Clustering

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Week 7

Clustering

How can we summarize or interpret an unknown dataset, with no labels?

$$\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$$

The idea behind **clustering** is that complex data can be described concisely by a small number of discrete components, each with its own clear and interpretable structure.

Clustering

How can we summarize or interpret an unknown dataset, with no labels?

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The idea behind **clustering** is that complex data can be described concisely by a small number of discrete components, each with its own clear and interpretable structure.

We'll look at a few algorithms for clustering. The key assumption we will need is that there is some reasonable notion of proximity, defined in terms of a **dissimilarity** $d(\mathbf{x}, \mathbf{x}')$, associated with our data points.

Many different domains

When might we want compact descriptions of data?

- "My clients can be considered to belong to 5 different groups, with a typical client from each group looking like this."
- Clustering web pages based on their content
- Clustering (and merging) web search results
- Clustering users based on their product preferences or purchase history
- Generally: to reduce apparent complexity in order to gain insight

Examples: David Barber

Clustering desiderata

1. Data points in the **same cluster** should have **high similarity**
2. Data points in **different clusters** should have **low similarity**

Notions of "dissimilarity" are data- and domain-specific, but squared (Euclidean) distance between points is pretty common...

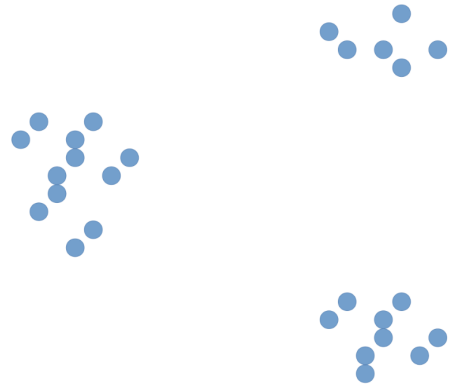

Figure: Andreas Müller

Intuitive clustering

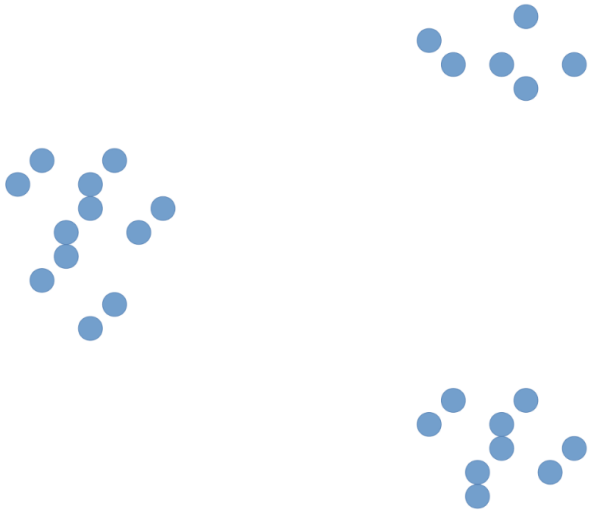

Figure: Andreas Müller

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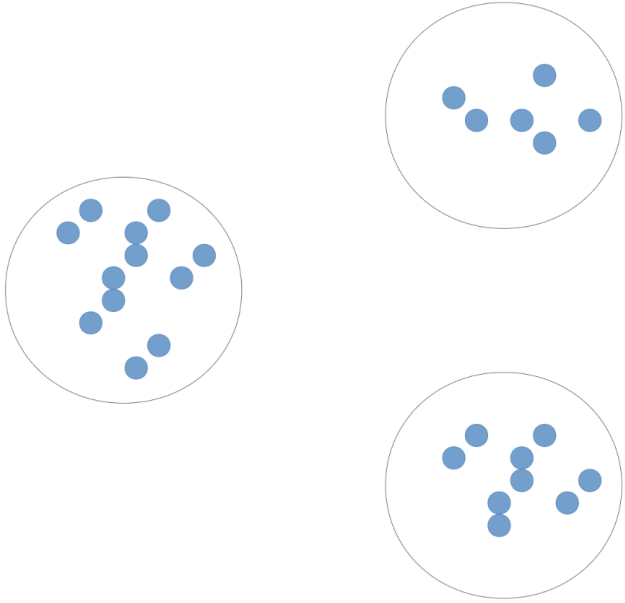

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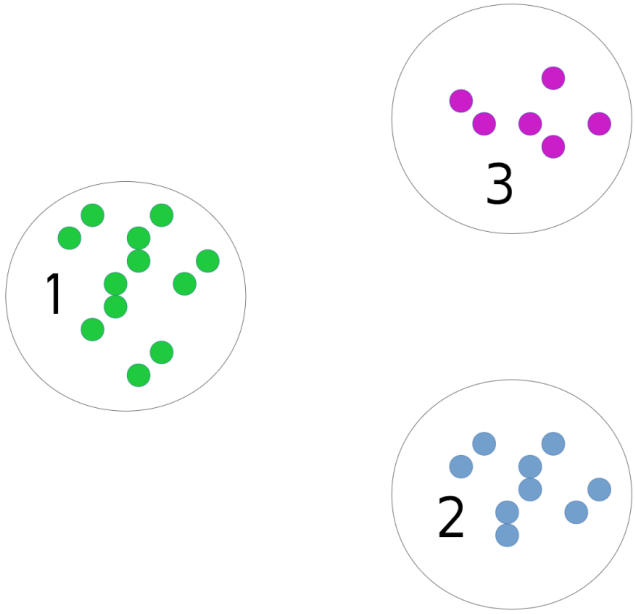

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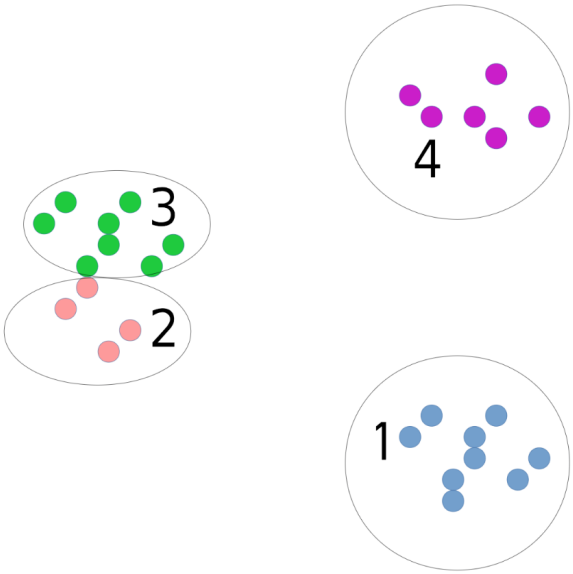

