EM Algorithm for Latent Variable Models

Julia Kempe & David S. Rosenberg

New York University

May 7, 2019

Contents

Latent Variable Models

General Latent Variable Model

- Two sets of random variables: z and x.
- z consists of unobserved **hidden variables**.
- x consists of **observed variables**.
- Joint probability model parameterized by $\theta \in \Theta$:

$$p(x, z \mid \theta)$$

Definition

A **latent variable model** is a probability model for which certain variables are never observed.

e.g. The Gaussian mixture model is a latent variable model.

Complete and Incomplete Data

- Suppose we observe some data $(x_1, \ldots, x_n)$.
- To simplify notation, take x to represent the entire dataset

$$x = (x_1, \ldots, x_n),$$

and z to represent the corresponding unobserved variables

$$z = (z_1, \ldots, z_n).$$

- An observation of x is called an **incomplete data set**.
- An observation (x, z) is called a **complete data set**.

Our Objectives

- **Learning problem**: Given incomplete dataset x, find MLE

$$\hat{\theta} = \arg\max_{\theta} p(x \mid \theta).$$

- **Inference problem**: Given x, find conditional distribution over z:

$$p(z \mid x, \theta).$$

- For Gaussian mixture model, learning is hard, inference is easy.
- For more complicated models, inference can also be hard. (See DSGA-1005)

Log-Likelihood and Terminology

- Note that
$$\arg\max_{\theta} p(x \mid \theta) = \arg\max_{\theta} \left[\log p(x \mid \theta)\right].$$
- Often easier to work with this "**log-likelihood**".
- We often call $p(x)$ the **marginal likelihood**,
    - because it is $p(x,z)$ with z "marginalized out":
$$p(x) = \sum_{z} p(x,z)$$
- We often call $p(x,z)$ the **joint**. (for "joint distribution")
- Similarly, $\log p(x)$ is the **marginal log-likelihood**.

EM Algorithm (and Variational Methods) – The Big Picture

Big Picture Idea

- Want to find θ by maximizing the likelihood of the observed data x:

$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\max} \left[\log p(x \mid \theta)\right]$$

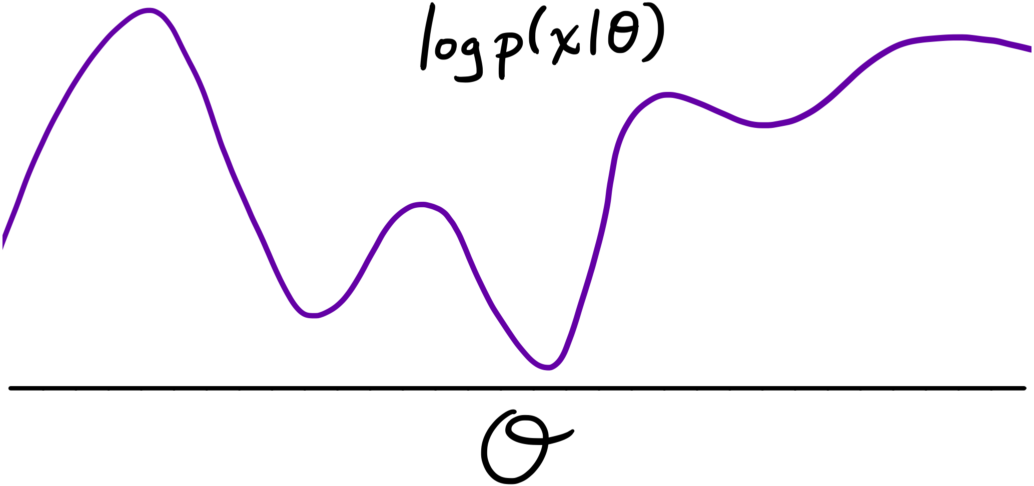
- Unfortunately this may be hard to do directly.
- Approach: Generate a **family of lower bounds** on $\theta \mapsto \log p(x \mid \theta)$.
- For every $q \in \mathcal{Q}$, we will have a lower bound:

$$\log p(x \mid \theta) \geqslant \mathcal{L}_q(\theta) \qquad \forall \theta \in \Theta$$

