Computational Data Analysis

Machine Learning

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Gaussian Mixture Model and EM Algorithm

Gaussian mixture model

- A density model $p(X)$ may be multi-modal: model it as a mixture of uni-modal distributions (e.g. Gaussians)

$$\mathcal{N}(X|\mu_k,\Sigma_k) := \frac{1}{|\Sigma|^{\frac{1}{2}}(2\pi)^{\frac{d}{2}}} exp\left(-\frac{1}{2}(X-\mu)^{\mathsf{T}}\Sigma^{-1}(X-\mu)\right)$$

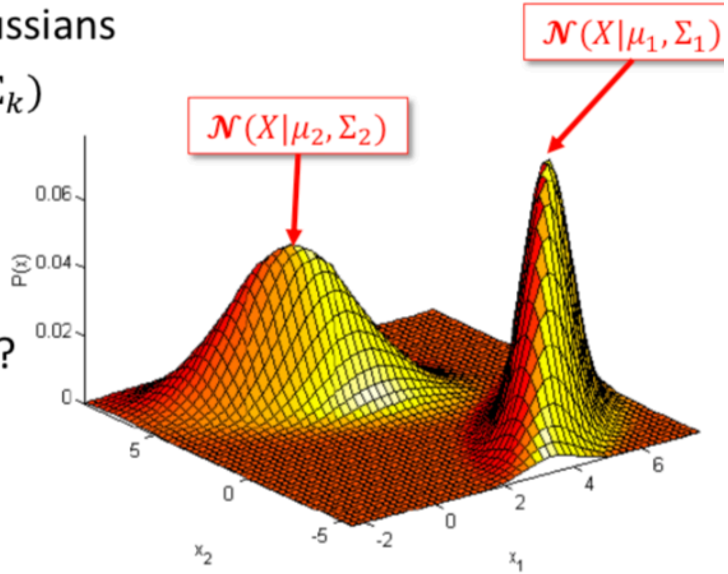
- Consider a mixture of K Gaussians
  - $p(X) = \sum_{k=1}^{K} \pi_k \mathcal{N}(X|\mu_k,\Sigma_k)$

mixing proportion

mixture Component

- Parametric or noparametric?

- Learn $\pi_k \in (0,1), \mu_k, \Sigma_k$;



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EM algorithm

- Associate each data and each component with a τ_k^i
- Initialize (π_k, μ_k, Σ_k), $k = 1 \dots K$
- Iterate the following two steps till convergence:
  - Expectation step (E-step): update τ_k^i given current (π_k, μ_k, Σ_k)

$$\tau_k^i = p\left(z_k^i = 1 \middle| D, \mu, \Sigma\right) = \frac{\pi_k \boldsymbol{\mathcal{N}}(x_i | \mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \boldsymbol{\mathcal{N}}(x_i | \mu_{k'}, \Sigma_{k'})}$$

