Expectation-Maximization

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Content

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- We want to group the data into a few cohesive clusters.
- This is an **unsupervised learning** problem.

K-means clustering algorithm

The k-means clustering algorithm is as follows:

1. Initialize cluster centroids $\mu_1, \mu_2, \ldots, \mu_k \in \mathbb{R}^n$ randomly.
2. Repeat until convergence {

   - For every i, set

   $$c^{(i)} := \arg\min_j ||x^{(i)} - \mu_j||2.$$

   - For every j, set

   $$\mu_j = \frac{\sum_{i=1}^m 1\{c^{(i)}=j\}x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)}=j\}}.$$

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1. Assigning each training example $x^{(i)}$ to the closest cluster centroid μ_j, and
2. Moving each cluster centroid μ_j to the mean of the points assigned to it.

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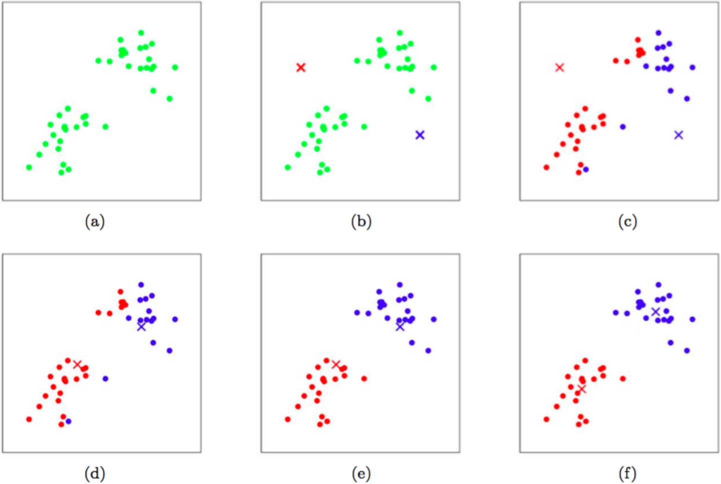
- We could choose k training examples randomly, and set the initial cluster centroids to be equal to the values of these k examples.
- Other initialization methods are also possible.

K-means clustering algorithm


(a) (b) (c) (d) (e) (f)

K-means clustering algorithm

Original image

$K = 2$

K-means clustering algorithm

Original image

$K = 3$

K-means clustering algorithm

Original image

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K-means clustering algorithm

- The k-means algorithm is guaranteed to converge in a certain sense. Let us define the distortion function to be:

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- In theory, it is possible for k-means to oscillate between a few different clusterings that have exactly the same value of J, but this almost never happens in practice.

- The distortion function J is a non-convex function, and then the algorithm can get stuck in local minima. Nevertheless, very often k-means will work fine and come up with very good clusterings.

K-means clustering algorithm

- Worried about getting stuck in bad local minima?

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- Worried about getting stuck in bad local minima?
- One common thing to do is run k-means many times using different random initial values for the cluster centroids μ_j.

Expectation-Maximization

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- The goal of ML estimation is to find the parameters that maximize the probability of having received certain measurements of a random variable, distributed by some probability density function.
- Given the density function $p(x|\theta)$ that is governed by a set of parameters θ, where p might be a set of Gaussians and θ could be the means and the covariances.

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- The function $\mathcal{L}(\theta|x)$ is called the likelihood of the parameters θ given the data.

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- Often we maximize $\log \mathcal{L}(\theta|x)$ instead because it is analytically easier.
- However, for many problems, it is not possible to solve this maximization problem analytically in closed form, and we must resort to more elaborate techniques.

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- The EM algorithm is useful when the data is incomplete or has missing values.

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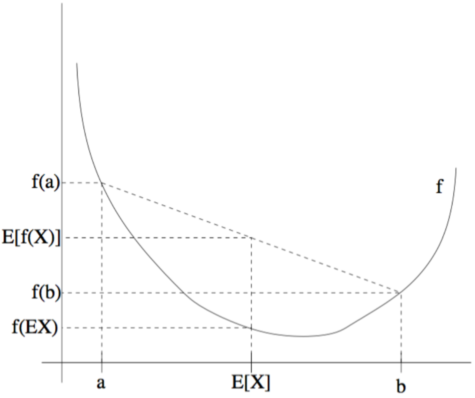
1. The first occurs when the data indeed has missing values, due to problems with or limitations of the observation process.
2. The second occurs when optimizing the likelihood function is analytically intractable, but the likelihood function can be simplified by assuming the existence of hidden parameters.