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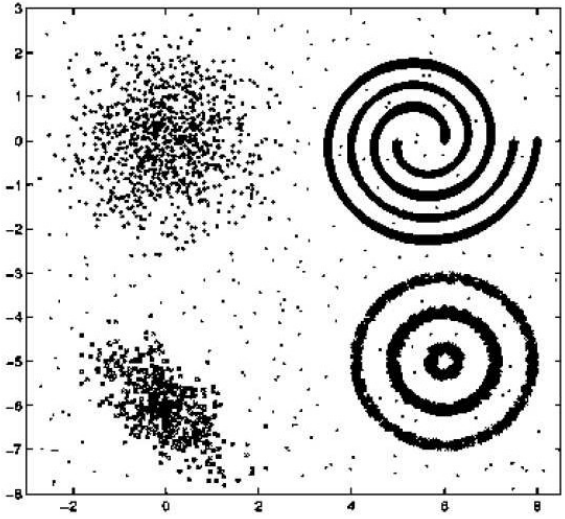
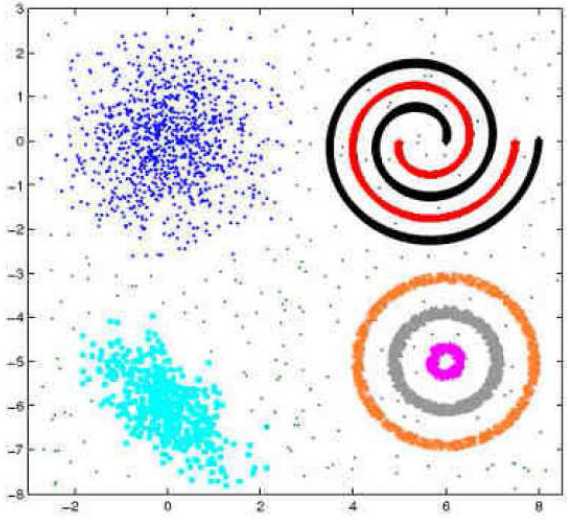


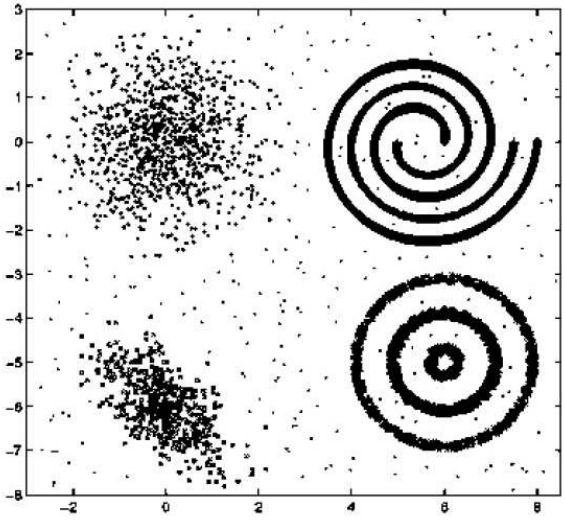
(a) Input data



(b) Desired clustering

Figure: Jain 2009

Intuitive clustering



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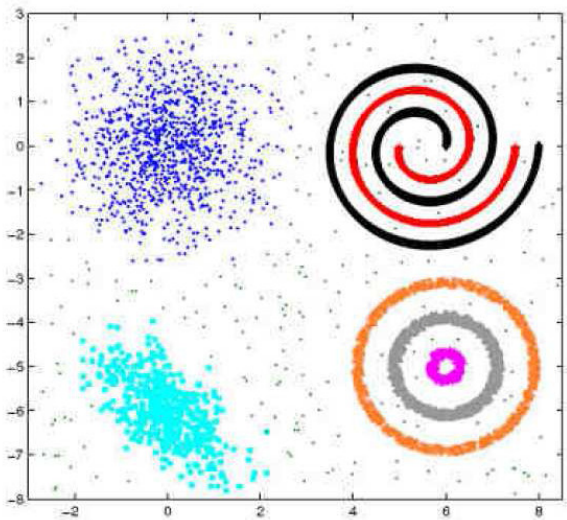


(b) Desired clustering

Warning: None of the algorithms we'll look at can do this!

Figure: Jain 2009

Market basket analysis

- Data: a list of items in each basket
- Useful to represent this as a matrix
- Typically **very sparse**!

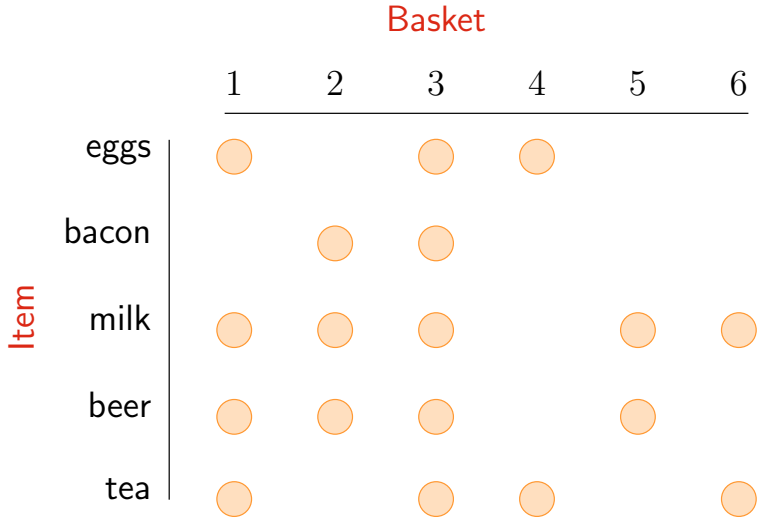


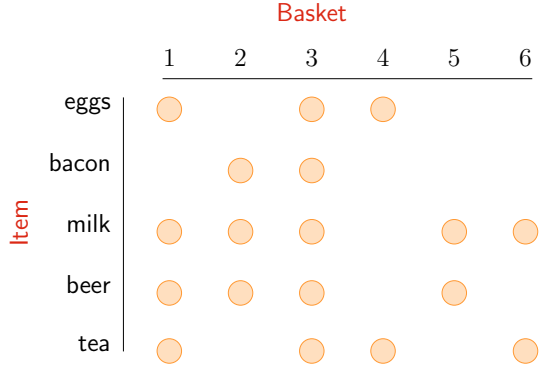
Figure: David Barber

Finding association rules

Finding frequent item sets:

- Find common single items, then common pairs, then triples, etc . . .
- For a threshold of 3: { Eggs }, { Milk }, { Beer }, {Tea }, { Eggs, Tea }, { Milk, Beer }, { Milk, Tea }

Clustering goal is slightly different: we want to find baskets that look similar and group them together into a single "cluster basket".



Clustering problem formulation

$\mathcal{D} = \{x_1, \ldots, x_N\}$ Encoder: $k = C(x_i)$

$k \in \{1, \ldots, K\}$ Dissimilarity: $d(x_i, x_j)$

Loss: $W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(x_i)=k} \sum_{C(x_{i'})=k} d(x_i, x_{i'})$

within-cluster "spread" for a "k"

$$T = \frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} d(x_i, x_{i'}) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(x_i)=k} \left(\sum_{C(x_{i'})=k} d_{ii'} + \sum_{C(x_{i'})\neq k} d_{ii'} \right)$$

$d_{ii'}$

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where $d(x_i, x_{i'}) = d_{ii'}$

$$= \left(\frac{1}{2}\sum_{k}\sum_{C(x_i)=k}\sum_{C(x_{i'})=k} d_{ii'}\right) + \left(\frac{1}{2}\sum_{k}\sum_{C(x_i)=k}\sum_{C(x_{i'})\neq k} d_{ii'}\right)$$

$W(C)$ (within cluster) $\qquad B(C)$ (between cluster)

$$\min_C W(C) = \min_C T - B(C) = \max_C B(C)$$

Combinatorial opt?

