Clustering

DSE 220

Roadmap for the course

1. Introduction
    - Nearest neighbor
    - Statistical learning theory setup

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   - Generative models: product distributions, multinomials, Gaussians
   - Discriminative models: logistic regression
   - Background in linear algebra and optimization
   - More linear classifiers: perceptrons and support vector machines
   - Kernels
   - Richer output spaces

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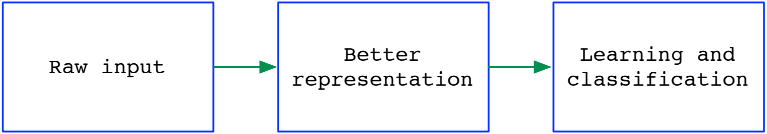
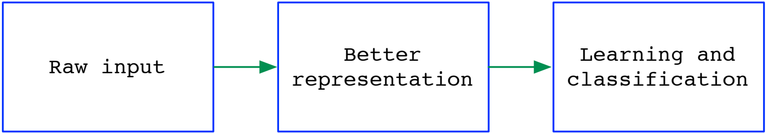
4. Combining simple classifiers

Representation learning



Good representations make learning easier.

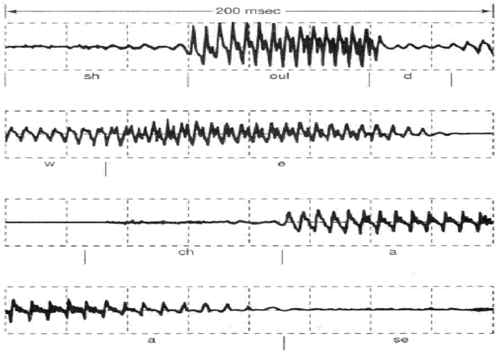
Representation learning



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.

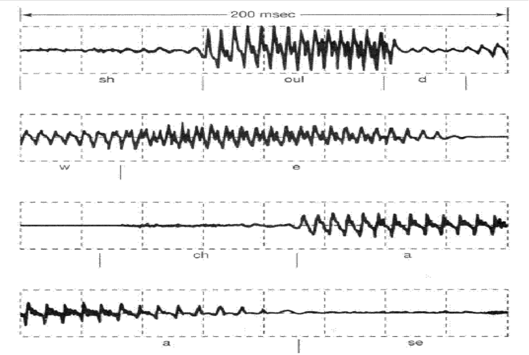
Degrees of freedom



Usual representation of speech:

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

Degrees of freedom



Usual representation of speech:

- Take overlapping windows of the speech signal
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But the speech is produced by a physical system (vocal tract) with a fixed number of degrees of freedom. And the phoneme being uttered can be characterized by the configuration of this apparatus.

Multiscale structure

Commonly-occurring structure at many levels:

- Low-level: like local edges
- Higher-level: like wheels, windows

Representation learning: goals

How, and to what extent, can underlying degrees of freedom and multiscale structure be learned from the statistics of unlabeled data?

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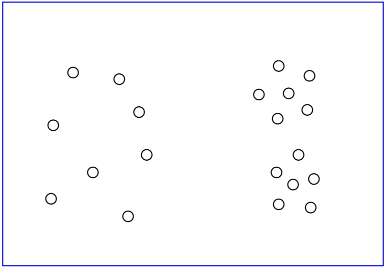
Topics:

- Clustering
- Informative linear projections
- Embedding and manifold learning
- Metric learning
- Autoencoders
- Deep nets

Clustering in $\mathbb{R}^p$



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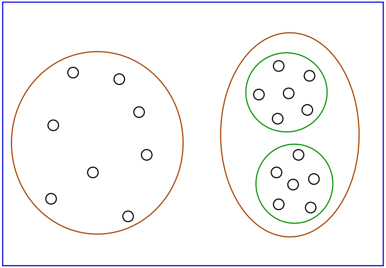