$$(k = 1 \dots K, i = 1 \dots m)$$

  - Maximization step (M-step): update (π_k, μ_k, Σ_k) given τ_k^i

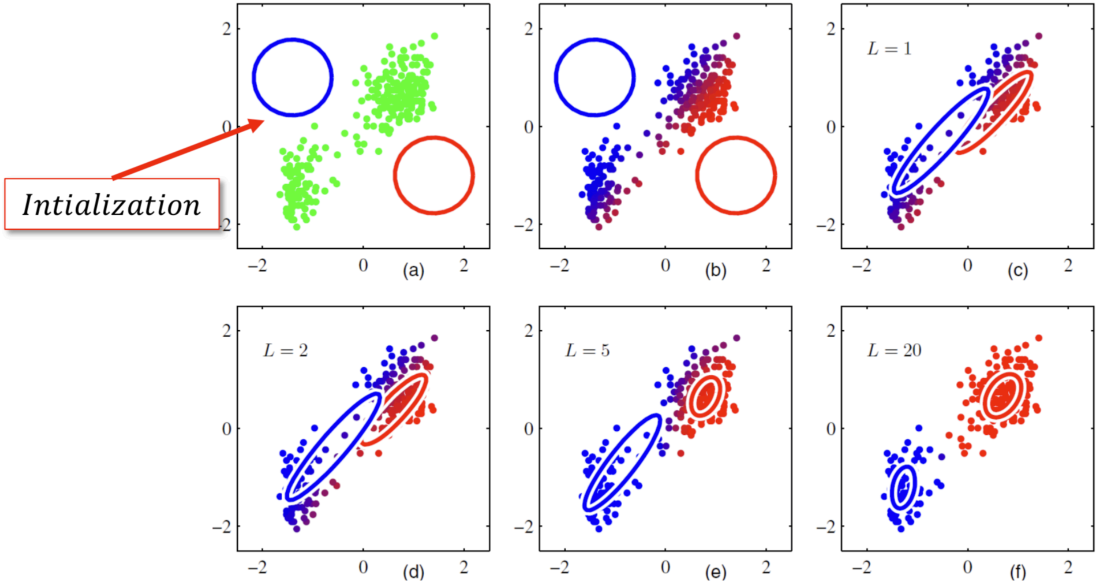
$$\pi_k = \frac{\sum_i \tau_k^i}{m}, \qquad \mu_k = \frac{\sum_i \tau_k^i x^i}{\sum_i \tau_k^i}$$

$$\Sigma_k = \frac{\sum_i \tau_k^i \left(x^i - \mu_k\right)\left(x^i - \mu_k\right)^T}{\sum_i \tau_k^i}$$

$$(k = 1 \dots K)$$

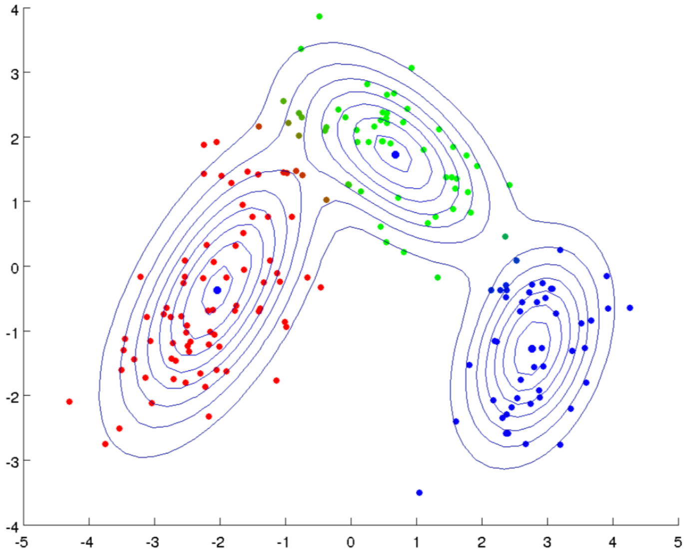
Expectation-Maximization Iterations

- $k = 1\ or\ 2$
- Use τ_1^i as the proportion of red, and τ_2^i proportion of blue
- Draw only one contour for each Gaussian component



Mixture of 3 Gaussians

- First run PCA to reduce the dimension to 2
- $k = 1 \; or \; 2 \; or \; 3$
- Use τ_1^i as the proportion of red, τ_2^i proportion of green, and τ_3^i proportion of green

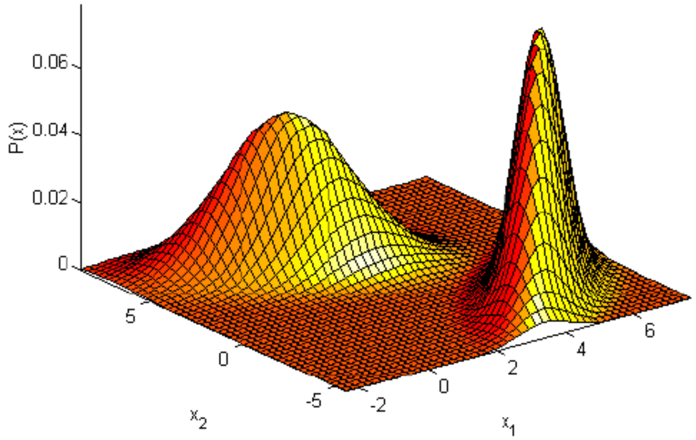


Generating a data point from GMM

- For each data point x^i:
  - Randomly choose a mixture component, $z^i = \{1,2, \dots K\}$, with probability π_{z^i}
  - Then sample the actual value of x^i from a Gaussian distribution $\boldsymbol{\mathcal{N}}\left(x \middle| \mu_{z^i}, \Sigma_{z^i}\right)$