$x_1, \ldots, x_N$

$c_1, \ldots, c_N \in \{1, \ldots, K\}$

# of possible assignments N data to K clusters?

$K = 4 \longrightarrow N = 10 \Rightarrow 34{,}105$ cluster assignments

$N = 19 \Rightarrow \approx 10^{10}$

K-means

K-means: $d(x_i, x_{i'}) \equiv \| x_i - x_{i'} \|_2^2$

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} \| x_i - x_{i'} \|_2^2$$

$$= \sum_{k=1}^{K} N_k \sum_{C(x_i)=k} \| x_i - \overline{x}_k \|_2^2$$

N_k: size of k

$\overline{x}_k$: mean of x_i where $C(x_i) = k$

$m_k \equiv \overline{x}_k \longleftrightarrow$ find C

(0) Initialize: K different values m_k, $1 \dots K$

Repeatedly:

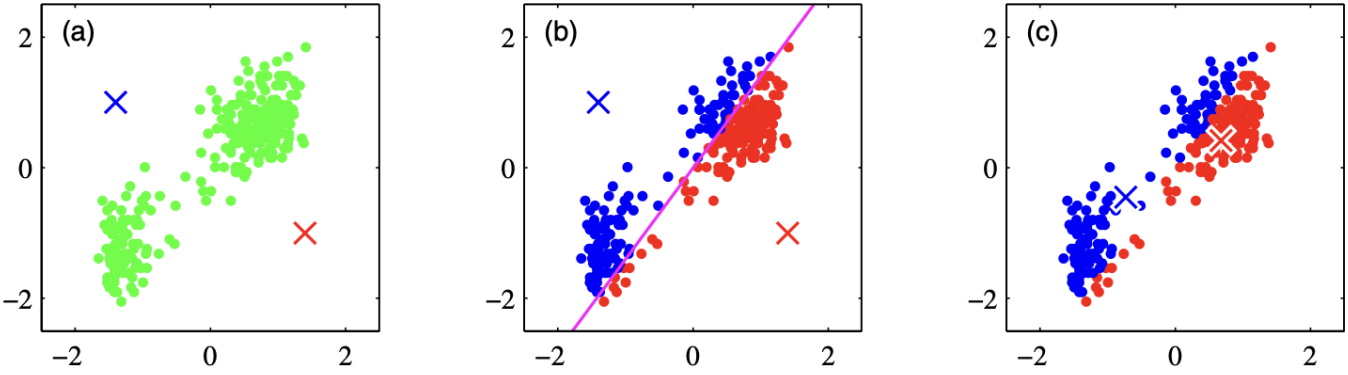
(1) Given $\{m_k\}$, assign $\underbrace{C(x_i)}_{c_i} = k$, $\forall i$

$$\Rightarrow \min_{c_i} \| x_i - m_{c_i} \|_2^2$$

(2) Given $C(x_i)$, update means:

$$m_k = \frac{1}{N_k} \sum_{c_i = k} x_i, \qquad N_k = \sum \mathbb{I}(C(x_i) = k)$$

