Machine Learning Course - CS-433
Expectation-Maximization Algorithm

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EPFL

Motivation

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

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

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

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

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

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

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

$\log \sum_{k=1}^K \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \geq \sum_{k=1}^K q_{kn} \log \frac{\pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{q_{kn}}$
with equality when,
$q_{kn} = \frac{\pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_{k=1}^K \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}$
This is not a coincidence.

The maximization step

Maximize the lower bound w.r.t. $\boldsymbol{\theta}$.
$\max_{\boldsymbol{\theta}} \sum_{n=1}^N \sum_{k=1}^K q_{kn}^{(t)} \left[\log \pi_k + \log \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right]$
Differentiating w.r.t. $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k^{-1}$, we
can get the updates for $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$.

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

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

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

2. Compute the marginal likelihood (cost).

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

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

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

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 $\sigma^2 \to 0$.

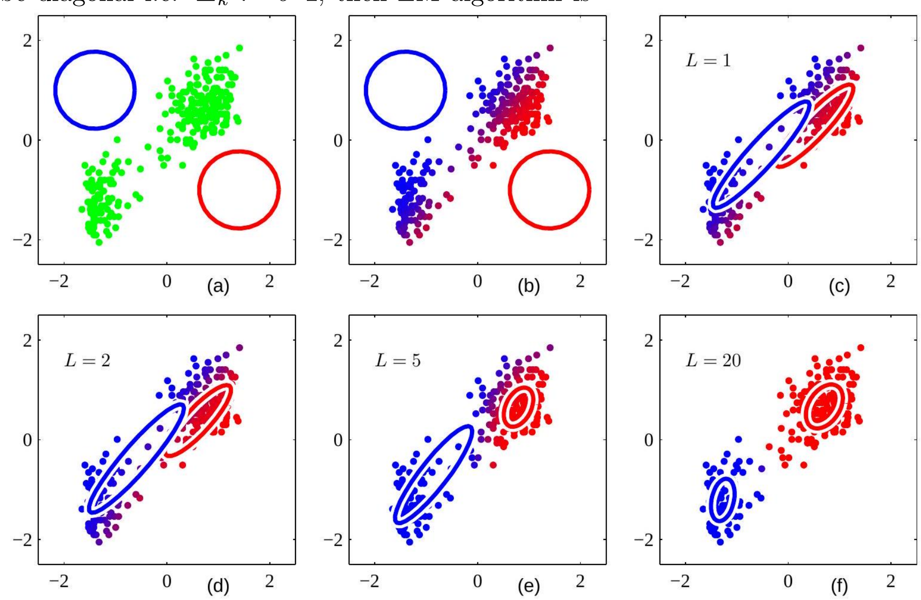
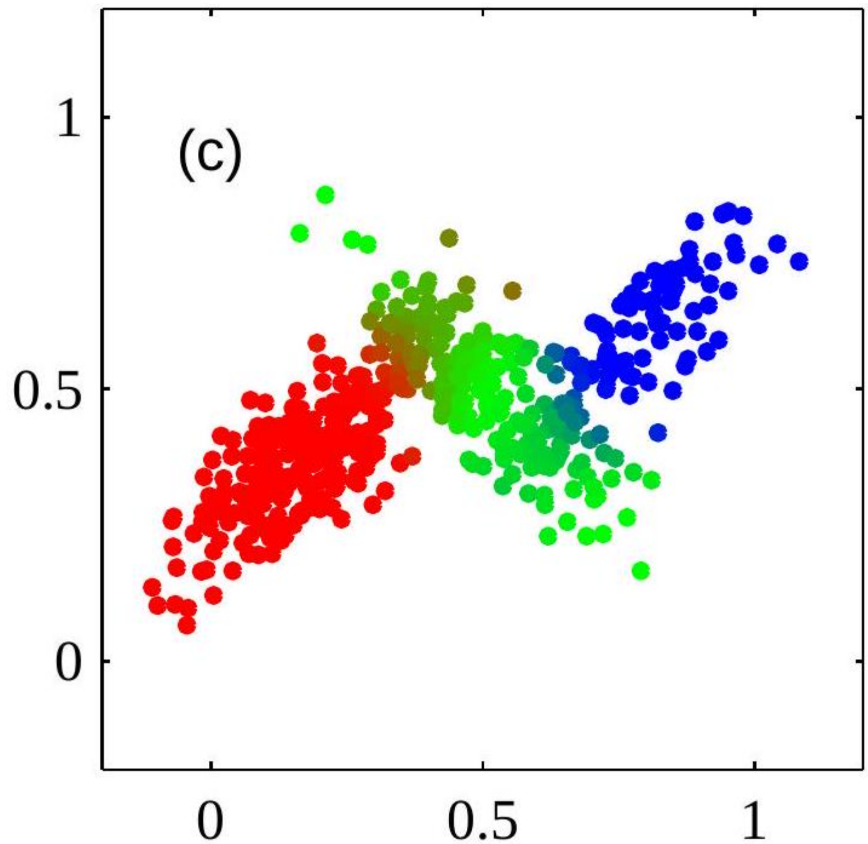


Figure 1: EM algorithm for GMM

Posterior distribution

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

$p\left(\mathbf{x}_n, z_n \mid \boldsymbol{\theta}\right) = p\left(\mathbf{x}_n \mid z_n, \boldsymbol{\theta}\right) p\left(z_n \mid \boldsymbol{\theta}\right) = p\left(z_n \mid \mathbf{x}_n, \boldsymbol{\theta}\right) p\left(\mathbf{x}_n \mid \boldsymbol{\theta}\right)$



EM in general

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

The EM algorithm can be compactly written as follows:
$\boldsymbol{\theta}^{(t+1)} := \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{p\left(z_n \mid \mathbf{x}_n, \boldsymbol{\theta}^{(t)}\right)} \left[\log p(\mathbf{x}_n, z_n \mid \boldsymbol{\theta})\right]$

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.