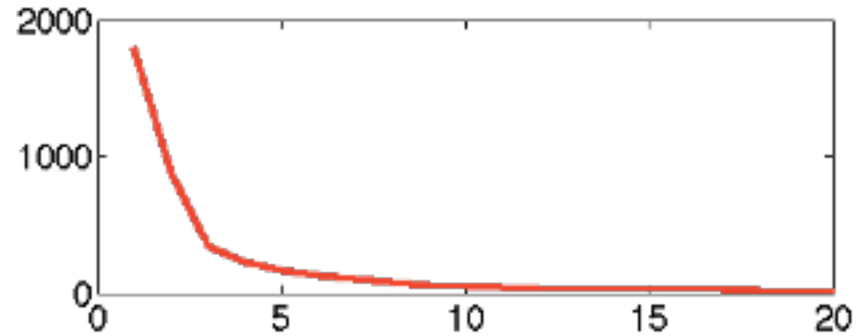


Choosing Number of Clusters

With cost function

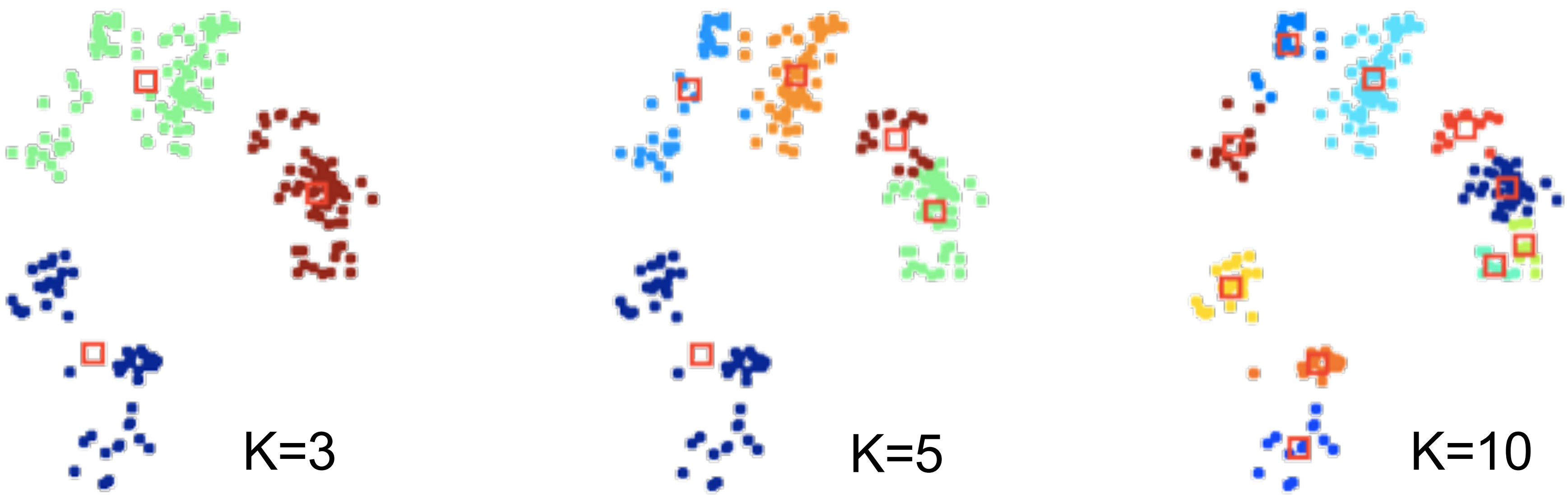
$$C(\underline{z}, \underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$$

what is the optimal value of k?



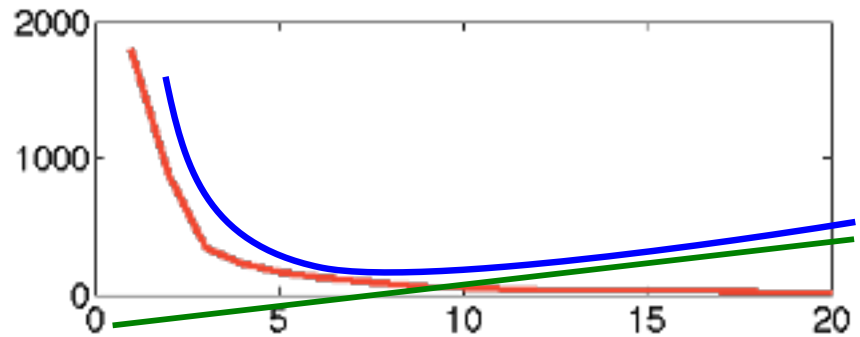
Cost always decreases with k!

A model complexity issue…



Choosing Number of Clusters

With cost function $C(\underline{z}, \underline{\mu}) = \sum_i \|x_i - \mu_{z_i}\|^2$



what is the optimal value of k?

Cost always decreases with k!

