Annotated version

Machine Learning Course - CS-433

Expectation-Maximization Algorithm

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changes by Martin Jaggi 2019, changes by Rüdiger Urbanke 2018, changes by Martin Jaggi 2016, 2017

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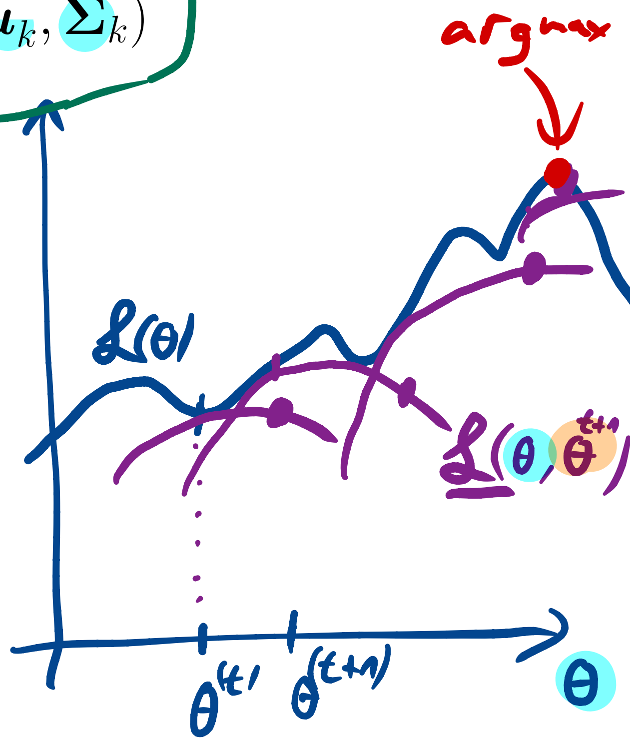
EPFL

$\theta = \left(\{\pi_k\}_{k=1}^K, \{\mu_k\}_{k=1}^K, \{\Sigma_k\}_{k=1}^K \right)$ with $\pi_k \in \mathbb{R}$, $\mu_k \in \mathbb{R}^D$, $\Sigma_k \in \mathbb{R}^{D\times D}$

Motivation

Computing maximum log-likelihood for Gaussian mixture model is difficult due to the log outside the sum.

$$\max_{\boldsymbol{\theta}} \ \mathcal{L}(\boldsymbol{\theta}) := \sum_{n=1}^{N} \underbrace{\log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \,|\, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\mathcal{L}_n}$$



Expectation-Maximization (EM) algorithm provides an elegant and general method to optimize such optimization problems. It uses an iterative two-step procedure where individual steps usually involve problems that are easy to optimize.

EM algorithm: Summary

Start with $\boldsymbol{\theta}^{(1)}$ and iterate:

1. Expectation step: Compute a lower bound to the cost such that it is tight at the previous $\boldsymbol{\theta}^{(t)}$:

- $\mathcal{L}(\boldsymbol{\theta}) \geq \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)})$ and $\quad \forall \theta \quad$ lower bound
- $\mathcal{L}(\boldsymbol{\theta}^{(t)}) = \underline{\mathcal{L}}(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t)})$. $\quad$ equality at $\theta = \theta^{(t)}$

2. Maximization step: Update $\boldsymbol{\theta}$:

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}).$$

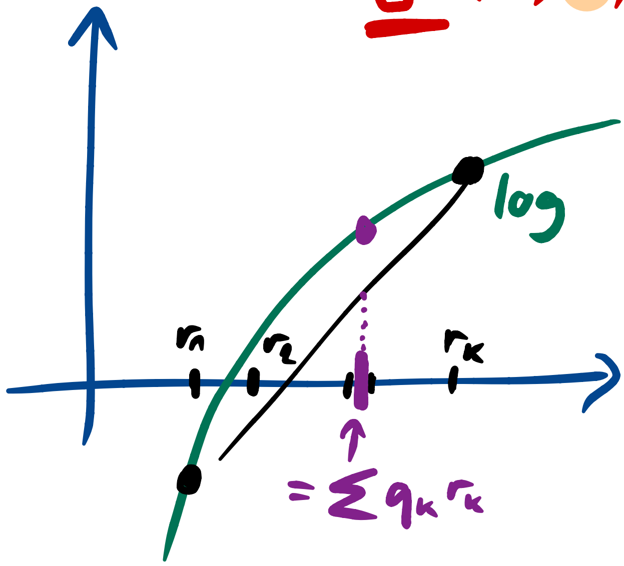
How to define $\mathcal{L}(\theta, \theta^{(t)})$