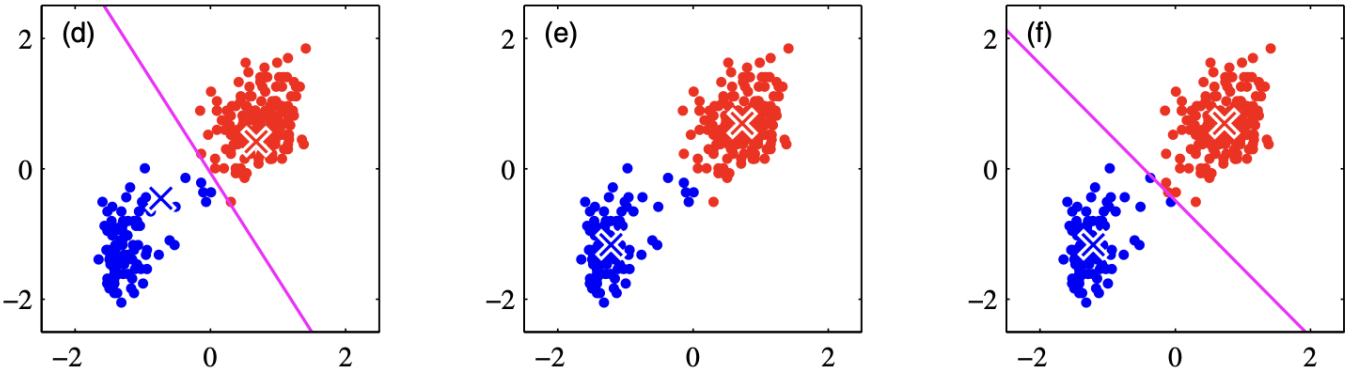
K-means estimation in action



(a) Initialization; (b) Cluster assignment; (c) Cluster center update

Figure: PRML

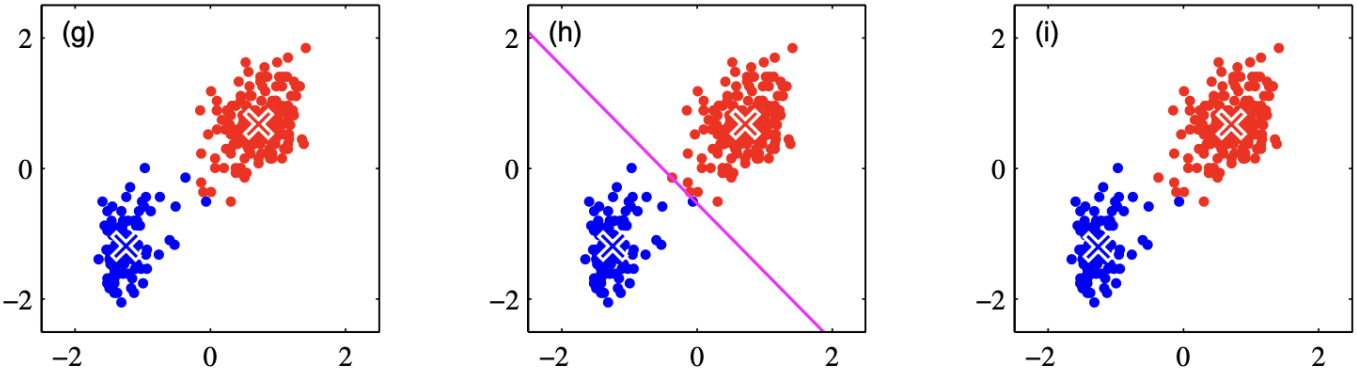
K-means estimation in action



Iteratively assign points to clusters and re-compute means

Figure: PRML

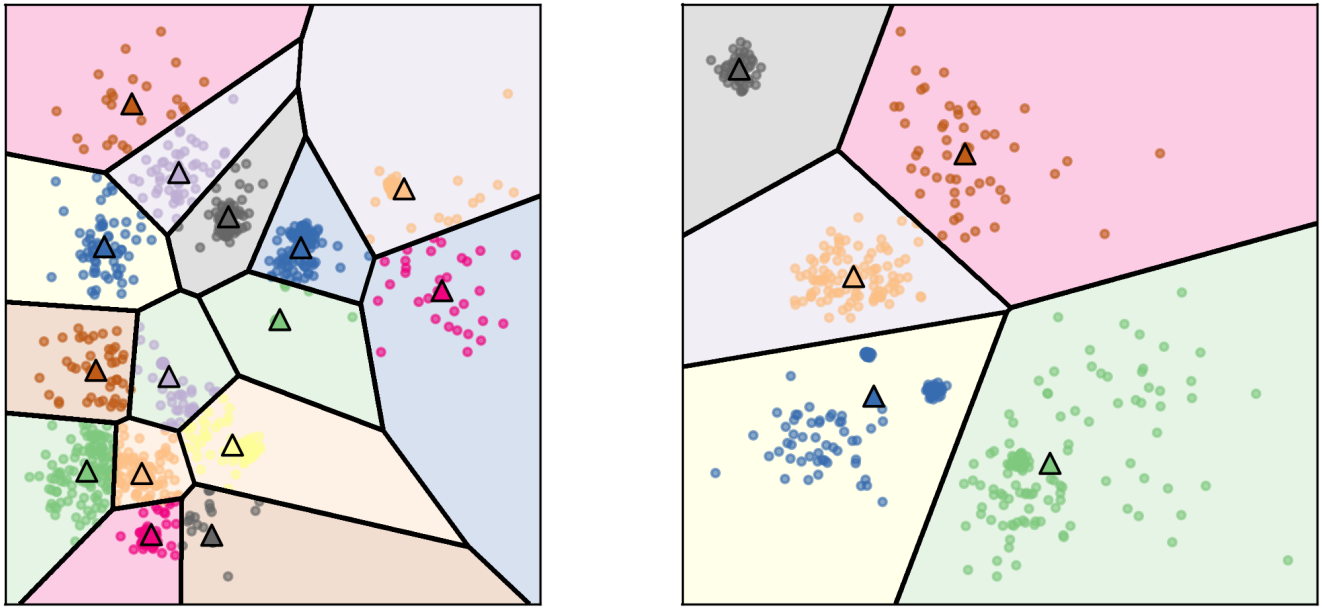
K-means estimation in action



Converges when no points change cluster given new mean

Figure: PRML

Cluster shapes (and generalization)



Cluster shapes are **Voronoi diagrams** of the centers

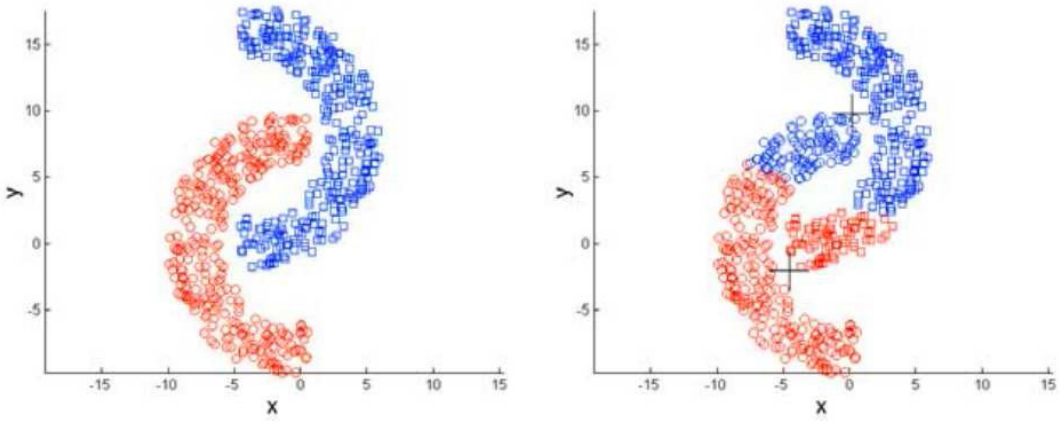
Figure: Andreas Müller

Application: Vector quantization

K-means in color space

Figure: PRML

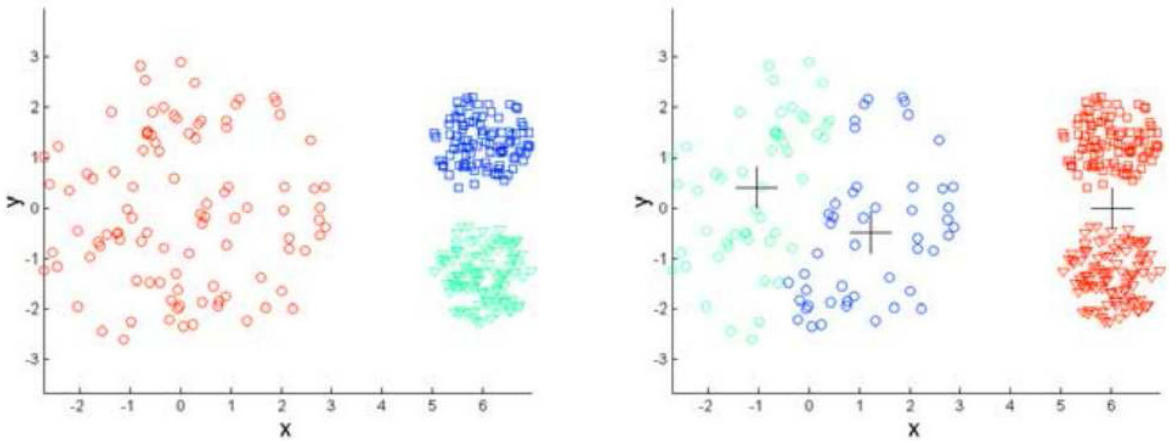
K-means limitations: non-spherical data



- Left: clustering we would like. Right: clustering K-means produces.
- Problem is that the clusters are not spherical and they are too close.

Figure: Christof Monz (Queen Mary, Univ. of London)

K-means limitations: unequal density



- Left: clustering we would like. Right: clustering K-means produces.
- Hard to address this with K-means.

Figure: David Barber

How can we improve this algorithm?

- K-medoids: robustness to outliers, works with arbitrary dissimilarities and data types
  - Simple idea: instead of computing the mean, select the data point which minimizes the average distance to all other points in the cluster
  - Problem: increased computational complexity

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  - Problem: increased computational complexity
- Gaussian mixture models: generalizes this to allow Gaussian-shaped clusters (as opposed to hyperspheres!)
- More general mixture models: can handle discrete observations and missing data
- Mixed-membership models: for when "hard" clustering isn't appropriate (e.g. a "customer" may be better modeled as a mixture of multiple groups...)