- Joint distribution over $p(x, z)$
- $p(x, z) = \pi_z \boldsymbol{\mathcal{N}}(x|\mu_z, \Sigma_z)$

- Marginal distribution $p(x)$
- $p(x) = \sum_{z=1}^{K} p(x, z) = \sum_{z=1}^{K} p(x|z)p(z)$



Learning the Parameters

- How to learn?

- Maximum likelihood learning (let $\theta = (\pi_k, \mu_k, \Sigma_k)$, $k = 1 \dots K$
- $\theta^* = \mathrm{argmax}\, l(\theta; D) = \log \prod_{i=1}^{m} p(x^i)$

- Write down the log-likelihood function (related to previous slide, generating a GMM sample)

$$l(\theta; D) = \log \prod_{i=1}^{m} \left(\sum_{z^i=1}^{K} p\left(x^i, z^i \middle| \theta\right) \right)$$

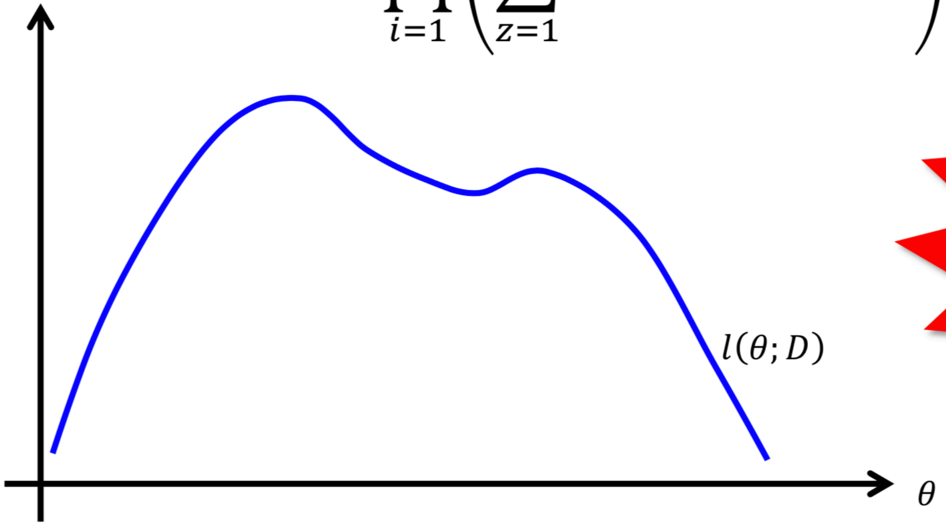
$$= \log \prod_{i=1}^{m} \left(\sum_{z^i=1}^{K} p\left(x^i \middle| \mu_{z^i}, \Sigma_{z^i}\right) p\left(z^i | \pi\right) \right)$$

Why is learning hard?

- With latent variables z, likelihood of the data becomes

$$l(\theta; D) = \log \prod_{i=1}^{m} \left(\sum_{z^i=1}^{K} p(x^i | \mu_{z^i}, \Sigma_{z^i}) p(z^i | \pi) \right)$$

$$= \log \prod_{i=1}^{m} \left(\sum_{z=1}^{K} \pi_{z^i} \mathcal{N}(x | \mu_{z^i}, \Sigma_{z^i}) \right)$$



Nonconvex
Difficult!

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Details of EM

- We intend to learn the parameters that maximizes the log–likelihood of the data

$$l(\theta; D) = \log \prod_{i=1}^{m} \left(\sum_{z^i=1}^{K} p\left(x^i, z^i \middle| \theta\right) \right)$$

Nonconvex
Difficult!

