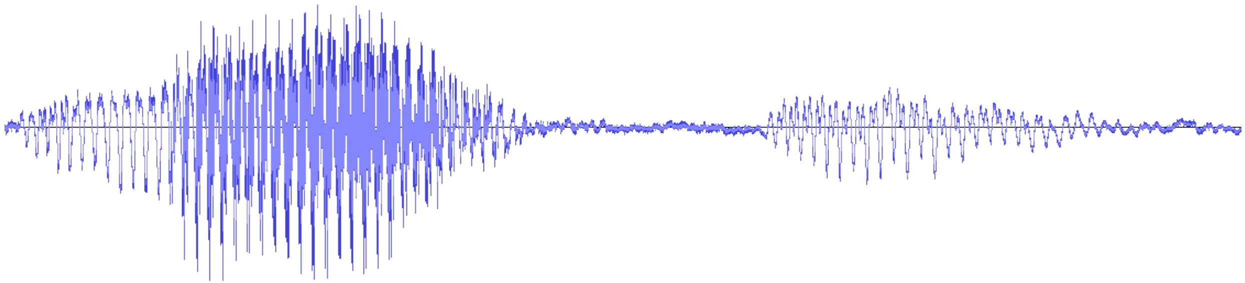
Representation learning

Representation learning

Good representations make learning easier.

- They bring out the true degrees of freedom in the data.
- They capture relevant structure at multiple scales.
- They screen out noisy or irrelevant structure.

Degrees of freedom



Usual representation of speech:

- Take overlapping windows of the speech signal
- Apply many filters within each window
- More filters $\Rightarrow$ higher dimensional

Yet it comes from a physical system with a few degrees of freedom.

Multiscale structure

Commonly-occurring structure at many levels.

Representation learning: goals

Learn underlying degrees of freedom and multiscale structure from the statistics of unlabeled data, e.g.:

- Clustering
- Linear projections
- Embedding and manifold learning
- Metric learning
- Autoencoders

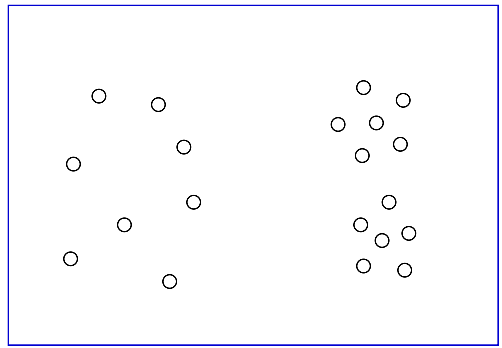
Or learn a representation in tandem with the classifier: deep learning.

Clustering with the k-means algorithm I

Topics we'll cover

1. The clustering problem
2. Two uses of clustering
3. The k-means cost function and algorithm
4. Initializing Lloyd's algorithm

Clustering in $\mathbb{R}^d$



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.

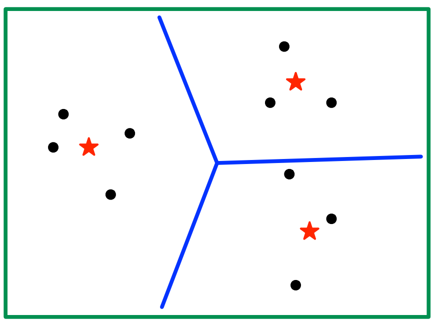
Widely-used clustering methods

1. K-means and its many variants
2. EM for mixtures of Gaussians
3. Agglomerative hierarchical 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:

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

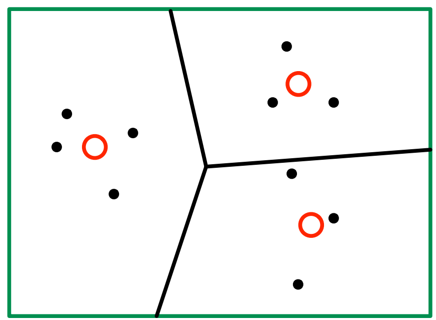


The centers partition $\mathbb{R}^d$ into k convex regions: μ_j's region consists of points for which it is the closest center.