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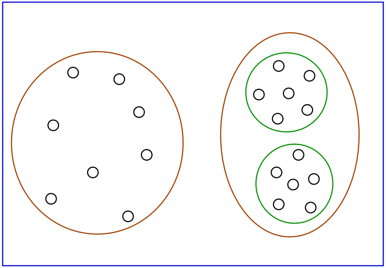
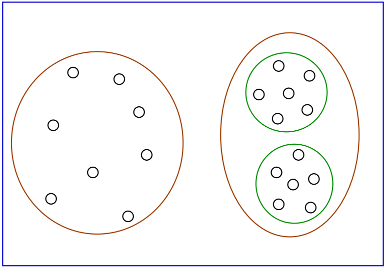


Two common uses of clustering:

Clustering in $\mathbb{R}^p$



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

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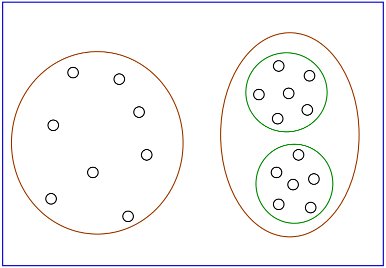


Two common uses of clustering:

- 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.

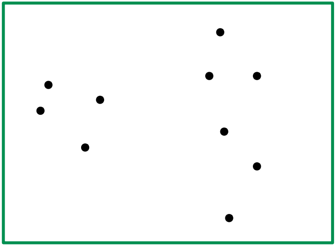
Widely-used clustering methods

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

The k-means optimization problem

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

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



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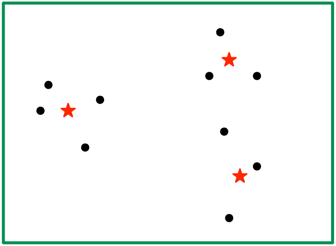

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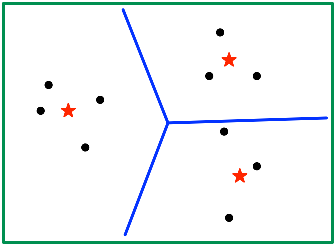

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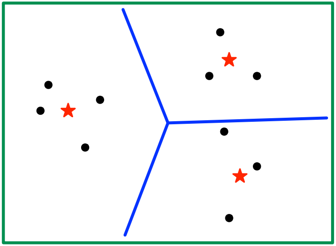

The centers carve $\mathbb{R}^p$ up into k convex regions: μ_j's region consists of points for which it is the closest center.

Lloyd's k-means algorithm

The k-means problem is NP-hard to solve. The most popular heuristic is called the "k-means algorithm".

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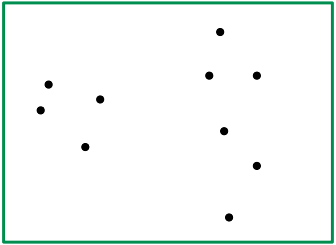

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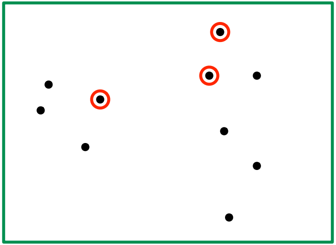

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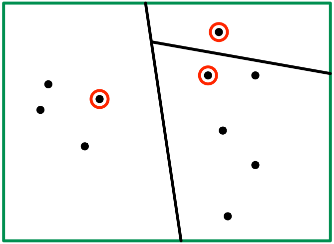

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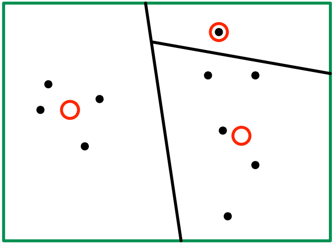

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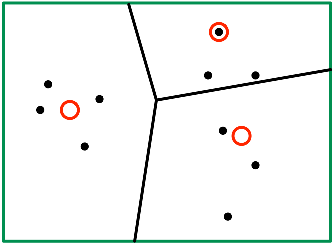