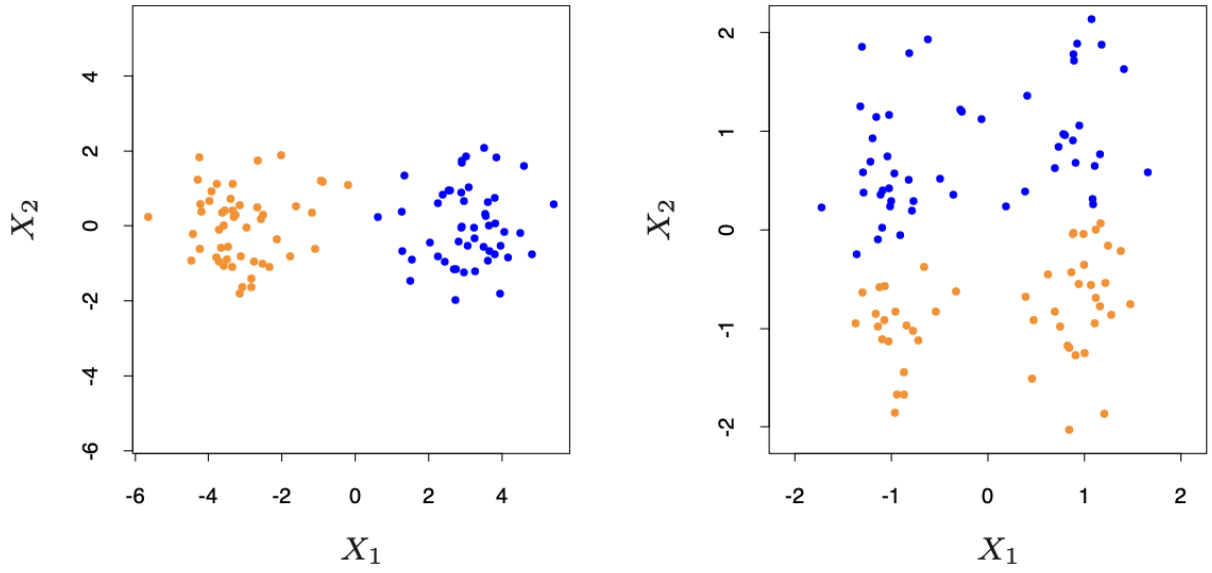
Practical challenges

- This only finds a local optima! Need to run K-means with different initial guesses for the cluster centers...
- K-means is generally fast, but in high dimensions finding the nearest cluster center can be slow (but we can use our fast nearest neighbor methods!)
- No great options for selecting K, other than to try different values and see when increasing no longer "helps"
- The cluster center is not necessarily close to an actual datapoint. This is particularly weird for e.g. one-hot encoded categorical data! (K-medoids does fix this though...)

Sensitivity to scaling

- Suppose each data-vector contains two attributes x_1 and x_2. x_1 represents the temperature in centigrade, and x_2 the distance.
- If we represent the distance in inches, then the Euclidean distance will be dominated by the difference in distance.
- If we represent the distance in miles, the distance will be most likely dominated by the difference in temperature.
- Rescaling / normalizing the dimensions one way around this. But...

Re-scaling dimensions can also be harmful



. . . "standardization" can remove otherwise obvious structure.

Figure: ESL

K-means as feature extractor

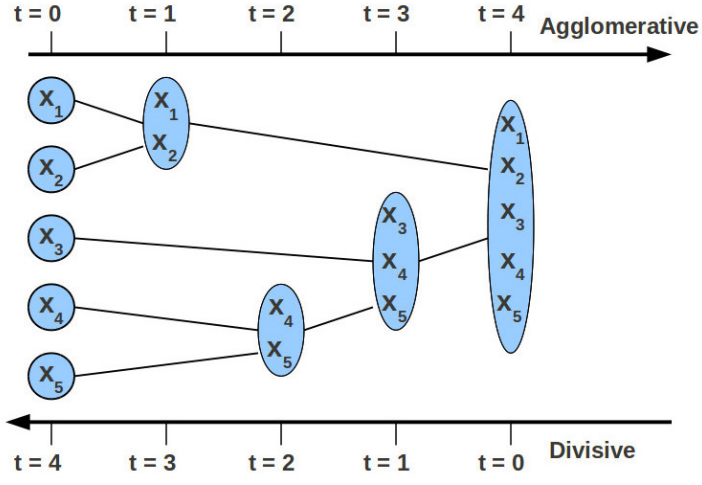
One interesting usage of K-means is as a way of defining a non-linear feature space.

- **Cluster membership**: Categorical feature
- **Distance to cluster centers**: K real-valued features

Can be used to construct useful feature spaces, particularly for low-dimensional data.

Agglomerative clustering

Hierarchical clustering



Hierarchical clustering forms a tree:
children are contained within their parent cluster.

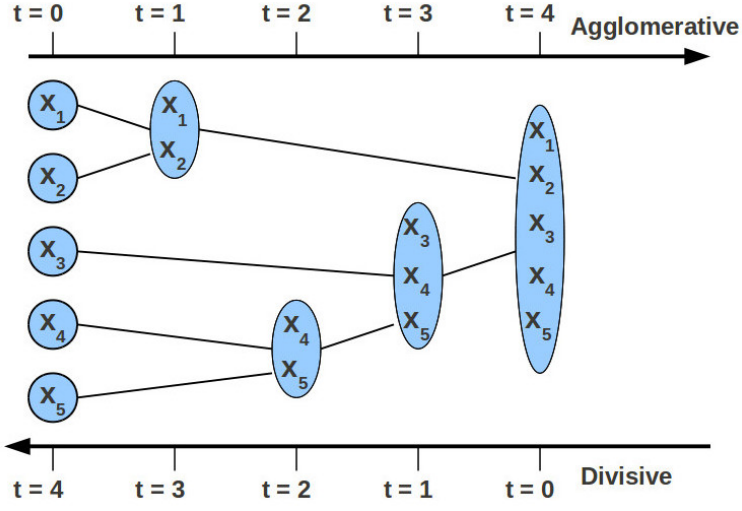
Two directions for clustering

Agglomerative (bottom-up)

- Start with each example in its own singleton cluster
- At each stage, greedily merge 2 most similar clusters

Divisive (top-down)

- Start with all examples in the same cluster
- At each stage, remove the 'outsiders' from the least cohesive cluster



Agglomerative clustering

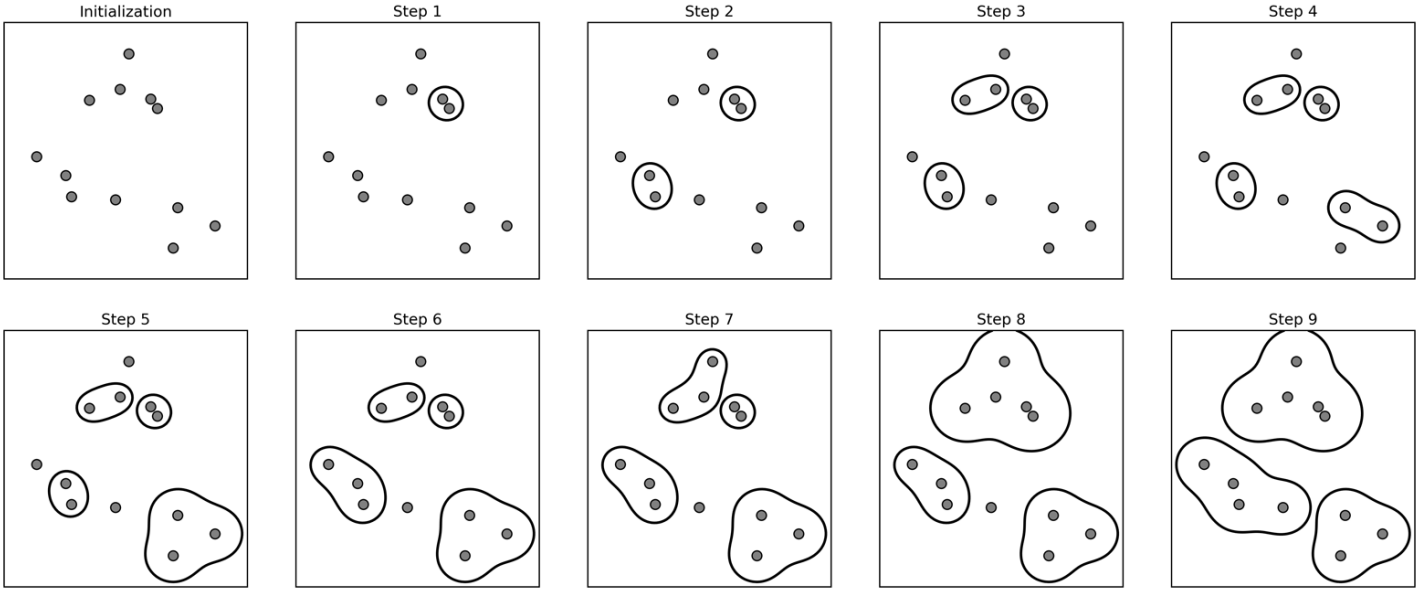
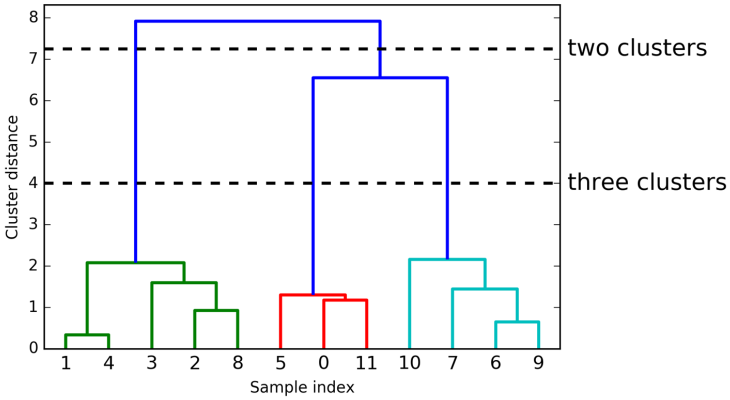
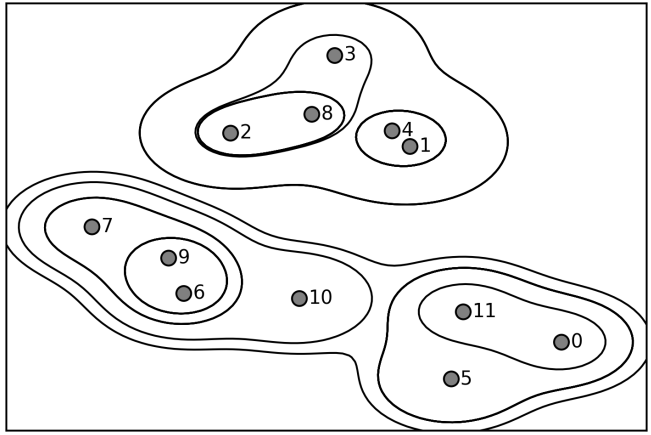