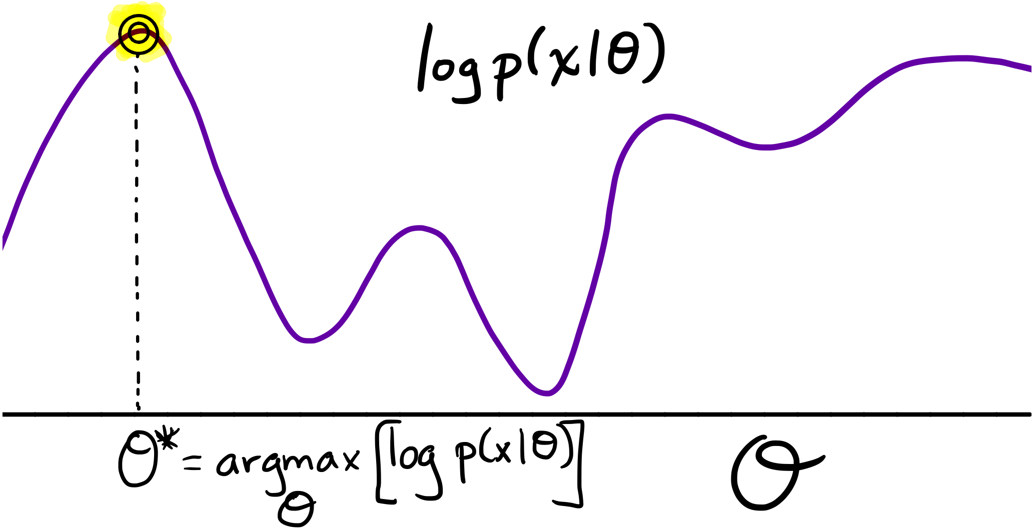
- We will try to find the maximum over all lower bounds:

$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\max} \left[\sup_{q \in \mathcal{Q}} \mathcal{L}_q(\theta) \right]$$