A model complexity issue…

One solution is to penalize for complexity

- Add penalty: Total = Error + Complexity
- Now more clusters can increase cost, if they don't help "enough"
- Ex: simplified BIC penalty $$J(\underline{z}, \underline{\mu}) = \log \left[\frac{1}{m\, d} \sum_i \|x_i - \mu_{z_i}\|^2 \right] + k \frac{\log m}{m}$$
- More precise version: see e.g. "X-means" (Pelleg & Moore 2000)

Summary

K-Means clustering

- Clusters described as locations (“centers”) in feature space

Procedure

- Initialize cluster centers
- Iterate: assign each data point to its closest cluster center
- : move cluster centers to minimize mean squared error

Properties

- Coordinate descent on MSE criterion
- Prone to local optima; initialization important
- Out-of-sample data

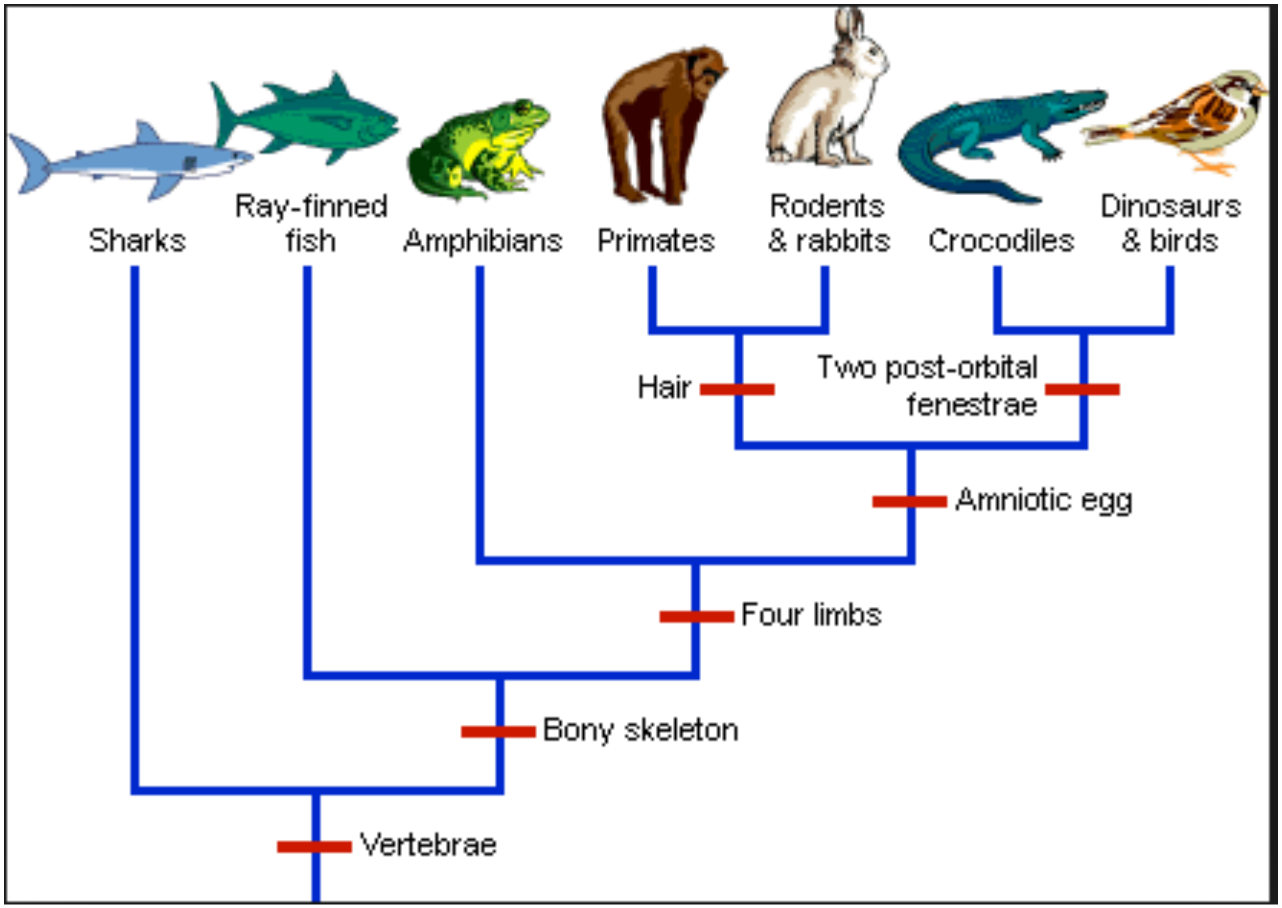
Choosing the # of clusters, K

- Model selection problem; penalize for complexity (BIC, etc.)