Lloyd's k-means algorithm

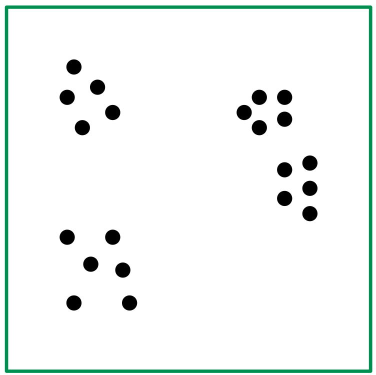
The k-means problem is NP-hard. Most popular heuristic: "k-means algorithm".

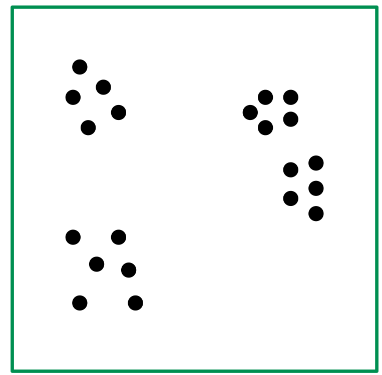
- Initialize centers $\mu_1, \ldots, \mu_k$ in some manner.
- Repeat until convergence:
  - Assign each point to its closest center.
  - Update each μ_j to the mean of the points assigned to it.



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:

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

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

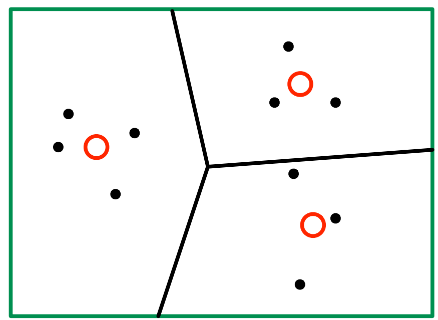
Clustering with the k-means algorithm II

Topics we'll cover

1. Two uses of k-means clustering
2. Clustering in a streaming or online setting
3. The good and bad of k-means

Lloyd's 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.

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

Streaming and online computation

Streaming computation: for data too large to fit in memory.

- Make one pass (or maybe a few passes) through the data.
- On each pass:
  - See data points one at a time, in order.
  - Update models/parameters along the way.
- Only enough space to store a tiny fraction of data, or perhaps a short summary.

Online computation: even more lightweight, for data continuously being collected.

- Initialize a model.
- Repeat forever:
  - See a new data point.
  - Update model if need be.

Example: sequential k-means

1. Set the centers $\mu_1, \ldots, \mu_k$ to the first k data points
2. Set their counts to $n_1 = n_2 = \cdots = n_k = 1$
3. Repeat, possibly forever:
   - Get next data point x
   - Let μ_j be the center closest to x
   - Update μ_j and n_j:

$$\mu_j = \frac{n_j \mu_j + x}{n_j + 1} \quad \text{and} \quad n_j = n_j + 1$$

K-means: the good and the bad

The good:

- Fast and easy.
- Effective in quantization.

The bad:

- Geared towards spherical clusters of roughly the same radius.

How to accommodate clusters of more general shape?

The EM algorithm for Gaussian mixture models

Topics we'll cover

1. Gaussian mixture models
2. The optimization problem
3. The EM algorithm
4. Examples

K-means: the good and the bad

The good:

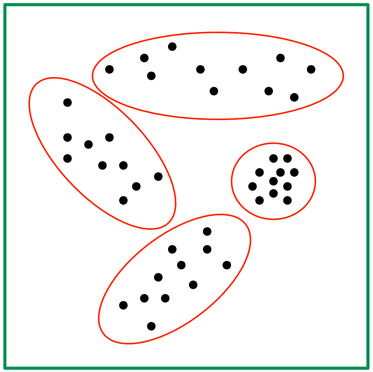
- Fast and easy.
- Effective in quantization.