convexity of $-\log$

Concavity of log

Given non-negative weights q s.t. $\sum_k q_k = 1$, the following holds for any $r_k > 0$:

$$\log\left(\sum_{k=1}^{K} q_k r_k\right) \geq \sum_{k=1}^{K} q_k \log r_k$$



$\Leftrightarrow$ Jensen's inequality

$\Leftrightarrow$ $-\log$ is convex

The expectation step

$$\mathcal{L}_n(\theta) = \log \sum_{k=1}^{K} \overbrace{\pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}^{q_k \cdot r_k} \geq \underbrace{\sum_{k=1}^{K} q_{kn}^{(t)} \log \overbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{q_{kn}^{(t)}}}^{r_k}}_{=: \mathcal{L}_n(\theta, \theta^{(t)})}$$

with equality when,

$$q_{kn} := \frac{\pi_k^{(t)} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{k=1}^{K} \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}$$

This is not a coincidence.

- lower bound ✓
- coincides with $\mathcal{L}$ at $\theta = \theta^{(t)}$

$$\mathcal{L}_n(\theta^{(t)}, \theta^{(t)}) = \sum_{k=1}^{K} \underbrace{\frac{\pi_k \mathcal{N}(.)}{\sum_{k'} \pi_{k'} \mathcal{N}(.)}}_{q_{kn}} \log \frac{\cancel{\pi_k \mathcal{N}(.)}}{\underbrace{\frac{\cancel{\pi_k \mathcal{N}(.)}}{\sum_{k'} \pi_{k'} \mathcal{N}(.)}}_{q_{kn}}}$$

$$= \log \sum_{k=1}^{K} \pi_k \mathcal{N}(.)$$

$$= \mathcal{L}_n(\theta^{(t)})$$

The maximization step

Maximize the lower bound w.r.t. $\boldsymbol{\theta}$.

$$\mathcal{L}_n(\theta, \theta^{(t)})$$

$$\log\left(\frac{\pi_k \mathcal{N}(x_n | ..)}{q_{kn}}\right)$$

$$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \sum_{k=1}^{K} q_{kn}^{(t)} \Big[\log \pi_k + \log \underbrace{\mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\exp -(x_n - \mu)\Sigma^{-1}(x_n - \mu)}] \underbrace{\cancel{- \log q_{kn}^{(t)}}}_{\text{independent of } \theta} \Big]$$

Differentiating w.r.t. $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k^{-1}$, we can get the updates for $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$.

$$\nabla_{\mu_k} \mathcal{L}(\theta, \theta^{(t)}) \overset{!}{=} 0$$

$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$$

$$\nabla_{\Sigma_k^{-1}} \mathcal{L}(\theta, \theta^{(t)}) \overset{!}{=} 0$$

$$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} (\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})^\top}{\sum_n q_{kn}^{(t)}}$$

$$v \cdot v^\top$$

$$v = x_n - \mu_k$$

For π_k, we use the fact that they sum to 1. Therefore, we add a Lagrangian term, differentiate w.r.t. π_k and set to 0, to get the following update:

want $\sum_k \pi_k = 1$

$$\mathcal{L}_n + \beta\left(\sum_{k=1}^{K} \pi_k - 1\right)$$

modified unconstrained objective.

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_{n=1}^{N} q_{kn}^{(t)}$$

$$\nabla_{\pi_k} \mathcal{L}_n(\theta, \theta^{(t)}) \overset{!}{=} 0$$

Summary of EM for GMM

Initialize $\boldsymbol{\mu}^{(1)}, \boldsymbol{\Sigma}^{(1)}, \boldsymbol{\pi}^{(1)}$ and iterate between the E and M step, until $\mathcal{L}(\boldsymbol{\theta})$ stabilizes.