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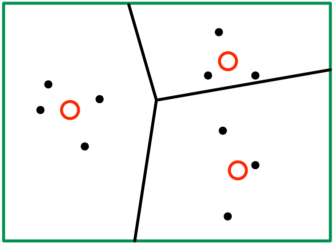

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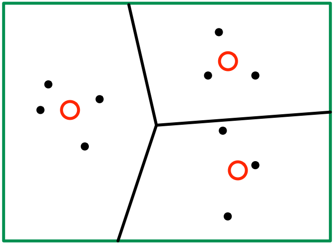

Each iteration reduces the cost $\Rightarrow$ convergence to a local optimum.

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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

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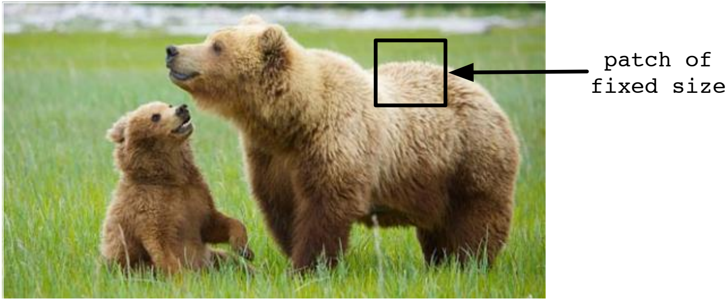

- Look at all $\ell \times \ell$ patches in all images. Extract features for each.
- Run k-means on this entire collection to get k centers.
- Now associate any image patch with its nearest center.
- Represent an image by a histogram over $\{1, 2, \ldots, k\}$.

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Such data sets are truly enormous.

Streaming and online computation

Streaming computation: for data sets that are 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.
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Online computation: an even more lightweight setup, for data that is 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:

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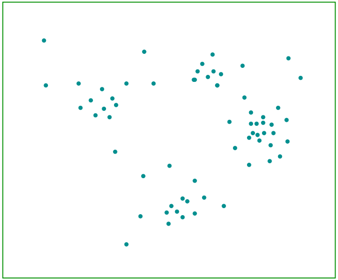
Is there is a similarly-simple algorithm in which clusters of more general shape are accommodated?

Mixtures of Gaussians

Idea: model each cluster by a Gaussian:



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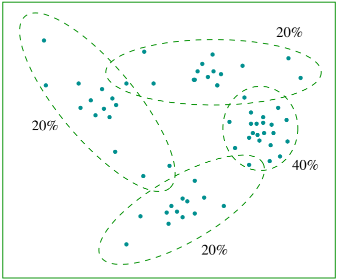

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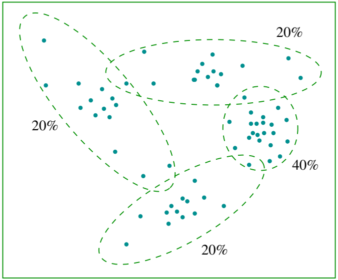

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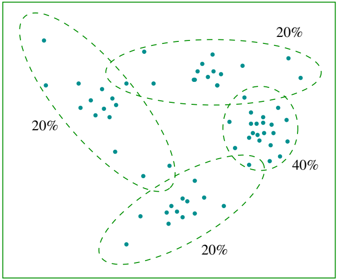

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Overall distribution over $\mathbb{R}^p$: a **mixture of Gaussians**

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

The clustering task

Given data $x_1, \ldots, x_n \in \mathbb{R}^P$, find the maximum-likelihood mixture of Gaussians: that is, find parameters

- $\pi_1, \ldots, \pi_k \geq 0$ summing to one
- $\mu_1, \ldots, \mu_k \in \mathbb{R}^p$
- $\Sigma_1, \ldots, \Sigma_k \in \mathbb{R}^{p \times p}$

to maximize

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

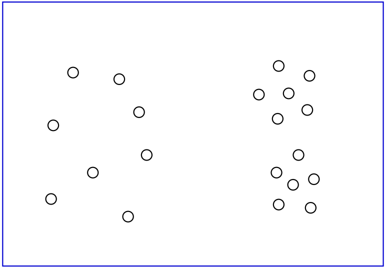
where P_j is the distribution of the jth cluster, $N(\mu_j, \Sigma_j)$.

