

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
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Motivation

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

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

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 $\boldsymbol{\theta}^{(t)}$:

$$\mathcal{L}(\boldsymbol{\theta}) \geq \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) \text{ and } \mathcal{L}(\boldsymbol{\theta}^{(t)}) = \underline{\mathcal{L}}(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t)}).$$

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

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

Concavity of log

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

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

The expectation step

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

with equality when,

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

This is not a coincidence.

The maximization step

Maximize the lower bound w.r.t. θ .

$$\max_{\theta} \sum_{n=1}^N \sum_{k=1}^K q_{kn}^{(t)} [\log \pi_k + \log \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$$

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

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

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:

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

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 $q_{kn}^{(t)}$:

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

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 $\boldsymbol{\mu}_k^{(t+1)}, \boldsymbol{\Sigma}_k^{(t+1)}, \pi_k^{(t+1)}$.

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

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 $\sigma^2 \rightarrow 0$.

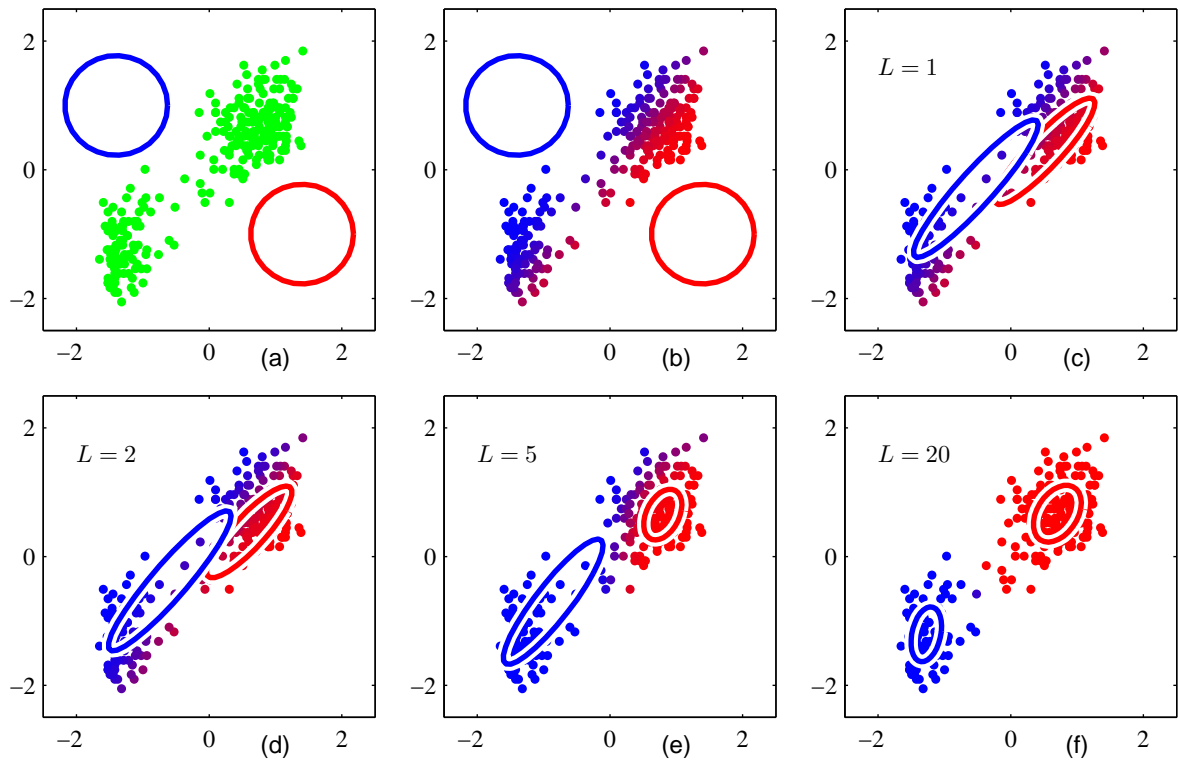
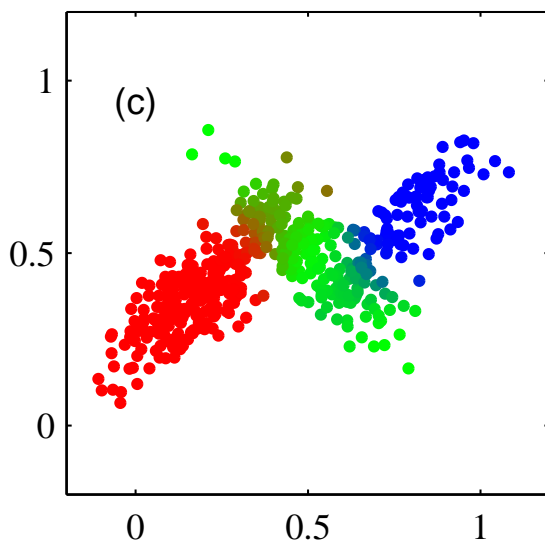


Figure 1: EM algorithm for GMM

Posterior distribution

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

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



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:

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

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.