Expectation-Maximization

Jensen's inequality

$E[f(X)] \geq f(E[X])$



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- When $f(X)$ is **concave** we have:

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We wish to fit the parameters θ of a model $p(x, z)$ to the data where the likelihood is given by

$$\begin{aligned} \ell(\theta) &= \sum_{i=1}^{m} \log p(x;\theta) \\ &= \sum_{i=1}^{m} \log \sum_{z} p(x, z; \theta). \end{aligned}$$

Expectation-Maximization

$$\begin{aligned}\sum_i \log p(x^{(i)};\theta) &= \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)};\theta) \\ &= \sum_i \log \sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})} \\ &\geq \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})}\end{aligned}$$

Expectation-Maximization

For each i let Q_i be some distribution over the z's , that is $\sum_z Q_i(z) = 1, Q_i(z) \geq 0$.

In the EM algorithm, you repeat until convergence:

(E-step) For each i, set

$$Q_i(z^{(i)}) := p(z^{(i)}|x^{(i)};\theta).$$

(M-step) Set

$$\theta := \arg\max_{\theta} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

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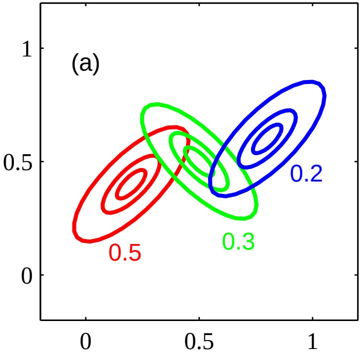
  $\phi_j \geq 0$,

  $\sum_{j=1}^{k} \phi_j = 1$.
- The parameter ϕ_j gives $p(z^{(i)} = j)$ and $x^{(i)}|z^{(i)} = j \sim \mathcal{N}(\mu_j, \Sigma_j)$.

Mixtures of Gaussians

$K = 3$ Gaussians



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- This is called the **mixture of Gaussians** model.
- Note that the $z^{(i)}$'s are **latent** random variables, meaning that they are hidden/unobserved.

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- However, if we set to zero the derivatives of this formula with respect to the parameters and try to solve, we will see that it is not possible to find the maximum likelihood estimates of the parameters in closed form.

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- Maximizing this with respect to ϕ, μ and Σ gives the parameters:

$$\begin{aligned}
\phi_j &= \tfrac{1}{m} \textstyle\sum_{i=1}^{m} 1\{z^{(i)} = j\}, \\
\mu_j &= \frac{\sum_{i=1}^{m} 1\{z^{(i)}=j\} x^{(i)}}{\sum_{i=1}^{m} 1\{z^{(i)}=j\}}, \\
\Sigma_j &= \frac{\sum_{i=1}^{m} 1\{z^{(i)}=j\}(x^{(i)}-\mu_j)(x^{(i)}-\mu_j)^\top}{\sum_{i=1}^{m} 1\{z^{(i)}=j\}}.
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- We can use the Expectation-Maximization (EM) algorithm that has two steps:

1. In the E-step, it tries to guess the values of the $z^{(i)}$'s.
2. In the M-step, it updates the parameters of our model based on our guesses.

Mixtures of Gaussians

- The EM algorithm would be implemented as follows:

Repeat until convergence {

1. (E-step) For each i, j set

$$w_j^{(i)} := p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$

2. (M-step) Update the parameters

$$\begin{aligned}
\phi_j &= \frac{1}{m} \sum_{i=1}^{m} w_j^{(i)}, \\
\mu_j &= \frac{\sum_{i=1}^{m} w_j^{(i)} x^{(i)}}{\sum_{i=1}^{m} w_j^{(i)}}, \\
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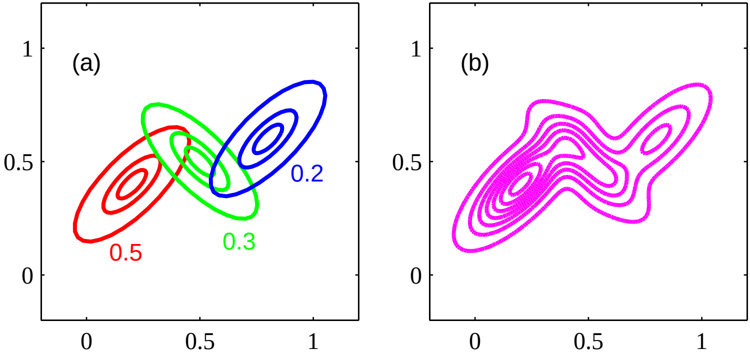