Machine Learning

- Clustering
- K-Means Clustering
- **Agglomerative Clustering**
- Gaussian Mixtures and EM

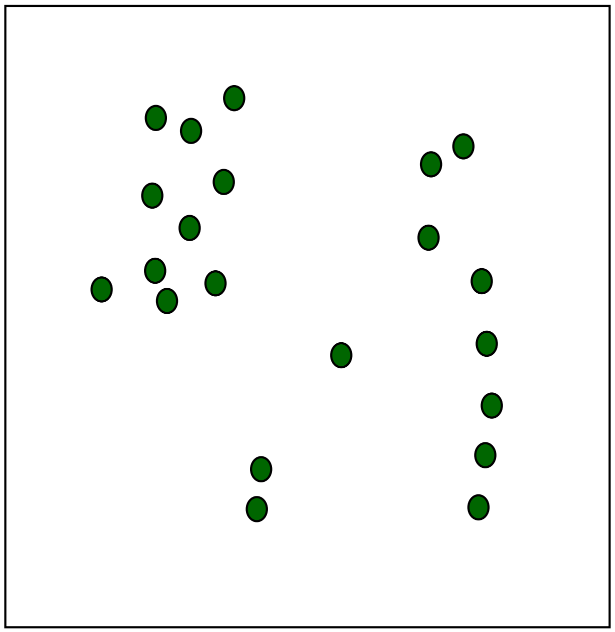
Hierarchical Clustering Example



Hierarchical Agglomerative Clustering

Initially, every datum is a cluster

Data:



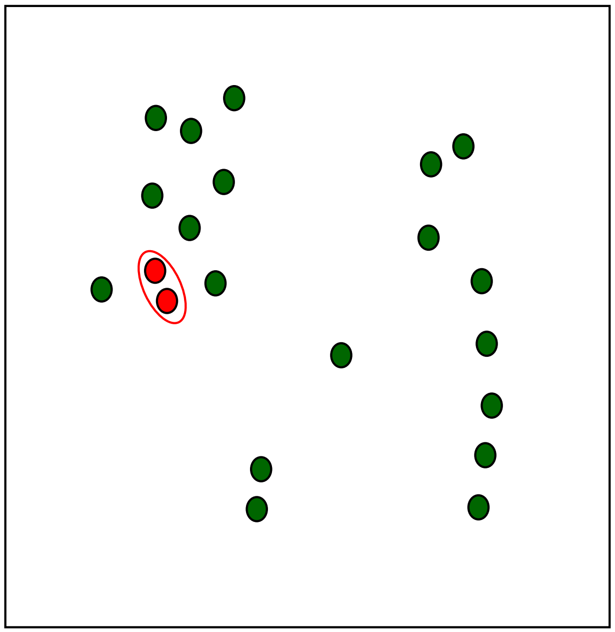
- A simple clustering algorithm
- Define a distance (or dissimilarity) between clusters (we'll return to this)
- Initialize: every example is a cluster
- Iterate:
  - Compute distances between all clusters (store for efficiency)
  - Merge two closest clusters
- Save both clustering and sequence of cluster operations
- "Dendrogram"

Algorithmic Complexity: $O(m^2 \log m)$ +

Iteration 1

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:

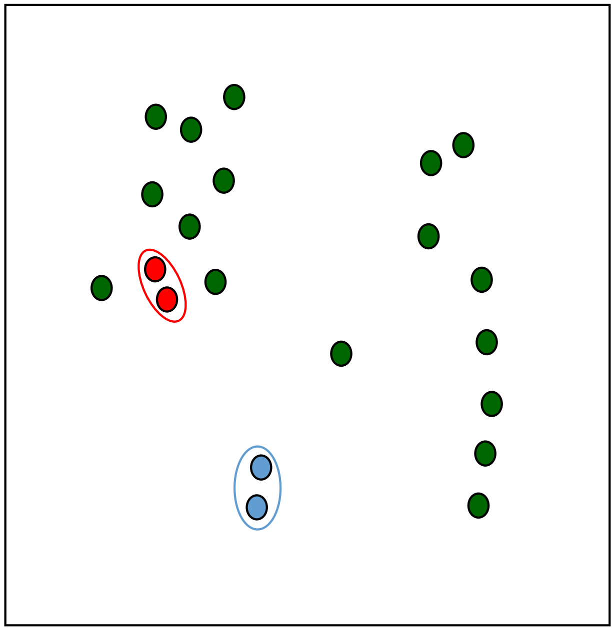
Height of the join indicates dissimilarity

Algorithmic Complexity: $O(m^2 \log m) + O(m \log m) +$

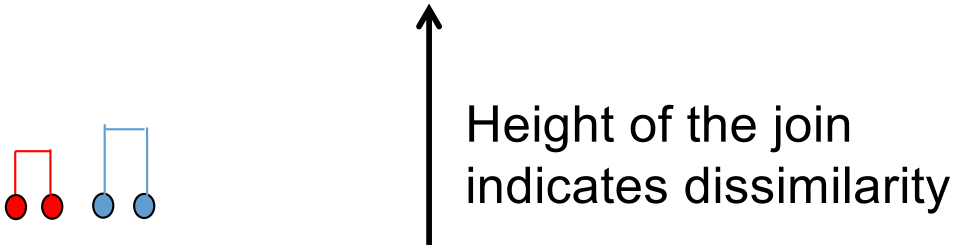
Iteration 2

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:

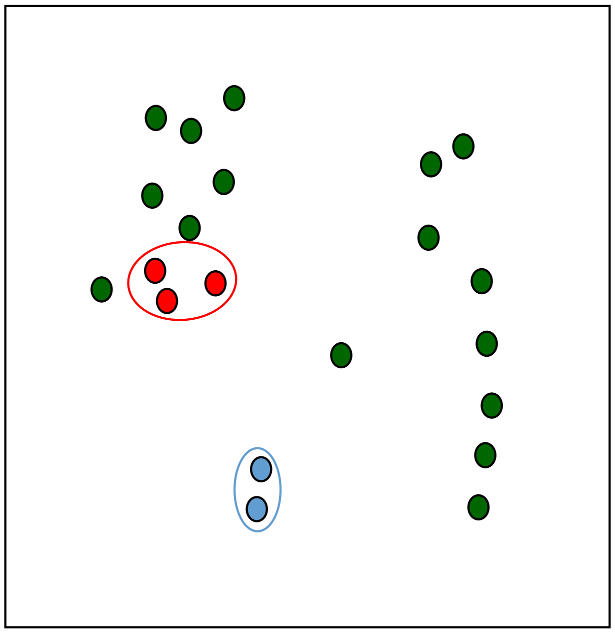


Algorithmic Complexity: $O(m^2 \log m) + 2*O(m \log m) +$

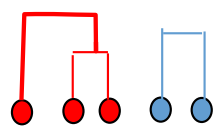
Iteration 3

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:



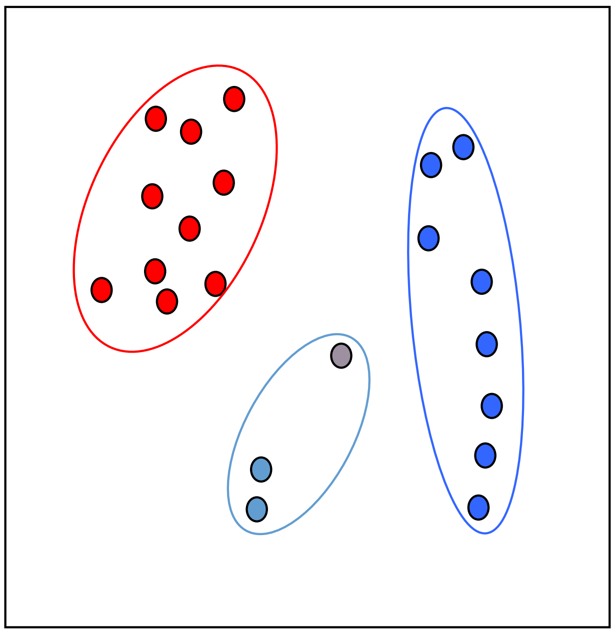
Height of the join indicates dissimilarity

Algorithmic Complexity: $O(m^2 \log m) + 3*O(m \log m) +$

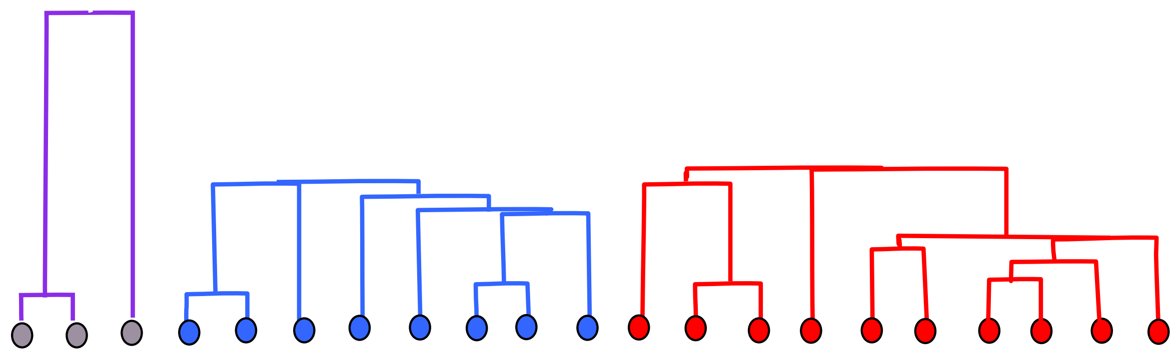
Iteration m-3

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:



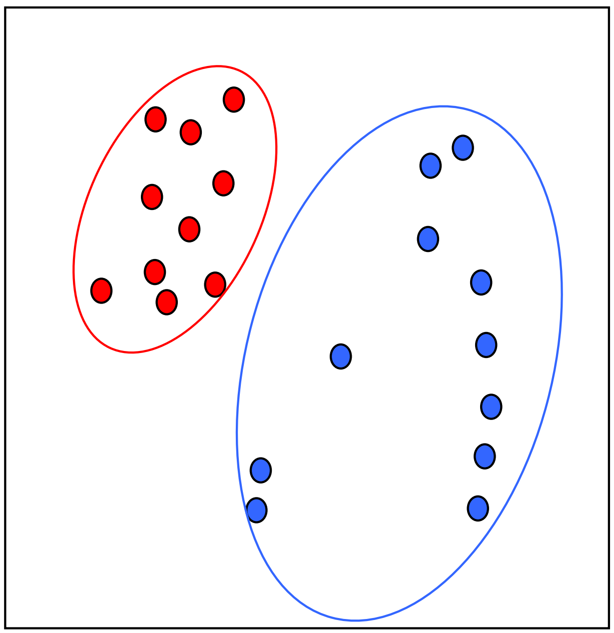
In mltools: "agglomerative"

Algorithmic Complexity: $O(m^2 \log m) + (m\text{-}3)*O(m \log m) +$

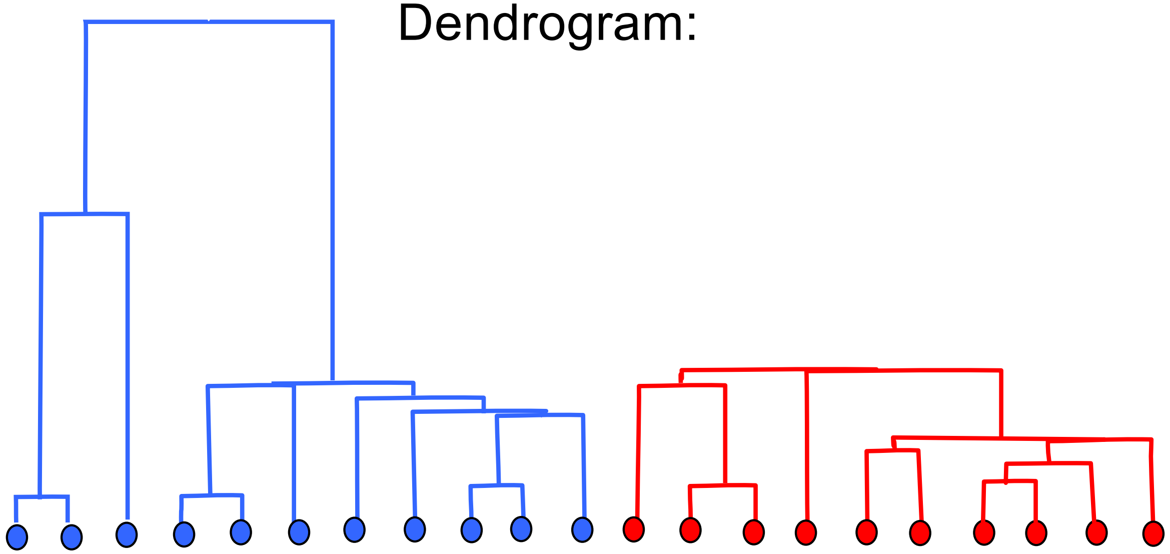
Iteration m-2

Builds up a sequence of clusters ("hierarchical")

Data:



Dendrogram:



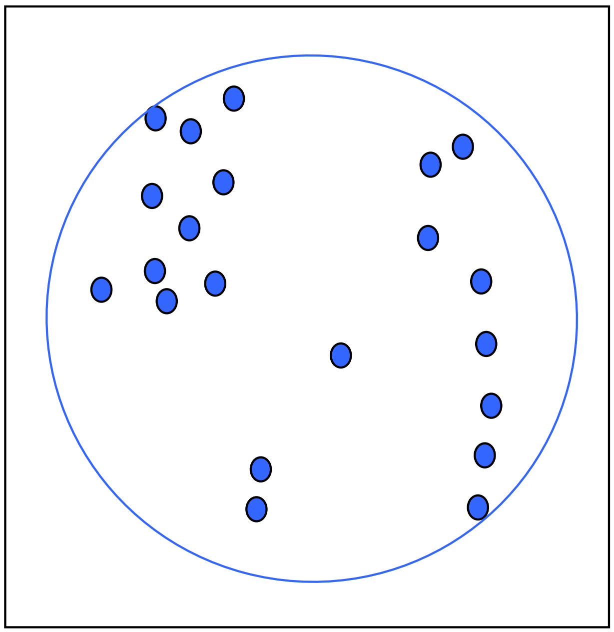
In mltools: "agglomerative"

