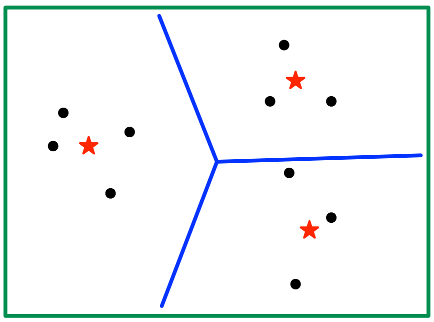
The basics of clustering

A: K-means clustering

The k-means optimization problem

- Input: Points $x_1, \ldots, x_n \in \mathbb{R}^d$; integer k
- Output: "Centers", or representatives, $\mu_1, \ldots, \mu_k \in \mathbb{R}^d$
- Goal: Minimize average squared distance between points and their nearest representatives:

$$\text{cost}(\mu_1, \ldots, \mu_k) = \sum_{i=1}^{n} \min_j \|x_i - \mu_j\|^2$$

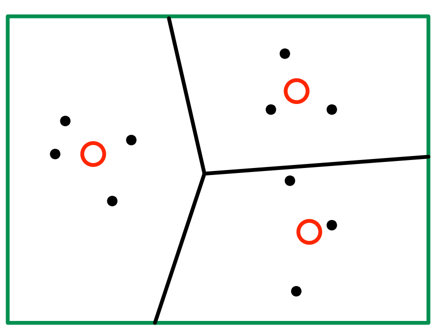


Centers carve $\mathbb{R}^d$ into k **convex** regions: μ_j's region consists of points for which it is the closest center.

Lloyd's k-means algorithm

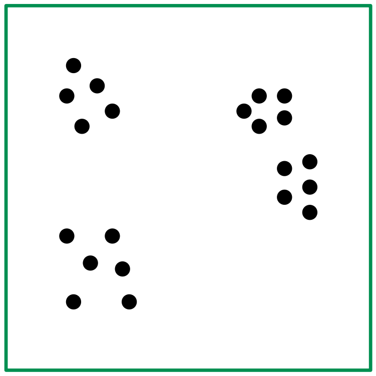
NP-hard optimization problem. Heuristic: "k-means algorithm".

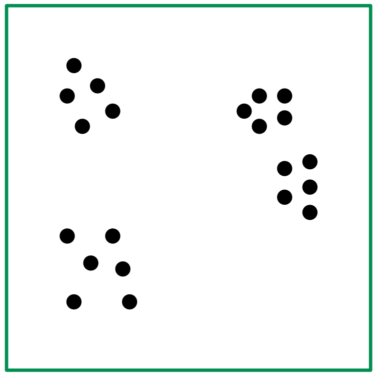
- Initialize centers $\mu_1, \ldots, \mu_k$ in some manner.
- Repeat until convergence:
  - Assign each point to its closest center.
  - Update each μ_j to the mean of the points assigned to it.



Each iteration reduces the cost $\Rightarrow$ convergence to a local optimum.

Initialization matters





Initializing the k-means algorithm

Typical practice: choose k data points at random as the initial centers.

Another common trick: start with extra centers, then prune later.

A particularly good initializer: **k-means++**

- Pick a data point x at random as the first center
- Let $C = \{x\}$ (centers chosen so far)
- Repeat until desired number of centers is attained:
  - Pick a data point x at random from the following distribution:

    $$\Pr(x) \propto \mathrm{dist}(x, C)^2,$$

    where $\mathrm{dist}(x, C) = \min_{z \in C} \|x - z\|$
  - Add x to C

B: Two uses of clustering

Two common uses of clustering

- Vector quantization
  Find a finite set of representatives that provides good coverage of a complex, possibly infinite, high-dimensional space.

- Finding meaningful structure in data
  Finding salient grouping in data.

Representing images using k-means codewords

How to represent a collection of images as fixed-length vectors?

- Take all $\ell \times \ell$ patches in all images. Extract features for each.
- Run k-means on this entire collection to get k centers.
- Now associate any image patch with its nearest center.
- Represent an image by a histogram over $\{1, 2, \ldots, k\}$.

Looking for natural groups in data

"Animals with attributes" data set

- 50 animals: antelope, grizzly bear, beaver, dalmatian, tiger, ...
- 85 attributes: longneck, tail, walks, swims, nocturnal, forager, desert, bush, plains, ...
- Each animal gets a score $(0 - 100)$ along each attribute
- 50 data points in $\mathbb{R}^{85}$

Apply k-means with $k = 10$ and look at grouping obtained.

1. zebra
2. spider monkey, gorilla, chimpanzee
3. tiger, leopard, wolf, bobcat, lion
4. hippopotamus, elephant, rhinoceros
5. killer whale, blue whale, humpback whale, seal, walrus, dolphin
6. giant panda
7. skunk, mole, hamster, squirrel, rabbit, bat, rat, weasel, mouse, raccoon
8. antelope, horse, moose, ox, sheep, giraffe, buffalo, deer, pig, cow
9. beaver, otter
10. grizzly bear, dalmatian, persian cat, german shepherd, siamese cat, fox, chihuahua, polar bear, collie

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8. antelope, horse, moose, ox, sheep, giraffe, deer, cow
9. hamster, rabbit
10. grizzly bear, polar bear

C: Beyond k-means

K-means: the good and the bad

The good:

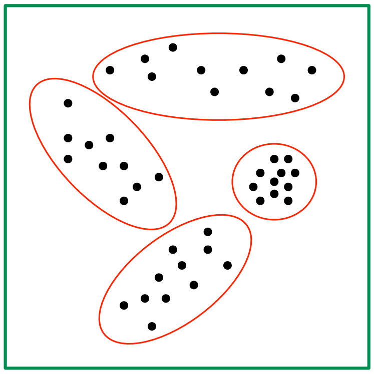
- Fast and easy.
- Effective in quantization.