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?

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**

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

The clustering task

We are given data $x_1, \ldots, x_n \in \mathbb{R}^d$.

For any mixture model $\pi_1, \ldots, \pi_k$, $P_1 = N(\mu_1, \Sigma_1), \ldots, P_k = N(\mu_k, \Sigma_k)$,

$$\begin{aligned}
&\Pr\left(\text{data} \mid \pi_1 P_1 + \cdots + \pi_k P_k\right) \\
&= \prod_{i=1}^{n} \left(\pi_1 P_1(x_i) + \cdots + \pi_k P_k(x_i)\right) \\
&= \prod_{i=1}^{n} \left(\sum_{j=1}^{k} \frac{\pi_j}{(2\pi)^{d/2} |\Sigma_j|^{1/2}} \exp\left(-\frac{1}{2} (x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j) \right) \right)
\end{aligned}$$

Find the **maximum-likelihood mixture of Gaussians**:
the parameters $\{\pi_j, \mu_j, \Sigma_j : j = 1 \ldots k\}$ that maximize this function.

Optimization surface

Minimize the negative log-likelihood,

$$L(\{\pi_j, \mu_j, \Sigma_j\}) \;=\; \sum_{i=1}^{n} \ln \left(\sum_{j=1}^{k} \frac{\pi_j}{(2\pi)^{d/2} |\Sigma_j|^{1/2}} \exp \left(-\frac{1}{2}(x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j) \right) \right)$$

The EM algorithm

1. Initialize $\pi_1, \ldots, \pi_k$ and $P_1 = N(\mu_1, \Sigma_1), \ldots, P_k = N(\mu_k, \Sigma_k)$.
2. Repeat until convergence:
   - Assign each point x_i fractionally between the k clusters:

$$w_{ij} = \Pr(\text{cluster } j \mid x_i) = \frac{\pi_j P_j(x_i)}{\sum_\ell \pi_\ell P_\ell(x_i)}$$

   - Update mixing weights, means, and covariances:

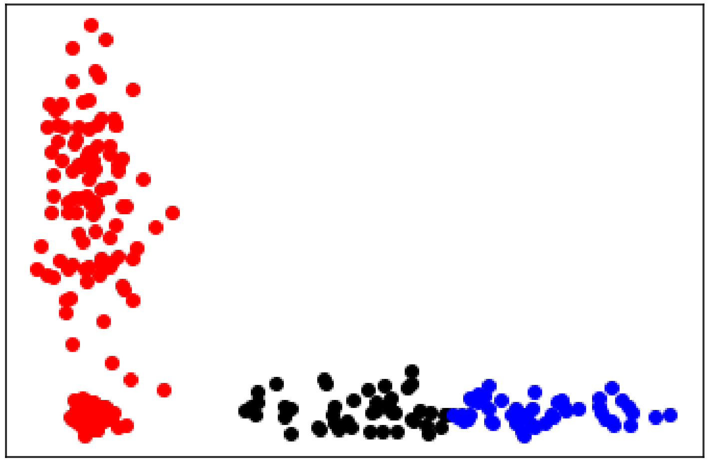
$$\pi_j = \frac{1}{n} \sum_{i=1}^{n} w_{ij}$$

$$\mu_j = \frac{1}{n\pi_j} \sum_{i=1}^{n} w_{ij} x_i$$

$$\Sigma_j = \frac{1}{n\pi_j} \sum_{i=1}^{n} w_{ij} (x_i - \mu_j)(x_i - \mu_j)^T$$