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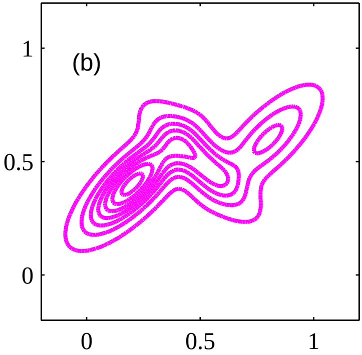

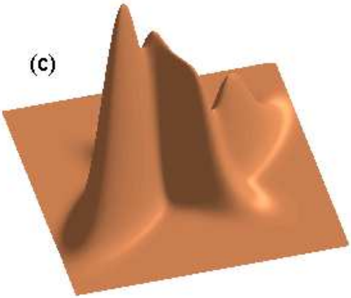

Mixtures of Gaussians

- Once we have estimated the parameters ϕ, μ and Σ, we could apply the following Bayes rule to classify a new point $x^{(i)}$:

$$p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma) = \frac{p(x^{(i)} | z^{(i)} = j; \mu, \Sigma) p(z^{(i)} = j; \phi)}{\sum_{l=1}^{k} p(x^{(i)} | z^{(i)} = l; \mu, \Sigma) p(z^{(i)} = l; \phi)}.$$

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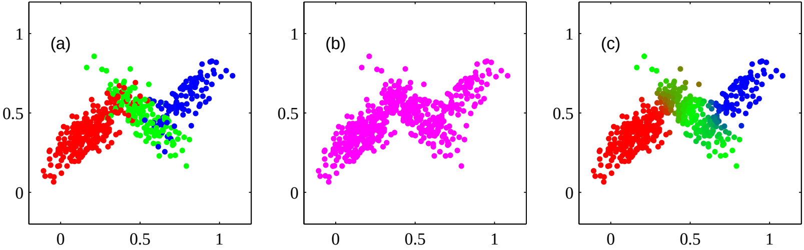
- Similarly, to K-means, it is also susceptible to local optima, so reinitializing at several different initial parameters may be a good idea.