1. E-step: Compute assignments $q_{kn}^{(t)}$:

$$q_{kn}^{(t)} := \frac{\pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{k=1}^K \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}$$

$\approx \exp\left(-\frac{\|x_n - \mu_k\|^2}{\sigma^2}\right)$

$\approx \sum_{k=1}^{K} \exp(\cdot\cdot/\sigma^2)$

$\xrightarrow{\sigma^2 \to 0} = \begin{cases} 1 & \text{closest } k \\ 0 & \text{others} \end{cases}$

K-means assignment

$q_{kn} \approx z_{kn}$

2. Compute the marginal likelihood (cost).

$$\mathcal{L}(\boldsymbol{\theta}^{(t)}) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})$$

3. M-step: Update $\boldsymbol{\mu}_k^{(t+1)}, \boldsymbol{\Sigma}_k^{(t+1)}, \pi_k^{(t+1)}$.

$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$$

mean

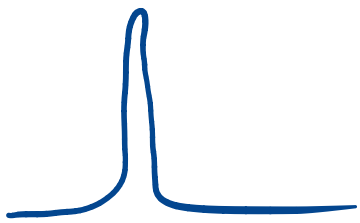
$$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} (\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})^\top}{\sum_n q_{kn}^{(t)}}$$

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_n q_{kn}^{(t)}$$

members of cluster k

If we let the covariance be diagonal i.e. $\boldsymbol{\Sigma}_k := \sigma^2 \mathbf{I}$, then EM algorithm is same as K-means as $\sigma^2 \to 0$.