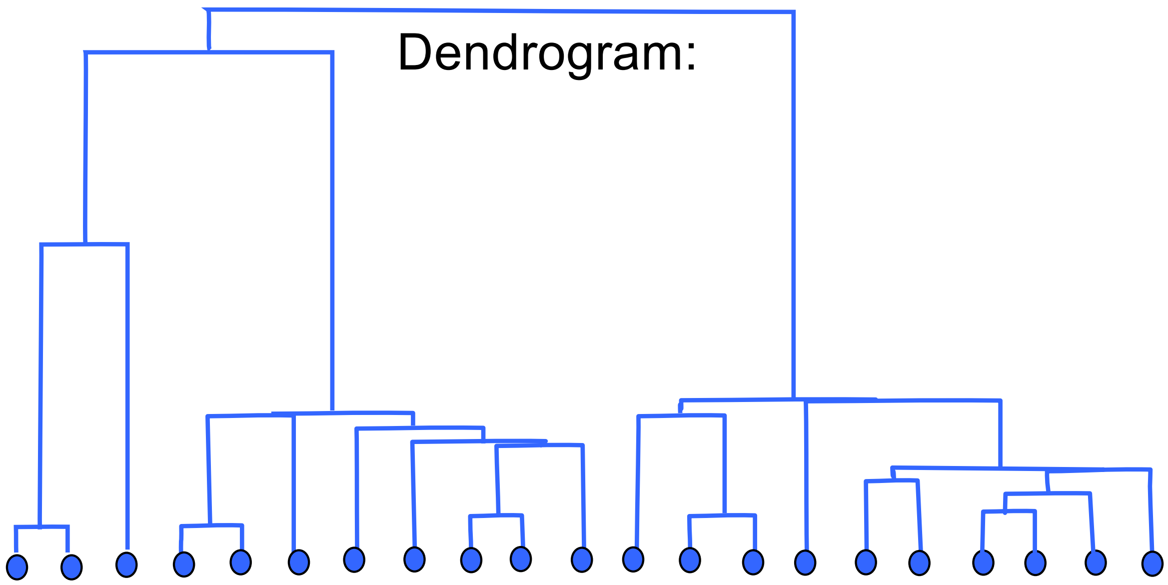
Algorithmic Complexity: $O(m^2 \log m) + (m-2)*O(m \log m) +$

Iteration m-1

Builds up a sequence of clusters (“hierarchical”)

Data:





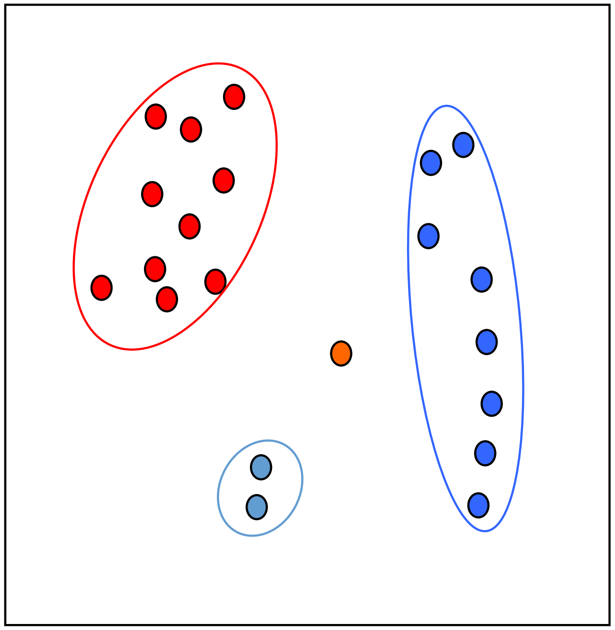
In mltools: “agglomerative”