Example

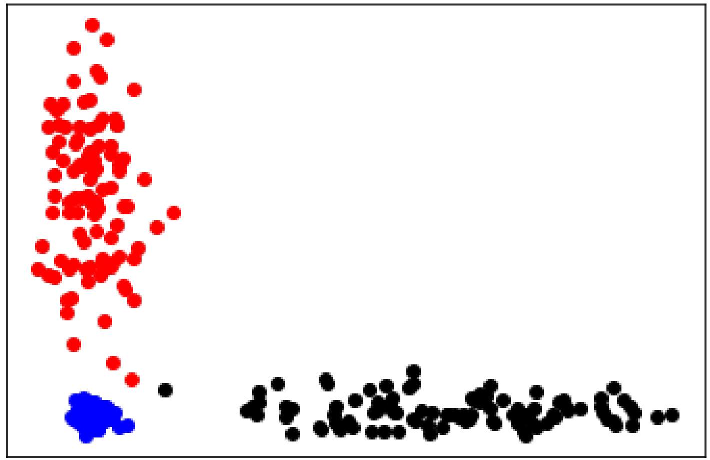
Data with 3 clusters, each with 100 points.



k-means solution 1

Example

Data with 3 clusters, each with 100 points.



EM for mixture of Gaussians

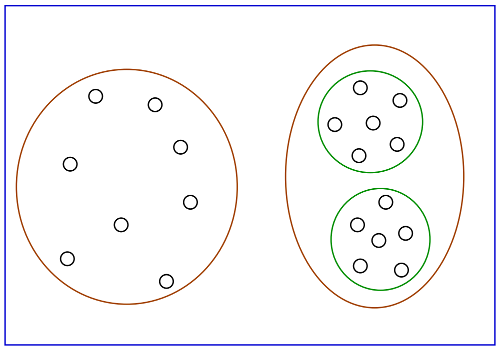
Hierarchical clustering

Topics we'll cover

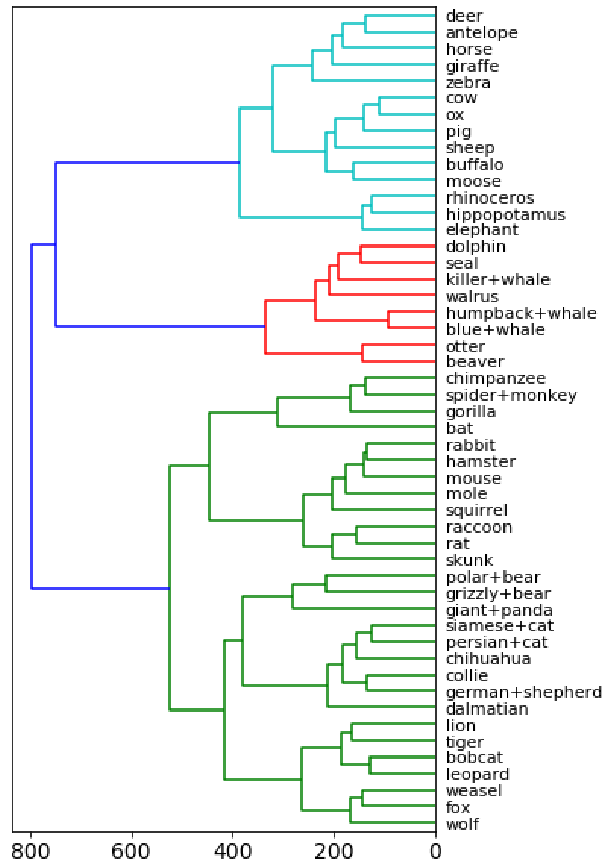
1. What is hierarchical clustering?
2. Single linkage
3. The other linkage schemes

Hierarchical clustering

Choosing the number of clusters (k) is difficult.



Often there is no single right answer, because of multiscale structure.