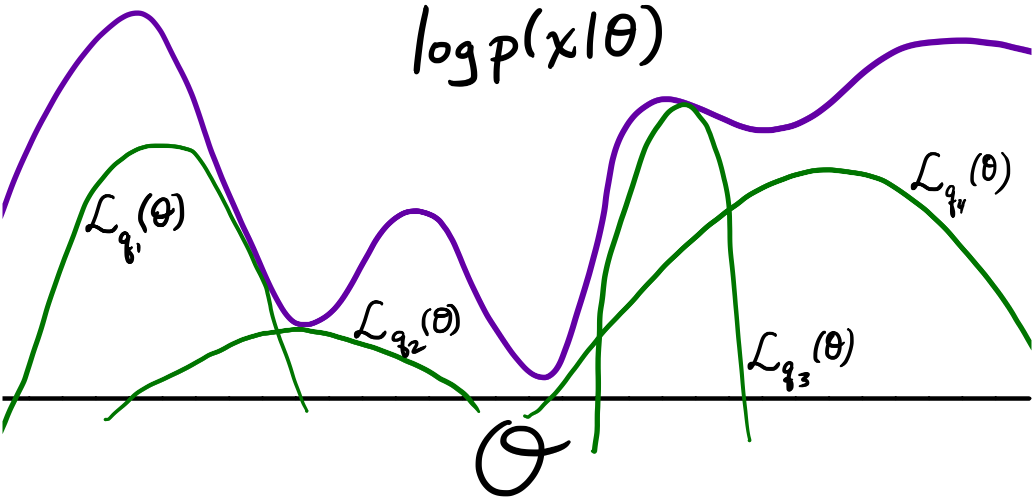
The Marginal Log-Likelihood Function



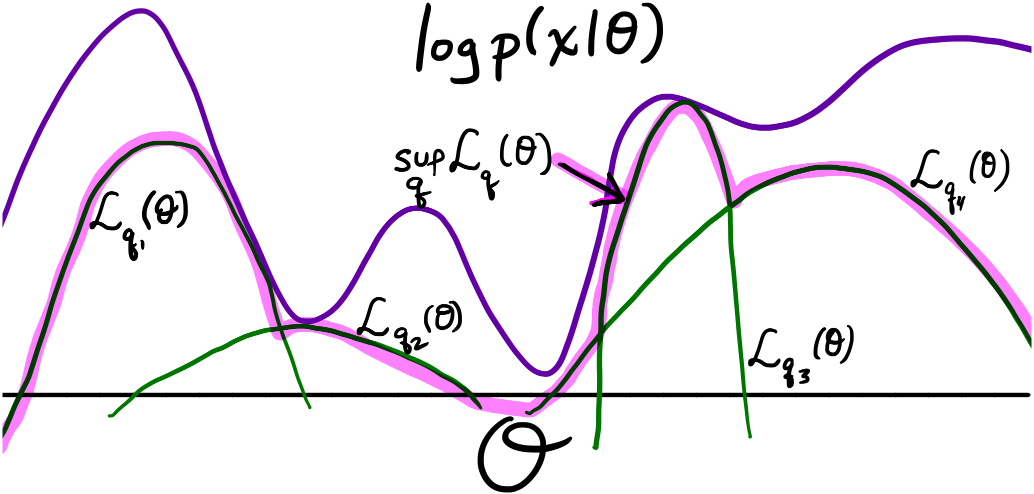
The Maximum Likelihood Estimator



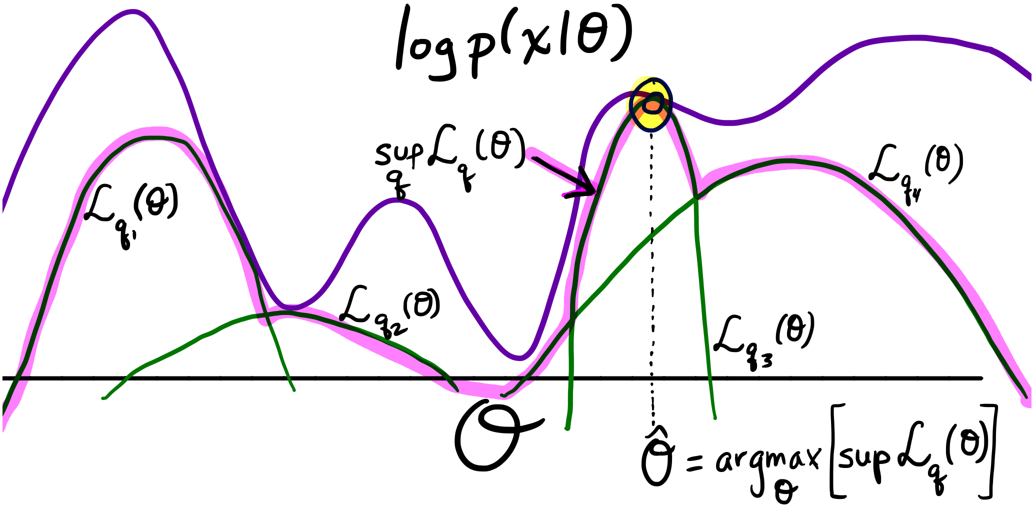
Lower Bounds on Marginal Log-Likelihood



Supremum over Lower Bounds is a Lower Bound



Parameter Estimate: Max over all lower bounds



The Expected Complete Data Log-Likelihood

- Marginal log-likelihood is hard to optimize:

$$\max_{\theta} \log p(x \mid \theta)$$

- **Typically** the complete data log-likelihood is easy to optimize:

$$\max_{\theta} \log p(x, z \mid \theta)$$

- What if we had a **distribution** $q(z)$ for the latent variables z?