Figure: Andreas Müller

Dendograms





Figures: Andreas Müller

Deciding what clusters to merge

Given a dissimilarity $d(\mathbf{x}, \mathbf{x}')$ between two points $\mathbf{x}, \mathbf{x}'$, there are a handful of different approaches to defining the dissimilarity $D(G, H)$ between existing clusters G, H, i.e. between sets of points.

These are known as different **linkage rules**.

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These are known as different **linkage rules**.

At each step of the algorithm, we merge whichever pair of clusters minimize the cluster dissimilarity $D(\cdot, \cdot)$.

Deciding what clusters to merge

- **Single Linkage**, also called the "nearest neighbor" approach, joins clusters based on their **minimum** distance between any two points:

$$D_{SL}(G, H) = \min_{\mathbf{x} \in G, \mathbf{x}' \in H} d(\mathbf{x}, \mathbf{x}')$$

- **Complete Linkage** (or "furthest neighbor") joins clusters based on their **maximum** distance between any two points:

$$D_{CL}(G, H) = \max_{\mathbf{x} \in G, \mathbf{x}' \in H} d(\mathbf{x}, \mathbf{x}')$$

- **Group Average Linkage** joins based on the average distance of points:

$$D_{GA}(G, H) = \frac{1}{|G||H|} \sum_{\mathbf{x} \in G} \sum_{\mathbf{x}' \in H} d(\mathbf{x}, \mathbf{x}')$$

Linkage rule behavior

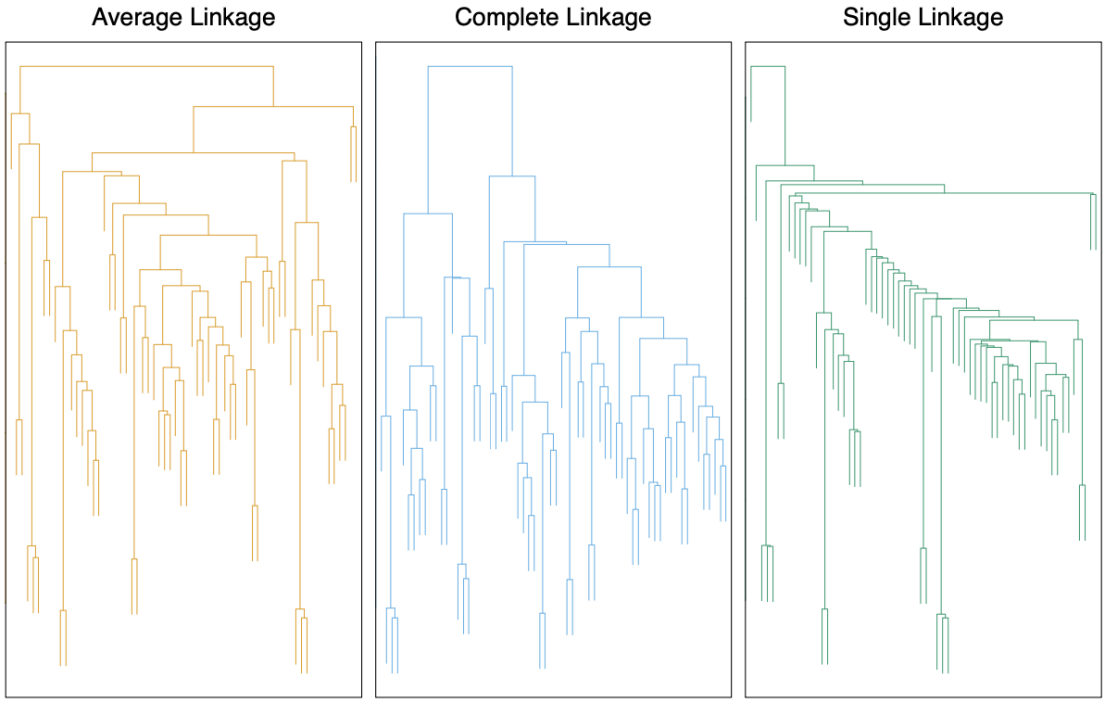

Figure: ESL

Deciding what clusters to merge

For real-valued data specifically, with the Euclidean distance $d(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|$, a different common choice is:

- **Ward's Linkage** looks at how much the within-cluster variances would increase after the merge.

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- **Ward's Linkage** looks at how much the within-cluster variances would increase after the merge. Letting $\boldsymbol{\mu}$ denote cluster means,

$$D_{WL}(G, H) = \frac{1}{|G| + |H|} \sum_{\mathbf{x}_i \in G \cup H} \|\mathbf{x}_i - \boldsymbol{\mu}_{G \cup H}\|^2$$

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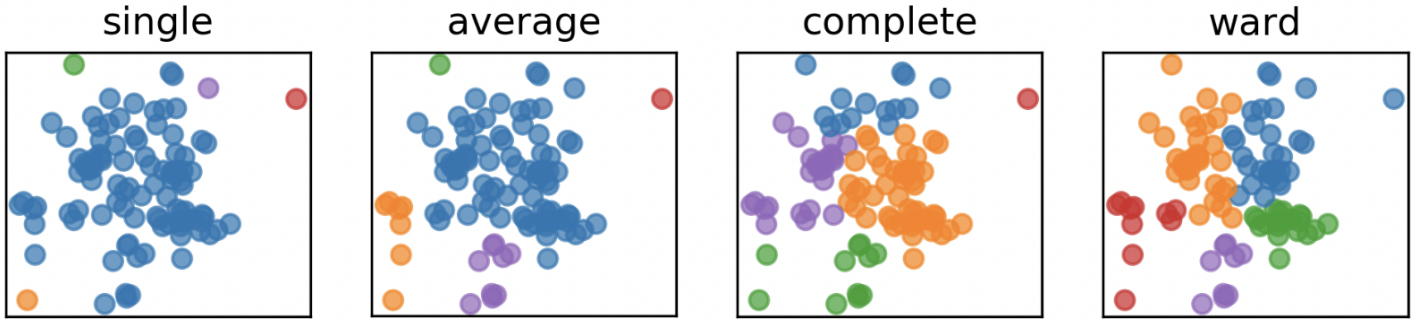
(This has some resemblance to K-means. . . !)