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giraffe
zebra
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buffalo
moose
rhinoceros
hippopotamus
elephant
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killer+whale
walrus
humpback+whale
blue+whale
otter
beaver
chimpanzee
spider+monkey
gorilla
bat
rabbit
hamster
mouse
mole
squirrel
raccoon
rat
skunk
polar+bear
grizzly+bear
giant+panda
siamese+cat
persian+cat
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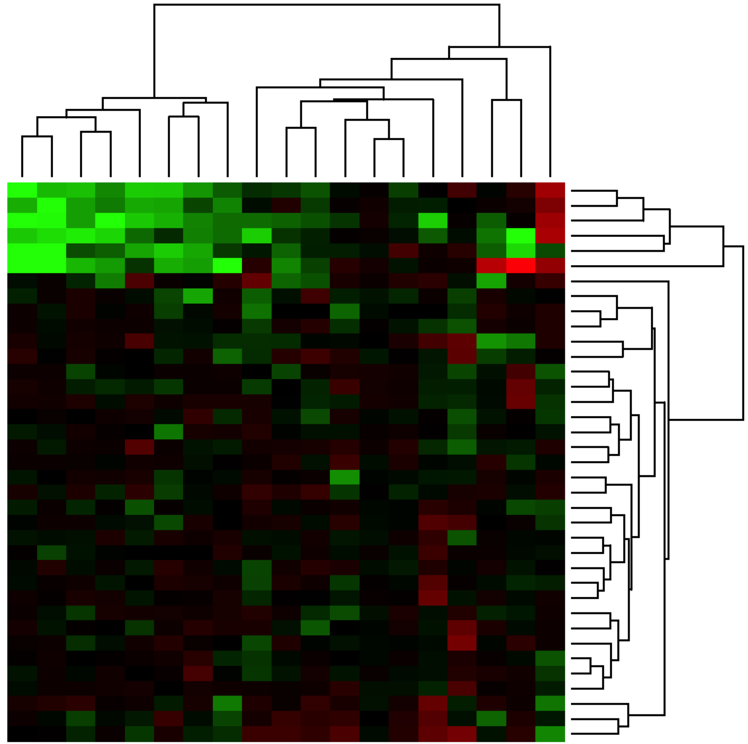
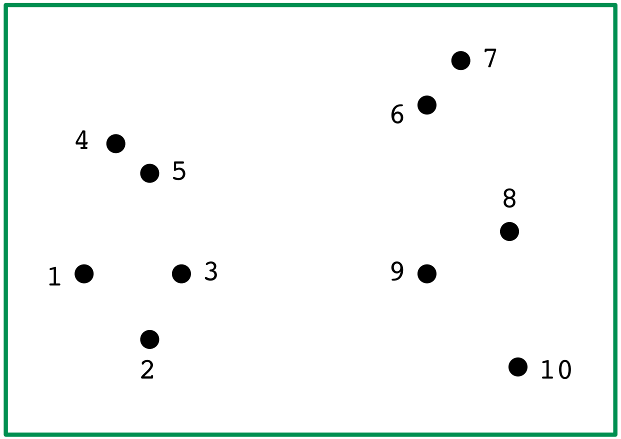


The single linkage algorithm

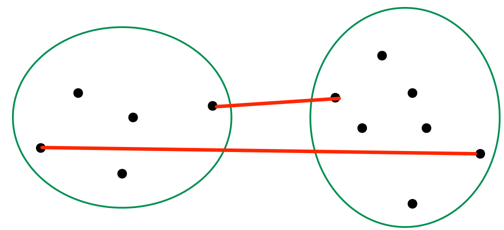


- Start with each point in its own, singleton, cluster
- Repeat until there is just one cluster:
  - Merge the two clusters with the closest pair of points

Linkage methods

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

How to measure the distance between two clusters C, C'?



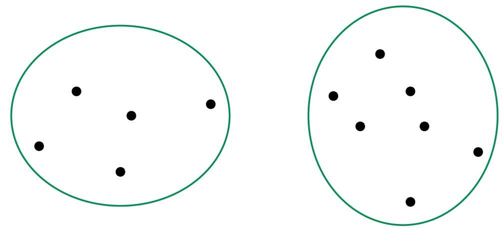
- Single linkage

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

- Complete linkage

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

Average linkage



1. Average pairwise distance between points in the two clusters

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

2. Distance between cluster centers

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

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

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