The Expected Complete Data Log-Likelihood

- Suppose we have a distribution $q(z)$ on latent variable z.
- Then maximize the **expected complete data log-likelihood**:

$$\max_{\theta} \sum_{z} q(z) \log p(x, z \mid \theta)$$

- If q puts lots of weight on actual z, this could be a good approximation to MLE
- EM **assumes this maximization is relatively easy**.
- (This is true for GMM.)

Math Prerequisites

Jensen's Inequality

Theorem (Jensen's Inequality)

If $f : \mathbf{R} \to \mathbf{R}$ is a ***convex*** *function, and x is a random variable, then*

$$\mathbb{E}f(x) \geqslant f(\mathbb{E}x).$$

Moreover, if f is ***strictly convex****, then equality implies that $x = \mathbb{E}x$ with probability 1 (i.e. x is a constant).*

- e.g. $f(x) = x^2$ is convex. So $\mathbb{E}x^2 \geqslant (\mathbb{E}x)^2$. Thus

$$\operatorname{Var}(x) = \mathbb{E}x^2 - (\mathbb{E}x)^2 \geqslant 0.$$

Kullback-Leibler Divergence

- Let $p(x)$ and $q(x)$ be probability mass functions (PMFs) on $\mathcal{X}$.
- How can we measure how "different" p and q are?
- The **Kullback-Leibler** or **"KL" Divergence** is defined by

$$\mathrm{KL}(p\|q) = \sum_{x\in\mathcal{X}} p(x)\log\frac{p(x)}{q(x)}.$$

(Assumes $q(x)=0$ implies $p(x)=0$.)

- Can also write this as

$$\mathrm{KL}(p\|q) = \mathbb{E}_{x\sim p}\log\frac{p(x)}{q(x)}.$$

Gibbs Inequality ($\mathrm{KL}(p\|q) \geqslant 0$ and $\mathrm{KL}(p\|p) = 0$)

Theorem (Gibbs Inequality)

Let $p(x)$ and $q(x)$ be PMFs on $\mathcal{X}$. Then

$$KL(p\|q) \geqslant 0,$$

with equality iff $p(x) = q(x)$ for all $x \in \mathcal{X}$.

- KL divergence measures the "distance" between distributions.
- Note:
  - KL divergence **not a metric**.
  - KL divergence is **not symmetric**.

Gibbs Inequality: Proof

$$\begin{aligned}
\mathrm{KL}(p\|q) &= \mathbb{E}_p\left[-\log\left(\frac{q(x)}{p(x)}\right)\right] \\
&\geqslant -\log\left[\mathbb{E}_p\left(\frac{q(x)}{p(x)}\right)\right] \qquad \text{(Jensen's)} \\
&= -\log\left[\sum_{\{x|p(x)>0\}} p(x)\frac{q(x)}{p(x)}\right] \\
&= -\log\left[\sum_{x\in\mathcal{X}} q(x)\right] \\
&= -\log 1 = 0.
\end{aligned}$$

- Since $-\log$ is strictly convex, we have strict equality iff $q(x)/p(x)$ is a constant, which implies $q = p$.

The ELBO: Family of Lower Bounds on $\log p(x \mid \theta)$

Lower Bound for Marginal Log-Likelihood

- Let $q(z)$ be any PMF on $\mathcal{Z}$, the support of z:

$$
\begin{aligned}
\log p(x \mid \theta) &= \log\left[\sum_z p(x, z \mid \theta)\right] \\
&= \log\left[\sum_z q(z)\left(\frac{p(x, z \mid \theta)}{q(z)}\right)\right] \quad \text{(log of an expectation)} \\
&\geqslant \underbrace{\sum_z q(z) \log\left(\frac{p(x, z \mid \theta)}{q(z)}\right)}_{\mathcal{L}(q,\theta)} \quad \text{(expectation of log)}
\end{aligned}
$$

- Inequality is by Jensen's, by concavity of the log.

This inequality is the basis for **"variational methods"**, of which EM is a basic example.