Algorithmic Complexity: $O(m^2 \log m) + (m-1)*O(m \log m) = O(m^2 \log m)$

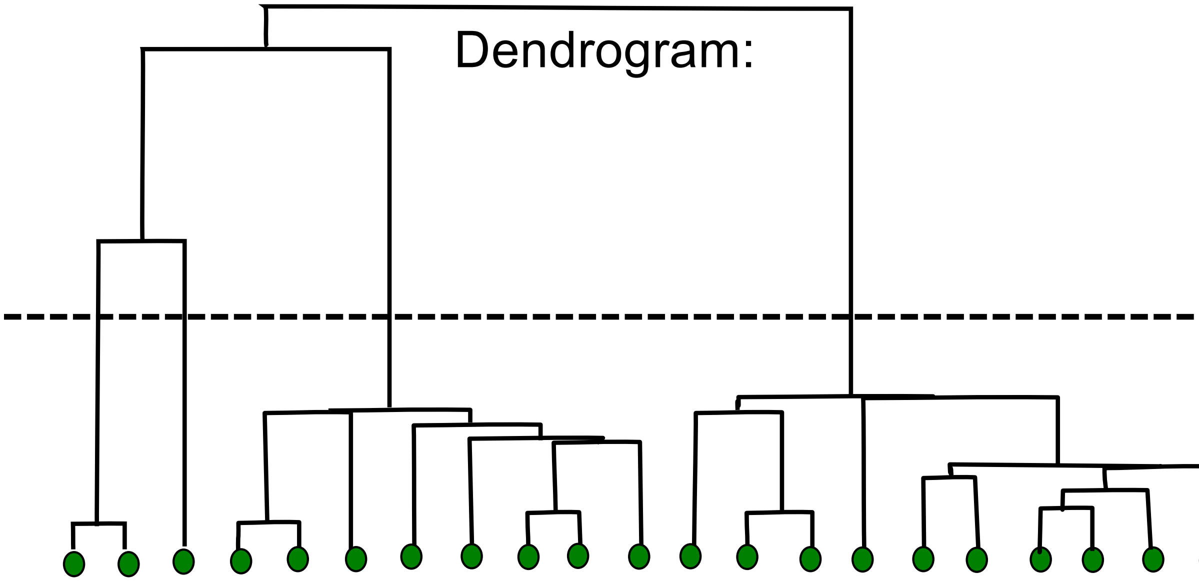
From dendrogram to clusters

Given the sequence, can select a number of clusters or a dissimilarity threshold:

Data:



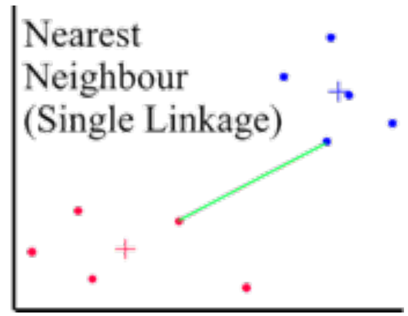
Dendrogram:



Algorithmic Complexity: $O(m^2 \log m) + (m-1)*O(m \log m) = O(m^2 \log m)$

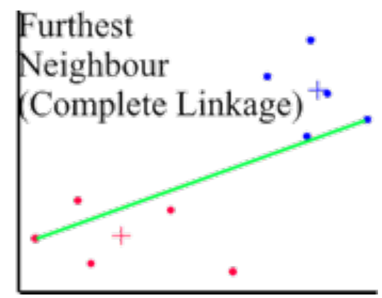
Cluster distances

$$D_{\min}(C_i, C_j) = \min_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



produces minimal spanning tree.

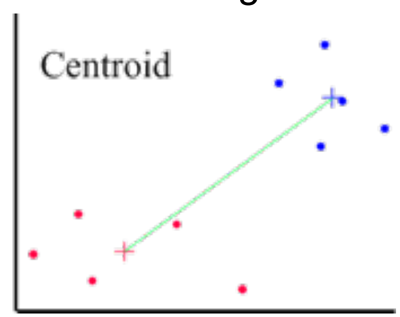
$$D_{\max}(C_i, C_j) = \max_{x \in C_i,\ y \in C_j} \|x - y\|^2$$



avoids elongated clusters.

$$D_{\mathrm{avg}}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i,\ y \in C_j} \|x - y\|^2$$