Consequences on cluster size distributions




```
single :   [96  1  1  1  1]
average :  [82  9  7  1  1]
complete : [50 24 14 11  1]
ward :     [31 30 20 10  9]
```

Ward's clustering tends to give more "evenly" sized clusters.

Figure: Andreas Müller

Mixture models

Probabilistic models

Basic idea: start with a simple probability distribution $p(\mathbf{x}|\theta)$, with parameters θ.

- Examples: Gaussian, Bernoulli, ...

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Here, the values $\pi_1, \ldots, \pi_K$ are the **mixture weights**, corresponding to the relative contribution of the different **mixture components** $p(\mathbf{x}|\theta_k)$.

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- Examples: Gaussian, Bernoulli, ...

Define a more complex distribution as a weighted sum of several of these distributions (indexed by k):

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\theta_k)$$

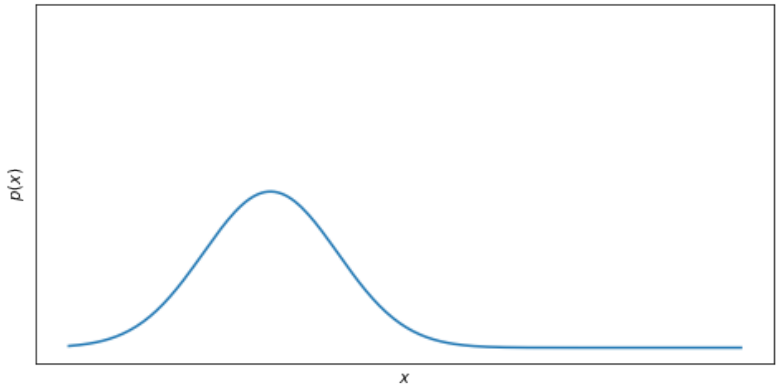
Here, the values $\pi_1, \ldots, \pi_K$ are the **mixture weights**, corresponding to the relative contribution of the different **mixture components** $p(\mathbf{x}|\theta_k)$.

Typically, this is a convex combination: $\pi_k \geq 0$ and $\sum_{k=1}^{K} \pi_k = 1$.

Gaussian mixture models

To make things more concrete, for the moment we will focus on Gaussian mixture models, where each mixture component is modeled by a Gaussian $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$.

Gaussian mixture cartoon



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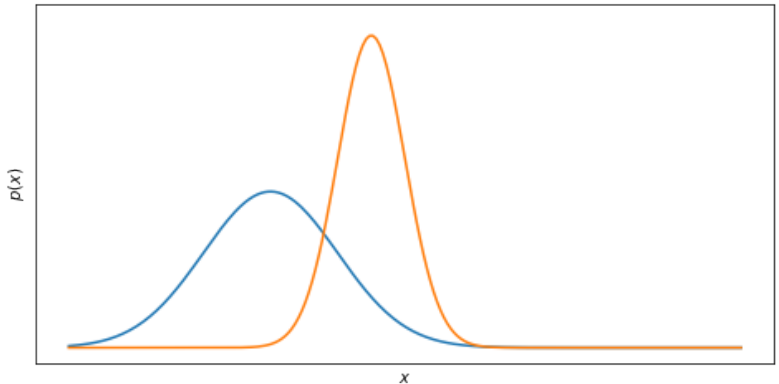

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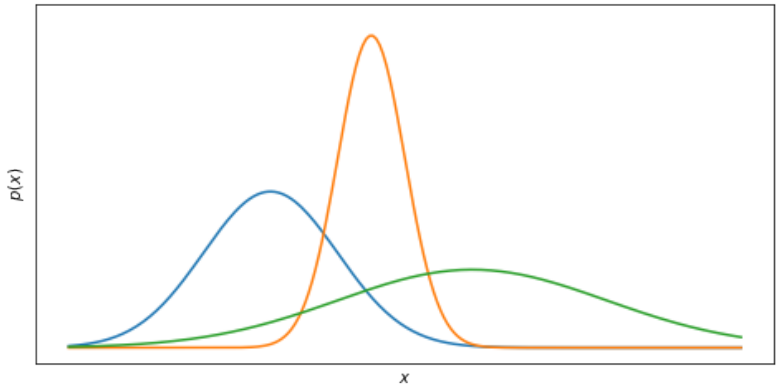

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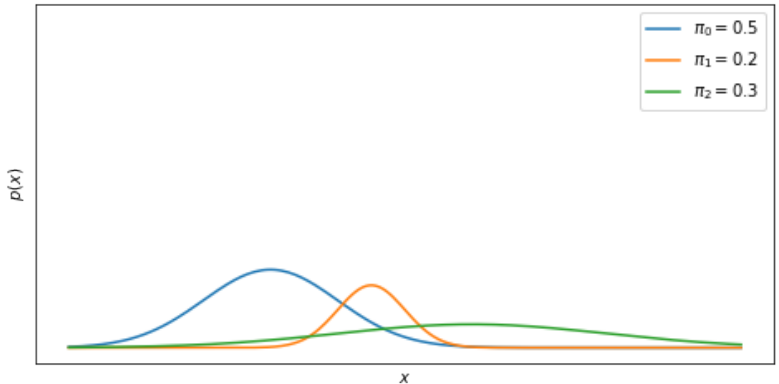

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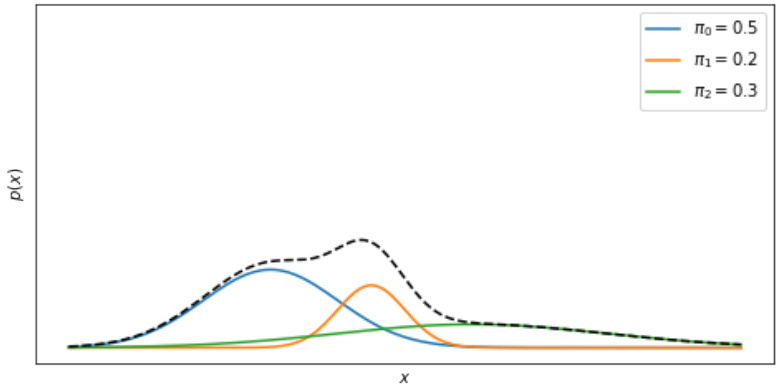