The ELBO

- For any PMF $q(z)$, we have a lower bound on the marginal log-likelihood

$$\log p(x \mid \theta) \geqslant \underbrace{\sum_z q(z) \log\left(\frac{p(x,z \mid \theta)}{q(z)}\right)}_{\mathcal{L}(q,\theta)}$$

- Marginal log likelihood $\log p(x \mid \theta)$ also called the **evidence**.
- $\mathcal{L}(q,\theta)$ is the **evidence lower bound**, or "**ELBO**".

In EM algorithm (and variational methods more generally), we maximize $\mathcal{L}(q,\theta)$ over q and θ.

MLE, EM, and the ELBO

- For any PMF $q(z)$, we have a lower bound on the marginal log-likelihood

$$\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta).$$

- The MLE is defined as a maximum over θ:

$$\hat{\theta}_{\text{MLE}} = \underset{\theta}{\arg\max} \left[\log p(x \mid \theta)\right].$$

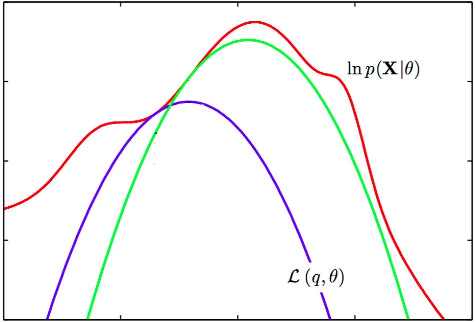
- In EM algorithm, we maximize the lower bound (ELBO) over θ and q:

$$\hat{\theta}_{\text{EM}} \approx \underset{\theta}{\arg\max} \left[\max_{q} \mathcal{L}(q, \theta)\right]$$

- In EM algorithm, q ranges over all distributions on z.

A Family of Lower Bounds

- For each q, we get a lower bound function: $\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta)\ \forall \theta$.
- Two lower bounds (blue and green curves), **as functions of** θ:



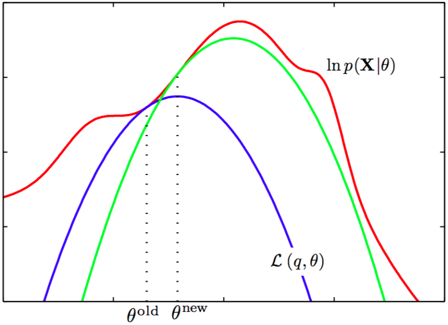
- Ideally, we'd find the maximum of the red curve. Maximum of green is close.

From Bishop's *Pattern recognition and machine learning*, Figure 9.14.

EM: Coordinate Ascent on Lower Bound

- Choose sequence of q's and θ's by "**coordinate ascent**" on $\mathcal{L}(q, \theta)$.
- EM Algorithm (high level):
  1. Choose initial θ^{old}.
  2. Let $q^* = \arg\max_q \mathcal{L}(q, \theta^{\text{old}})$
  3. Let $\theta^{\text{new}} = \arg\max_\theta \mathcal{L}(q^*, \theta^{\text{old}})$.
  4. Go to step 2, until converged.
- Will show: $p(x \mid \theta^{\textbf{new}}) \geqslant p(x \mid \theta^{\textbf{old}})$
- **Get sequence of θ's with monotonically increasing likelihood.**

EM: Coordinate Ascent on Lower Bound



1. Start at θ^{old}.
2. Find q giving best lower bound at $\theta^{\text{old}} \implies \mathcal{L}(q, \theta)$.
3. $\theta^{\text{new}} = \arg\max_{\theta} \mathcal{L}(q, \theta)$.

From Bishop's *Pattern recognition and machine learning*, Figure 9.14.

EM: Next Steps

- In EM algorithm, we need to repeatedly solve the following steps:
  - $\arg\max_q \mathcal{L}(q,\theta)$, for a given θ, and
  - $\arg\max_\theta \mathcal{L}(q,\theta)$, for a given q.
- We now give two re-expressions of ELBO $\mathcal{L}(q,\theta)$ that make these easy to compute...