The bad:

- Geared towards data in which the clusters are spherical, and of roughly the same radius.

Is there is a similarly-simple algorithm in which clusters of more general shape are accommodated?

Preview: Mixtures of Gaussians



Each of the k clusters is specified by:

- a Gaussian distribution $P_j = N(\mu_j, \Sigma_j)$
- a mixing weight π_j

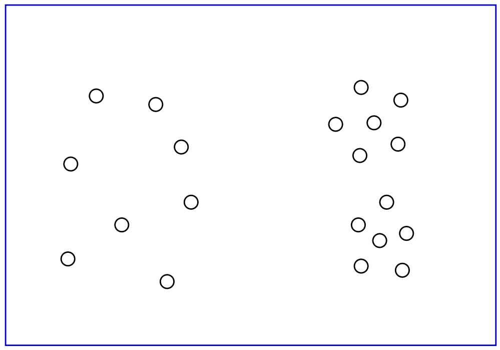
Overall distribution over $\mathbb{R}^d$: a **mixture of Gaussians**

$$\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x)$$

D: Hierarchical clustering

Hierarchical clustering

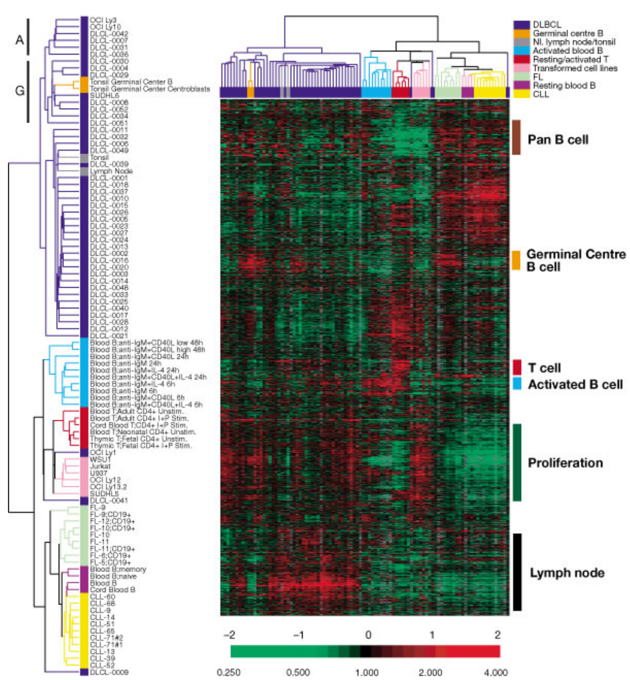
Choosing the number of clusters (k) is difficult.



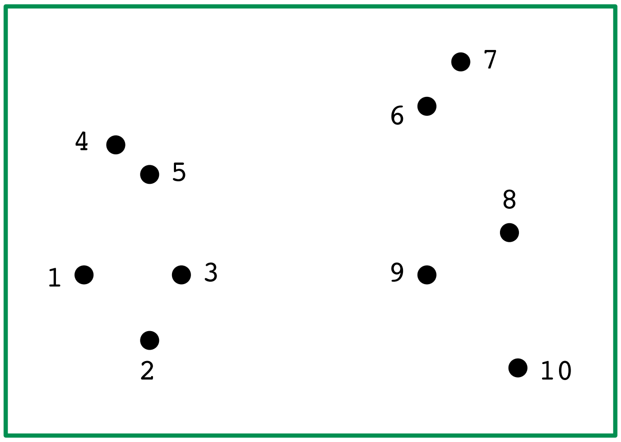
Often: no single right answer, because of multiscale structure.

Hierarchical clustering avoids these problems.

Example: gene expression data



The single linkage algorithm

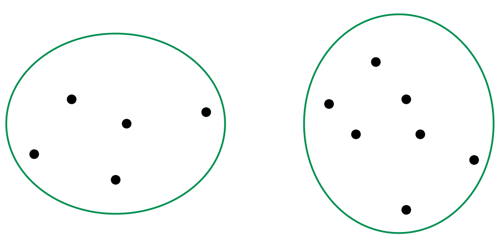


- Start with each point in its own, singleton, cluster
- Repeat until there is just one cluster:
  - Merge the two clusters with the closest pair of points
- Disregard singleton clusters

Linkage methods

- Start with each point in its own, singleton, cluster
- Repeat until there is just one cluster:
  - Merge the two "closest" clusters

How to measure distance between two clusters C and C'?



- Single linkage

$$\text{dist}(C, C') = \min_{x \in C, x' \in C'} \|x - x'\|$$

- Complete linkage

$$\text{dist}(C, C') = \max_{x \in C, x' \in C'} \|x - x'\|$$

Average linkage

Three commonly-used variants:

1. Average pairwise distance between points in the two clusters

$$\text{dist}(C, C') = \frac{1}{|C| \cdot |C'|} \sum_{x \in C} \sum_{x' \in C'} \|x - x'\|$$

2. Distance between cluster centers

$$\text{dist}(C, C') = \|\text{mean}(C) - \text{mean}(C')\|$$

3. Ward's method: the increase in k-means cost occasioned by merging the two clusters

$$\text{dist}(C, C') = \frac{|C| \cdot |C'|}{|C| + |C'|} \|\text{mean}(C) - \text{mean}(C')\|^2$$