- Expectation step (E-step): What do we take expectation over?

$$l(\theta; D) \geq f(\theta) = E_{q(z^1, z^2, \ldots, z^m)}[\log \prod_{i=1}^{m} p\left(x^i, z^i \middle| \theta\right)]$$

- Maximization step (M-step): how to maximize?

$$\theta^{t+1} = argmax_{\theta}\ f(\theta)$$

Bayes rule

likelihood Prior

$$P(z|x) = \frac{P(x|z)P(z)}{P(x)} = \frac{P(x,z)}{\sum_{z'} P(x,z')}$$

posterior normalization constant

Prior: $p(z) = \pi_z$

Likelihood: $p(x|z) = \mathcal{N}(x|\mu_z, \Sigma_z)$

Posterior: $p(z|x) = \frac{\pi_z \mathcal{N}(x|\mu_z, \Sigma_z)}{\sum_{z'} \pi_{z'} \mathcal{N}(x|\mu_{z'}, \Sigma_{z'})}$

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E-step: what is $q(z^1, z^2, .., z^m)$

- $q(z^1, z^2, .., z^m)$: posterior distribution of the latent variables

$$q(z^1, z^2, .., z^m) = \prod_{i=1}^{m} p(z^i | x^i, \theta^t)$$

- For each data point x^i, compute $p(z^i = k | x^i)$ for each k

$$\tau_k^i = p\left(z^i = k \middle| x^i\right) = \frac{p(z^i = k\ , x^i)}{\sum_{k'=1..K} p(z^i = k', x^i)}$$

$$= \frac{\pi_k \boldsymbol{\mathcal{N}}\left(x^i \middle| \mu_k, \Sigma_k\right)}{\sum_{k'=1..K} \pi_{k'} \boldsymbol{\mathcal{N}}(x^i | \mu_{k'}, \Sigma_{k'})}$$

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E-step: compute the expectation

$$f(\theta) = E_{q(z^1,z^2,\ldots,z^m)}\left[\log \prod_{i=1}^{m} p\left(x^i, z^i | \theta\right)\right]$$

$$= \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}\left[\log p\left(x^i, z^i | \theta\right)\right]$$

$$= \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}\left[\log \pi_{z^i} \mathcal{N}\left(x^i | \mu_{z^i}, \Sigma_{z^i}\right)\right]$$

- Expand log of Gaussian $\log \mathcal{N}\left(x^i | \mu_{z^i}, \Sigma_{z^i}\right)$

$$f(\theta) = \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}\left[\log \pi_{z^i} - \left(x^i - \mu_{z^i}\right)^{\top} \Sigma_{z^i}\left(x^i - \mu_{z^i}\right) + \log \Sigma_{z^i} + c\right]$$

$$= \sum_{i=1}^{m} \sum_{k=1}^{K} \tau_k^i \left[\log \pi_k - \left(x^i - \mu_k\right)^{\top} \Sigma_k \left(x^i - \mu_k\right) + \log \Sigma_k + c\right]$$

M-step: maximize $f(\theta)$

- $f(\theta) = \sum_{i=1}^{m} \sum_{k=1}^{K} \tau_i^k \left[\log \pi_k - \left(x^i - \mu_k\right)^\top \Sigma_k \left(x^i - \mu_k\right) + \log \Sigma_k + c\right]$

For instance, we want to find π_k, and $\sum_{i=1}^{K} \pi_k = 1$

- Form Lagrangian

$$L = \sum_{i=1}^{m} \sum_{k=1}^{K} \tau_k^i [\log \pi_k + other\ terms] + \lambda(1 - \sum_{i=1}^{K} \pi_k)$$