ELBO in Terms of KL Divergence and Entropy

- Let's investigate the lower bound:

$$
\begin{aligned}
\mathcal{L}(q,\theta) &= \sum_z q(z)\log\left(\frac{p(x,z\mid\theta)}{q(z)}\right) \\
&= \sum_z q(z)\log\left(\frac{p(z\mid x,\theta)p(x\mid\theta)}{q(z)}\right) \\
&= \sum_z q(z)\log\left(\frac{p(z\mid x,\theta)}{q(z)}\right) + \sum_z q(z)\log p(x\mid\theta) \\
&= -\mathrm{KL}[q(z),p(z\mid x,\theta)] + \log p(x\mid\theta)
\end{aligned}
$$

- Amazing! We get back an equality for the marginal likelihood:

$$
\log p(x\mid\theta) = \mathcal{L}(q,\theta) + \mathrm{KL}[q(z),p(z\mid x,\theta)]
$$

Maximizing over q for fixed θ.

- Find q maximizing

$$\mathcal{L}(q,\theta) = -\mathrm{KL}[q(z), p(z \mid x,\theta)] + \underbrace{\log p(x \mid \theta)}_{\text{no } q \text{ here}}$$

- Recall $\mathrm{KL}(p\|q) \geqslant 0$, and $\mathrm{KL}(p\|p) = 0$.
- Best q is $q^*(z) = p(z \mid x,\theta)$ and

$$\mathcal{L}(q^*,\theta) = -\underbrace{\mathrm{KL}[p(z \mid x,\theta), p(z \mid x,\theta)]}_{=0} + \log p(x \mid \theta)$$

- Summary:

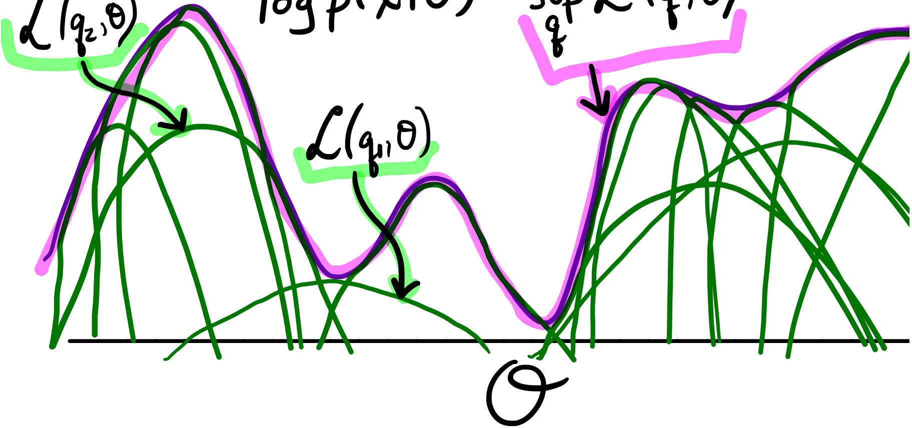
$$\log p(x \mid \theta) = \sup_q \mathcal{L}(q,\theta) \qquad \forall\theta$$

- For any θ, **sup is attained** at $q(z) = p(z \mid x,\theta)$.

Marginal Log-Likelihood **IS** the Supremum over Lower Bounds

sup is over all distributions on z

$$\log p(x|\theta) = \sup_q \mathcal{L}(q,\theta)$$



Maximum of ELBO is MLE

- Suppose we find a **maximum** of $\mathcal{L}(q,\theta)$ over **all distributions** q on z and all $\theta \in \Theta$:

$$\mathcal{L}(q^*,\theta^*) = \sup_\theta \sup_q \mathcal{L}(q,\theta).$$

(where of course $q^*(z) = p(z \mid x, \theta^*)$.)

- Claim: θ^* is a maximizes $\log p(x \mid \theta)$.
- Proof: Trivial, since $\log p(x \mid \theta) = \sup_q \mathcal{L}(q,\theta)$.