The EM algorithm

1. Initialize $\pi_1, \ldots, \pi_k$ and $P_1 = N(\mu_1, \Sigma_1), \ldots, P_k = N(\mu_k, \Sigma_k)$ in some manner.
2. Repeat until convergence:
   - Assign each point x_i fractionally between the k clusters:
   $$w_{ij} = \Pr(\text{cluster } j \mid x_i) = \frac{\pi_j P_j(x_i)}{\sum_\ell \pi_\ell P_\ell(x_i)}$$
   - Now update the mixing weights, means, and covariances:
   $$\pi_j = \frac{1}{n} \sum_{i=1}^n w_{ij}$$
   $$\mu_j = \frac{1}{n\pi_j} \sum_{i=1}^n w_{ij} x_i$$
   $$\Sigma_j = \frac{1}{n\pi_j} \sum_{i=1}^n w_{ij} (x_i - \mu_j)(x_i - \mu_j)^T$$

Hierarchical clustering

Choosing the number of clusters (k) is difficult.



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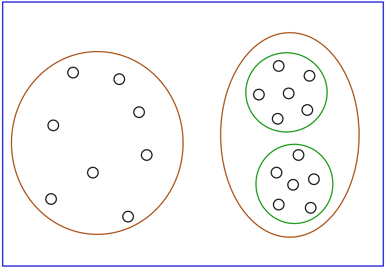

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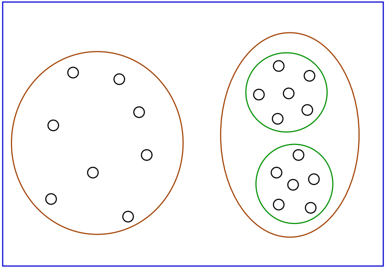

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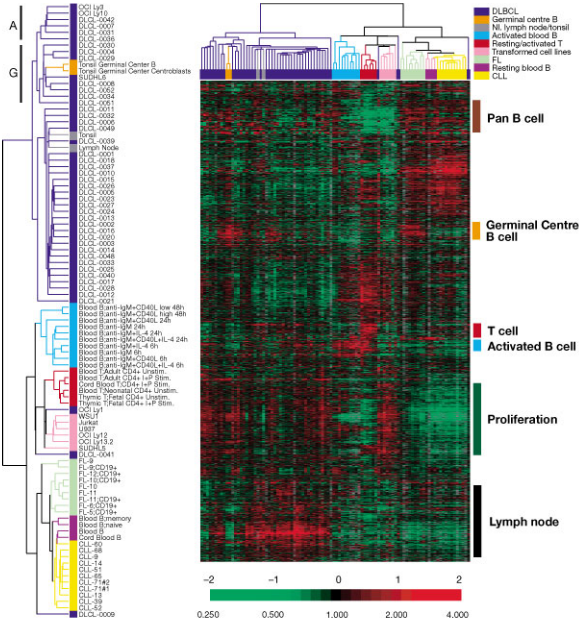
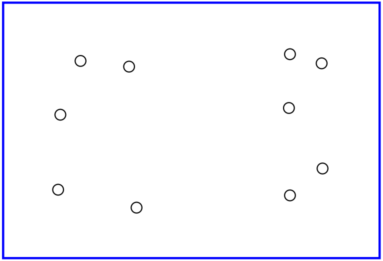
Hierarchical clustering avoids these problems.