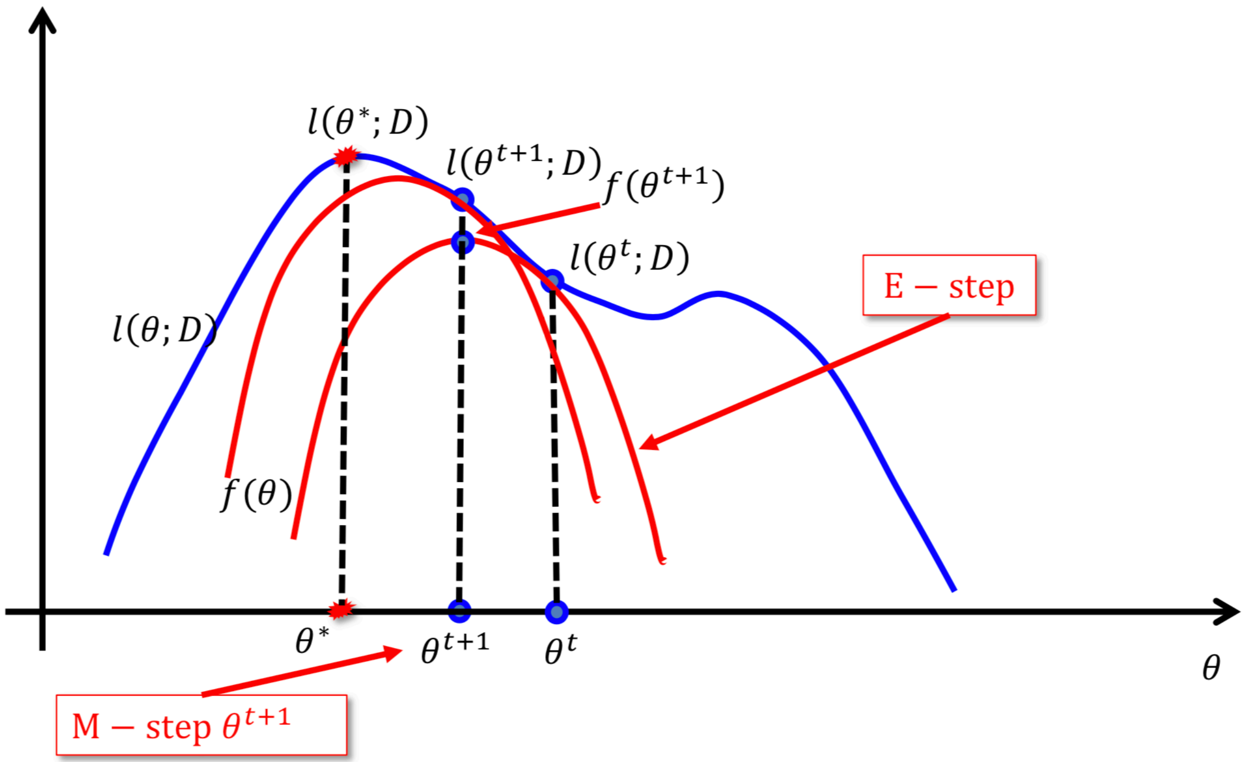
- Take partial derivative and set to 0

$$\frac{\partial L}{\partial \pi_k} = \sum_{i=1}^{m} \frac{\tau_k^i}{\pi_k} - \lambda = 0$$

$$\Rightarrow \pi_k = \frac{1}{\lambda} \sum_{i=1}^{m} \tau_k^i$$

$$\Rightarrow \lambda = m$$

EM graphically



EM vs. modified K-means

- The EM algorithm for mixture of Gaussian is like a soft clustering algorithm

- K-means:
  - "E-step", we do hard assignment:
    - $z^i = argmax_k (x^i - \mu_k)\, \Sigma_k^{-1} (x^i - \mu_k)$
  - "M-step", we update the means and covariance of cluster using maximum likelihood estimate:
    - $\mu_k = \frac{\sum_i \delta(z^i, k) x^i}{\sum_i \delta(z^i, k)}$
    - $\Sigma_k = \frac{\sum_i \delta(z^i, k)(x^i - \mu_k)\,(x^i - \mu_k)^T}{\sum_i \delta(z^i, k)}$

$\delta(z^i, k) = 1 \; if \; z^i = k$; otherwise 0.