large σ^2



small σ^2

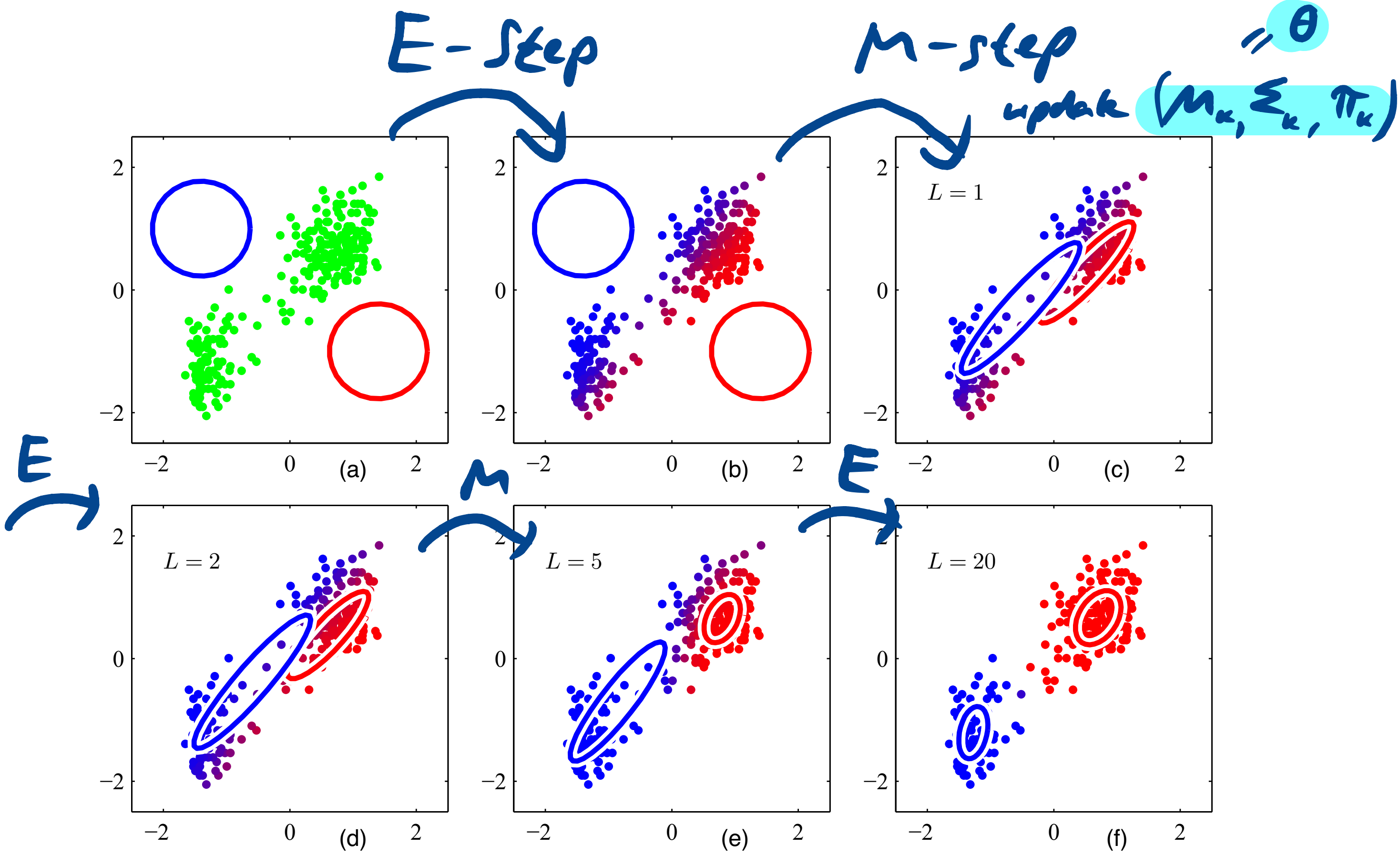


Figure 1: EM algorithm for GMM

Posterior distribution

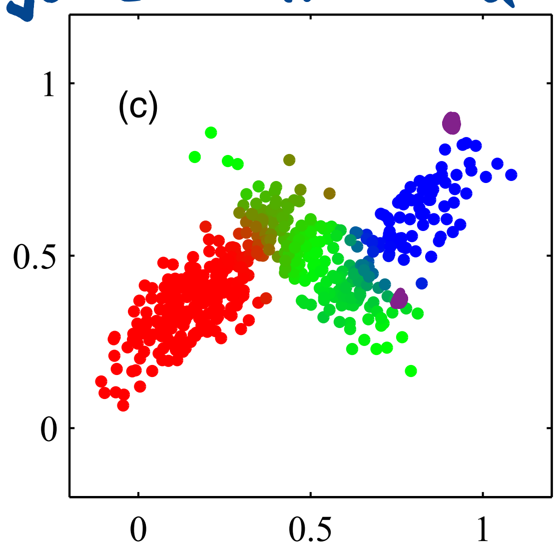
We now show that $q_{kn}^{(t)}$ is the posterior distribution of the latent variable, i.e. $q_{kn}^{(t)} = p(z_n = k \,|\, \mathbf{x}_n, \boldsymbol{\theta}^{(t)})$ posterior

Bayes

$p(A|B) \cdot p(B) = p(B|A) \cdot p(A)$

$$p(\mathbf{x}_n, z_n|\boldsymbol{\theta}) = p(\mathbf{x}_n|z_n, \boldsymbol{\theta})p(z_n|\boldsymbol{\theta}) = p(z_n|\mathbf{x}_n, \boldsymbol{\theta})p(\mathbf{x}_n|\boldsymbol{\theta})$$

joint $\quad$ likelihood · prior $\quad$ posterior · marginal likelihood



$$p(z_n = k | x_n, \theta) = \frac{\text{prior} \cdot \text{likelihood}}{ML}$$

$$= \frac{\overset{\pi_k}{p(z_n = k|\theta)}\; p(x_n|z_n = k, \theta)}{\sum_{k=1}^{K} p(z = k)\, p(x_n|z_n = k, \theta)}$$

$$p(x) = \sum_{k=1}^{K} \overset{\pi_k}{p(z_n = k)}\, p(x_n|z_n = k, \theta)$$

$$= \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_k \pi_k \mathcal{N}(x_n| \;.\;\; .\;)} =: q_{kn}$$

EM in general

Given a general joint distribution $p(\mathbf{x}_n, z_n|\boldsymbol{\theta})$, the marginal likelihood can be lower bounded similarly:

The EM algorithm can be compactly written as follows:

$$\boldsymbol{\theta}^{(t+1)} := \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{p(z_n|\mathbf{x}_n, \boldsymbol{\theta}^{(t)})}\big[\log p(\mathbf{x}_n, z_n|\boldsymbol{\theta})\big]$$

Another interpretation is that part of the data is missing, i.e. $(\mathbf{x}_n, z_n)$ is the "complete" data and z_n is missing. The EM algorithm averages over the "unobserved" part of the data.