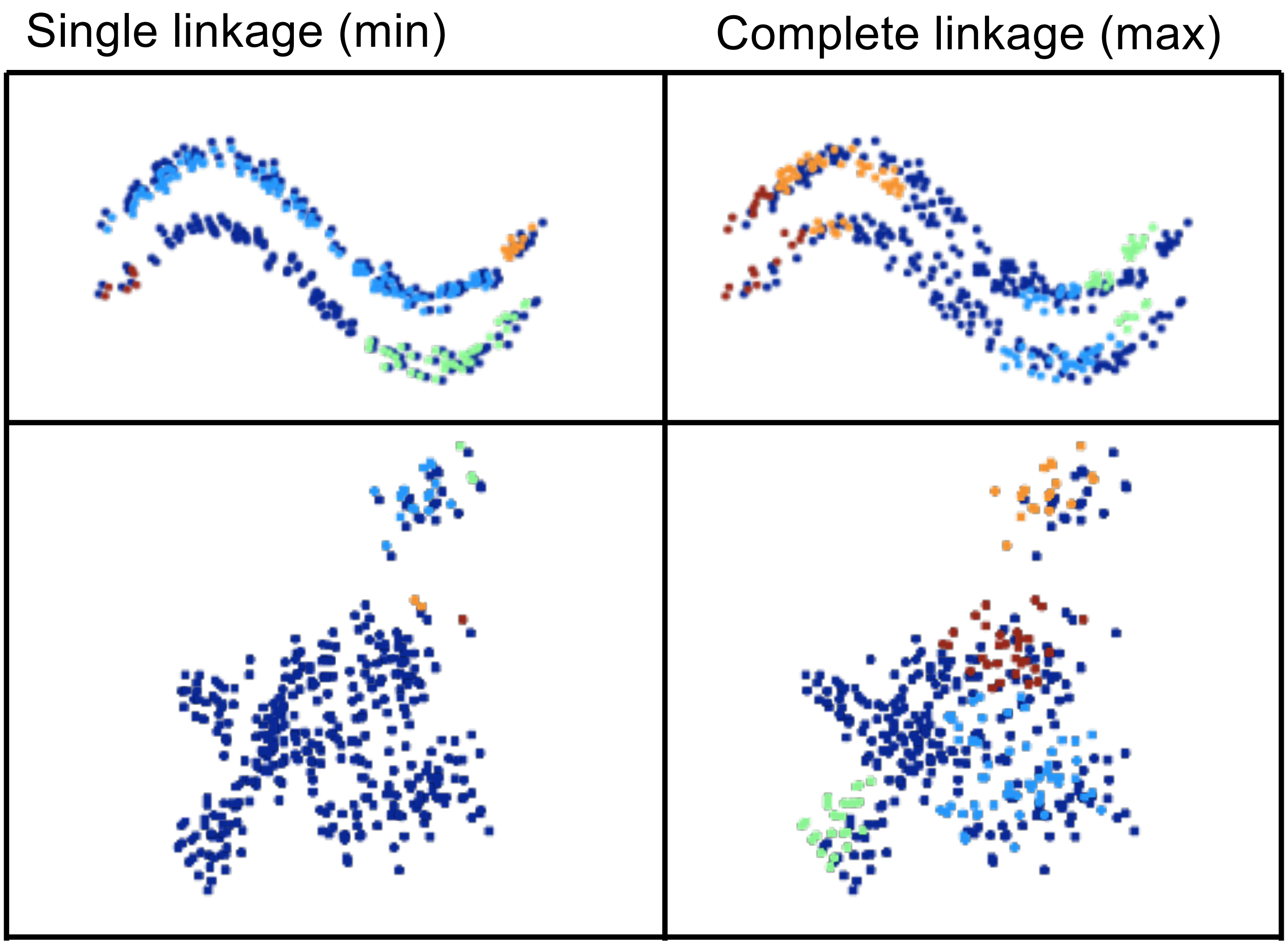
$$D_{\mathrm{means}}(C_i, C_j) = \|\mu_i - \mu_j\|^2$$



Constant time (WHY?): D(A,C) → D(A+B,C)
D(B,C) → D(A+B,C)

Dissimilarity choice will affect clusters created

Cluster distances



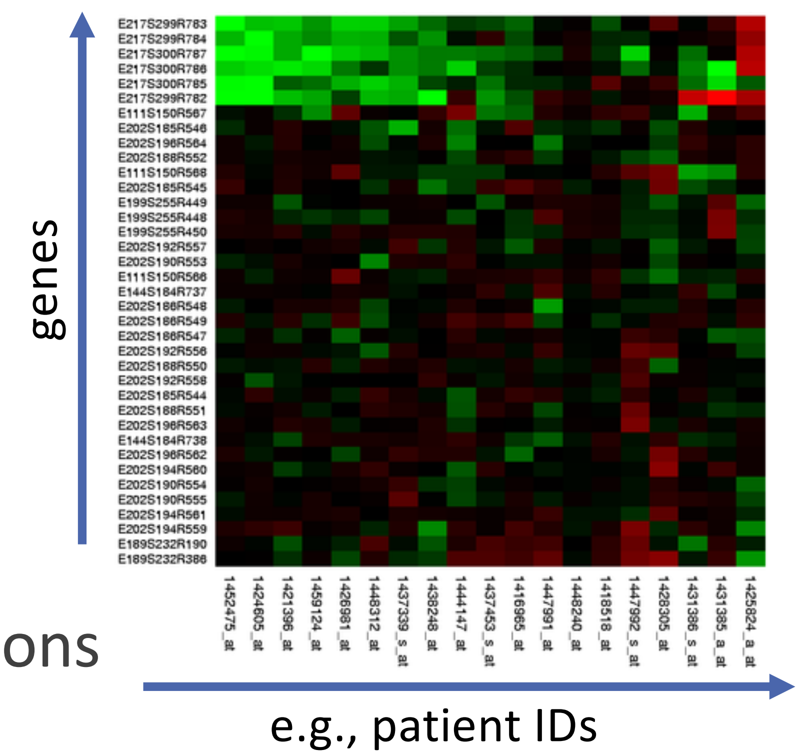
Example: microarray expression

Measure gene expression

Various experimental conditions
- Disease v. normal
- Time
- Patient identities

Explore similarities
- Which genes are similar to which?
- Which patients are similar?

Cluster on both genes and conditions



Summary

Agglomerative clustering

- Choose a cluster distance / dissimilarity scoring method
- Successively merge closest pair of clusters
- "Dendrogram" shows sequence of merges & distances
- Complexity: $O(m^2 \log m)$

Agglomerative clusters depend critically on dissimilarity

- Choice determines characteristics of "found" clusters

"Clustergram" for understanding data matrix

- Build clusters on rows (data) and columns (features)
- Reorder data & features to expose behavior across groups