Summary: Maximizing over q for fixed $\theta = \theta^{\text{old}}$.

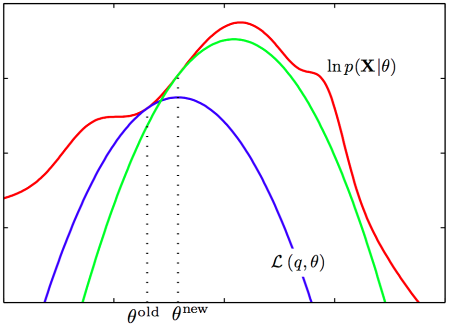
- At given $\theta = \theta^{\text{old}}$, want to find q giving best lower bound.
- Answer is $q^* = p(z \mid x, \theta^{\text{old}})$.
- This gives lower bound $\mathcal{L}(q^*, \theta)$ that is tight (equality) at θ^{old}

$$\log p(x \mid \theta^{\text{old}}) = \mathcal{L}(q^*, \theta^{\text{old}}) \quad (\text{tangent at } \theta^{\text{old}}).$$

- And elsewhere, of course, $\mathcal{L}(q^*, \theta)$ is just a lower bound:

$$\log p(x \mid \theta) \geqslant \mathcal{L}(q^*, \theta) \quad \forall \theta$$

Tight lower bound for any chosen θ



For θ^{old}, take $q(z) = p(z \mid x, \theta^{\text{old}})$. Then

1. $\log p(x \mid \theta^{\text{old}}) = \mathcal{L}(q, \theta^{\text{old}})$. [Lower bound is **tight** at $\theta^{\textbf{old}}$.]
2. $\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta)\ \forall \theta$. [Global lower bound].

From Bishop's *Pattern recognition and machine learning*, Figure 9.14.

Maximizing over θ for fixed q

- Consider maximizing the lower bound $\mathcal{L}(q,\theta)$:

$$\begin{aligned}\mathcal{L}(q,\theta) &= \sum_z q(z)\log\left(\frac{p(x,z\mid\theta)}{q(z)}\right)\\ &= \underbrace{\sum_z q(z)\log p(x,z\mid\theta)}_{\mathbb{E}[\text{complete data log-likelihood}]} - \underbrace{\sum_z q(z)\log q(z)}_{\text{no } \theta \text{ here}}\end{aligned}$$

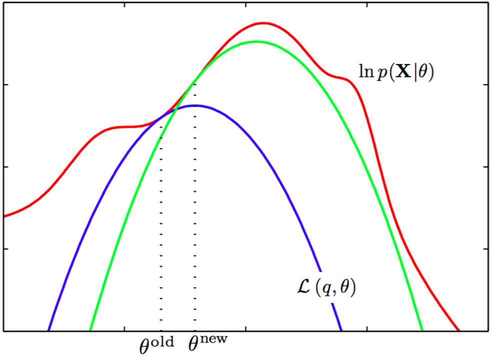
- Maximizing $\mathcal{L}(q,\theta)$ equivalent to maximizing $\mathbb{E}$[complete data log-likelihood] (for fixed q).

General EM Algorithm

1. Choose initial θ^{old}.
2. **Expectation Step**
   - Let $q^*(z) = p(z \mid x, \theta^{\text{old}})$. [$q^*$ gives best lower bound at θ^{old}]
   - Let
$$J(\theta) := \mathcal{L}(q^*, \theta) = \underbrace{\sum_z q^*(z) \log \left(\frac{p(x, z \mid \theta)}{q^*(z)} \right)}_{\textbf{expectation} \text{ w.r.t. } z \sim q^*(z)}$$
3. **Maximization Step**
$$\theta^{\text{new}} = \arg\max_\theta J(\theta).$$
   [Equivalent to maximizing expected complete log-likelihood.]
4. Go to step 2, until converged.

Does EM Work?