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

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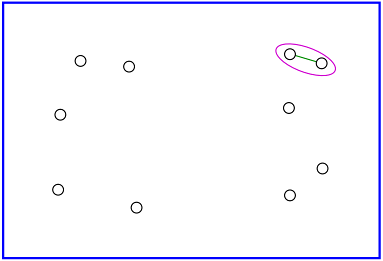

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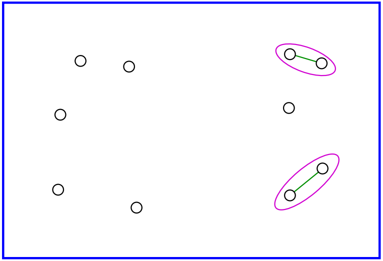

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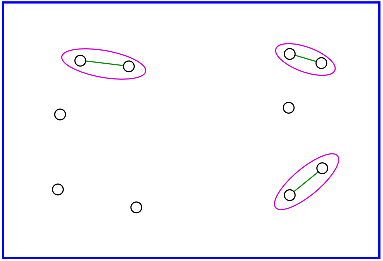

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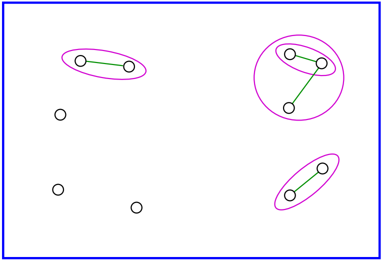

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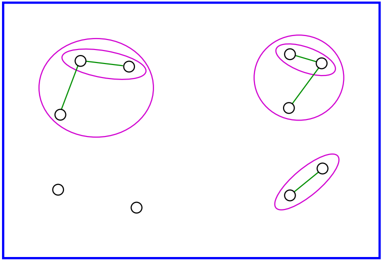

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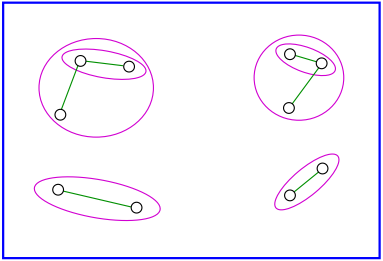

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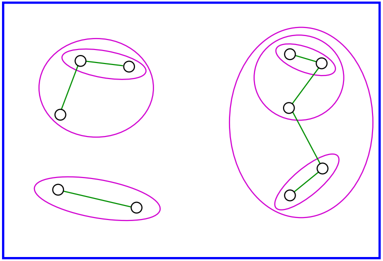

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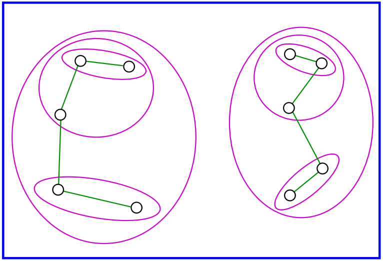

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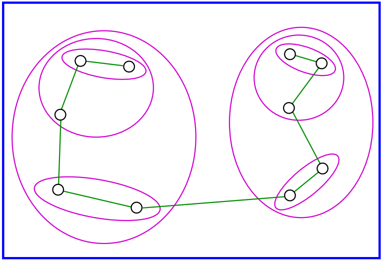

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Linkage methods

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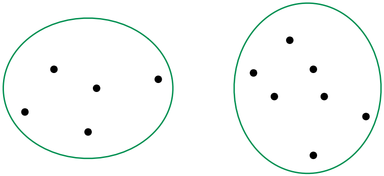
How to measure the distance between two clusters of points, C and C'?



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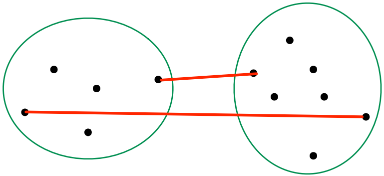

- Single linkage

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

- Complete linkage

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

Average linkage

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

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