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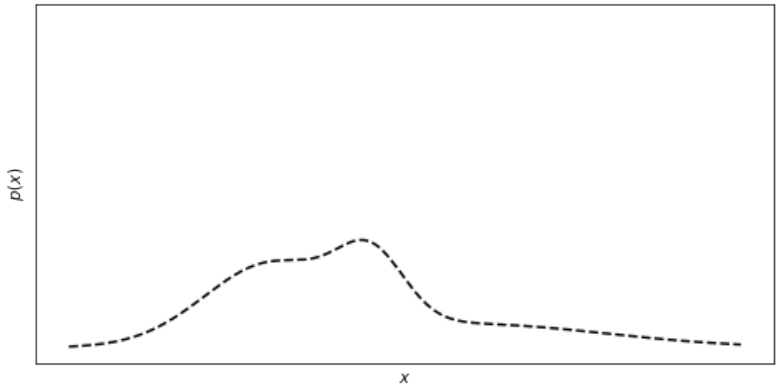
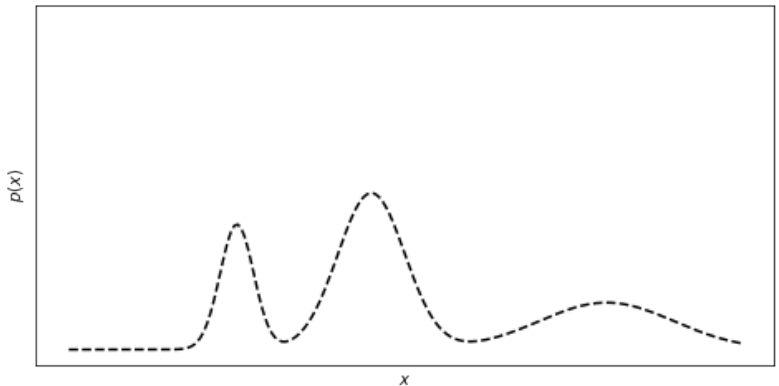


Relevance to clustering



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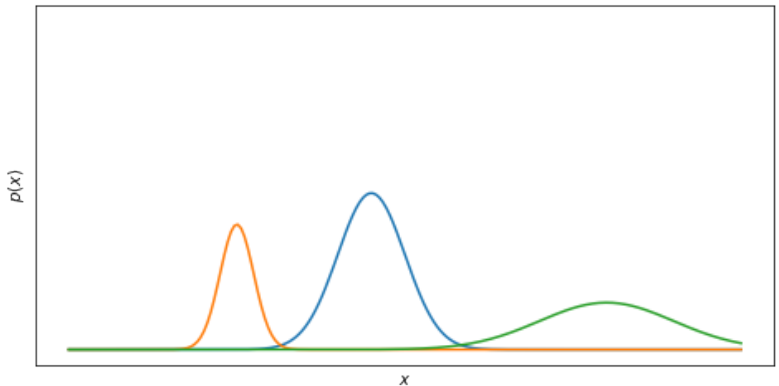

Mixtures as latent variable models

Since the values of π_k are nonnegative and sum to one, we can also view them as a probability distribution over the different components, and write the model as

$$p(z_n) = \text{Discrete}(\boldsymbol{\pi})$$
$$p(\mathbf{x}_n | z_n = k) = \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

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Each data point $\mathbf{x}_n$ then is distributed

$$p(\mathbf{x}_n) = \sum_k p(z_n = k) p(\mathbf{x}_n | z_n = k) = \sum_k \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

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- Estimate the parameters $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ which correspond to cluster means and cluster covariances.

Gaussian mixtures: intuition

We'll go over the math behind estimating Gaussian mixture models (GMMs) in the next lecture. Algorithmically, it's simple enough to understand:

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- Update cluster parameters $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ by computing a mean and covariance of data points $\mathbf{x}_n$, weighted by the probability that $z_n = k$
  - *(Analogous to re-computing cluster centers in K-means)*

Gaussian mixture estimation

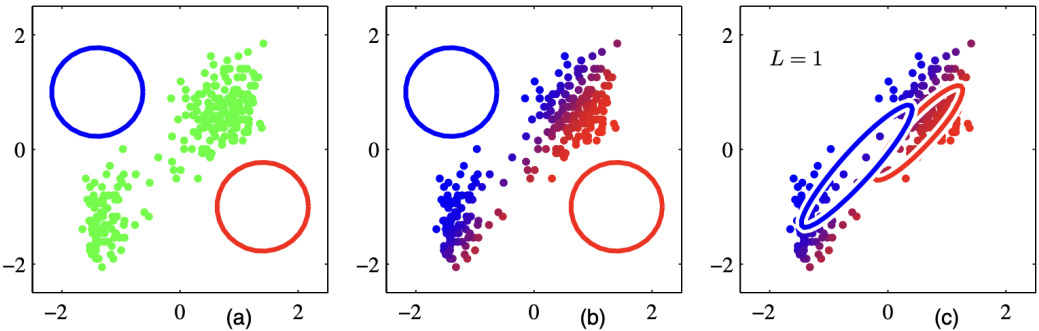

Figure: PRML

Gaussian mixture estimation

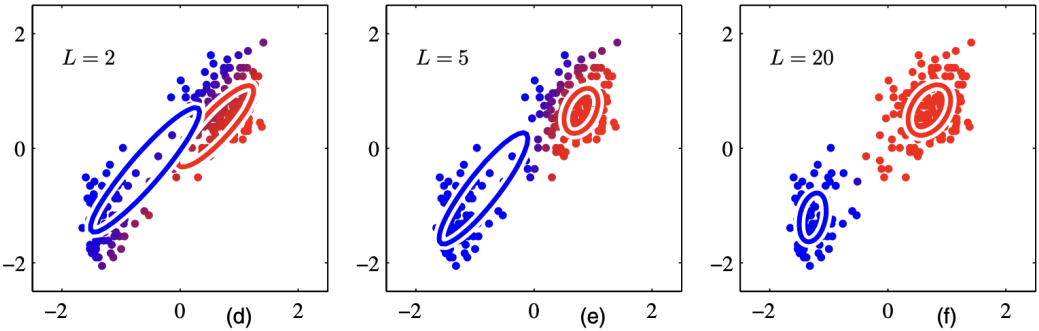

Figure: PRML

GMM or K-means?

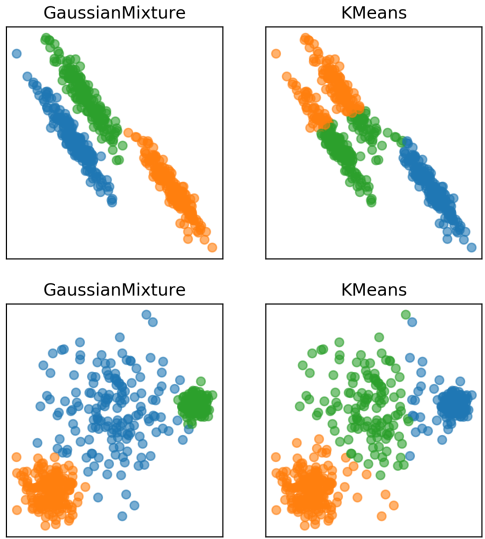

Figure: Andreas Müller

Thoughts on mixture models

Good things:

- Natural probabilistic model for clustering; generalizes K-means nicely
- Easy to expand to other data types (e.g. mixtures of Bernoullis, etc); different data types or likelihoods per-dimension are fine
- Choosing the number K can be done by looking at the likelihood on held-out test data, or using a Bayesian approach

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Less good things:

- Only can really find "compact" clusters
- Non-convex objective; initialization dependent
- GMMs are sensitive to outliers — consider using mixtures of Student-t distributions instead