Mixtures of Gaussians

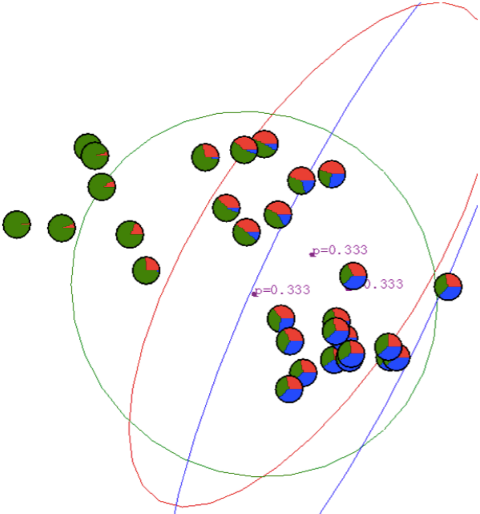
$K = 3$ Gaussians and 500 data points



(a) Complete data; (b) Incomplete data; (c) Final solution

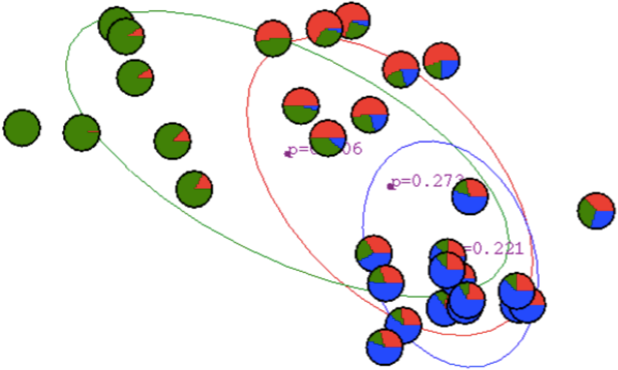
Mixtures of Gaussians

Start



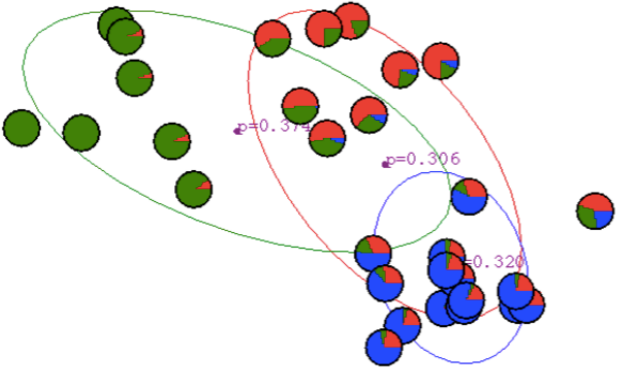
Mixtures of Gaussians

Iteration 1



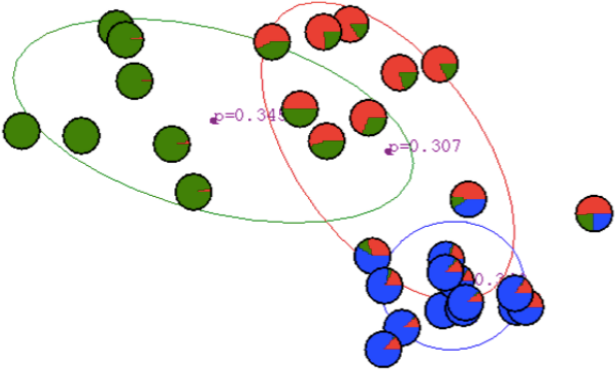
Mixtures of Gaussians

Iteration 2



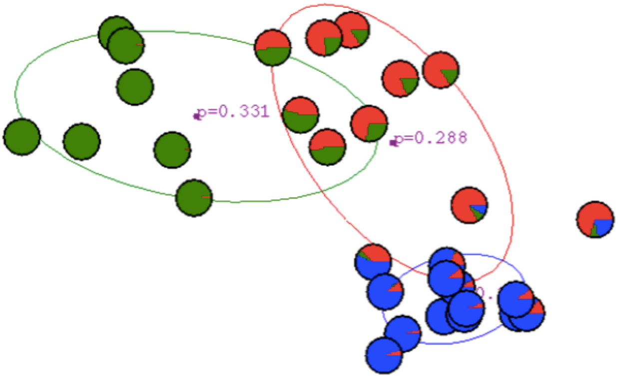
Mixtures of Gaussians

Iteration 3



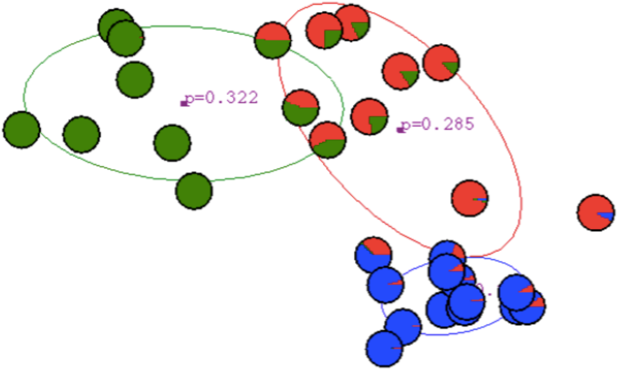
Mixtures of Gaussians

Iteration 4



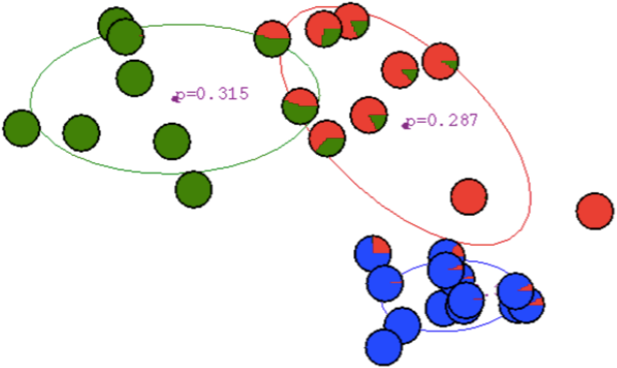
Mixtures of Gaussians

Iteration 5



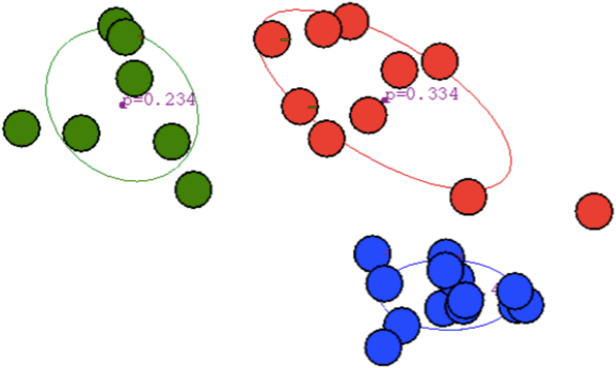
Mixtures of Gaussians

Iteration 6



Mixtures of Gaussians

Iteration 20



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Thank you!

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