EM Gives Monotonically Increasing Likelihood: By Picture



From Bishop's *Pattern recognition and machine learning*, Figure 9.14.

EM Gives Monotonically Increasing Likelihood: By Math

1. Start at θ^{old}.
2. Choose $q^*(z) = \arg\max_q \mathcal{L}(q, \theta^{\text{old}})$. We've shown

$$\log p(x \mid \theta^{\text{old}}) = \mathcal{L}(q^*, \theta^{\text{old}})$$

3. Choose $\theta^{\text{new}} = \arg\max_\theta \mathcal{L}(q^*, \theta)$. So

$$\mathcal{L}(q^*, \theta^{\text{new}}) \geqslant \mathcal{L}(q^*, \theta^{\text{old}}).$$

Putting it together, we get

$$\begin{aligned}
\log p(x \mid \theta^{\text{new}}) &\geqslant \mathcal{L}(q^*, \theta^{\text{new}}) && \mathcal{L} \text{ is a lower bound} \\
&\geqslant \mathcal{L}(q^*, \theta^{\text{old}}) && \text{By definition of } \theta^{\text{new}} \\
&= \log p(x \mid \theta^{\text{old}}) && \text{Bound is tight at } \theta^{\text{old}}.
\end{aligned}$$

Convergence of EM

- Let θ_n be value of EM algorithm after n steps.
- Define "transition function" $M(\cdot)$ such that $\theta_{n+1} = M(\theta_n)$.
- Suppose log-likelihood function $\ell(\theta) = \log p(x \mid \theta)$ is differentiable.
- Let S be the set of stationary points of $\ell(\theta)$. (i.e. $\nabla_\theta \ell(\theta) = 0$)

Theorem

Under mild regularity conditions[a]*, for any starting point* θ_0*,*

- $\lim_{n\to\infty} \theta_n = \theta^*$ *for some stationary point* $\theta^* \in S$ *and*
- θ^* *is a fixed point of the EM algorithm, i.e.* $M(\theta^*) = \theta^*$*. Moreover,*
- $\ell(\theta_n)$ *strictly increases to* $\ell(\theta^*)$ *as* $n \to \infty$*, unless* $\theta_n \equiv \theta^*$*.*

[a] For details, see "Parameter Convergence for EM and MM Algorithms" by Florin Vaida in *Statistica Sinica* (2005). http://www3.stat.sinica.edu.tw/statistica/oldpdf/a15n316.pdf

Variations on EM

EM Gives Us Two New Problems

- The "E" Step: Computing

$$J(\theta) := \mathcal{L}(q^*, \theta) = \sum_z q^*(z) \log\left(\frac{p(x, z \mid \theta)}{q^*(z)}\right)$$

- The "M" Step: Computing

$$\theta^{\text{new}} = \arg\max_\theta J(\theta).$$

- Either of these can be too hard to do in practice.

Generalized EM (GEM)

- Addresses the problem of a difficult "M" step.
- Rather than finding
$$\theta^{\text{new}} = \underset{\theta}{\arg\max}\, J(\theta),$$
find **any** θ^{new} for which
$$J(\theta^{\text{new}}) > J(\theta^{\text{old}}).$$
- Can use a standard nonlinear optimization strategy
  - e.g. take a gradient step on J.
- We still get monotonically increasing likelihood.

EM and More General Variational Methods

- Suppose "E" step is difficult:
  - Hard to take expectation w.r.t. $q^*(z) = p(z \mid x, \theta^{\text{old}})$.
- Solution: Restrict to distributions $\mathcal{Q}$ that are easy to work with.
- Lower bound now looser:

$$q^* = \underset{q \in \mathcal{Q}}{\arg\min} \, \mathrm{KL}[q(z), p(z \mid x, \theta^{\text{old}})]$$

EM in Bayesian Setting

- Suppose we have a prior $p(\theta)$.
- Want to find MAP estimate: $\hat{\theta}_{\text{MAP}} = \arg\max_\theta p(\theta \mid x)$:

$$
\begin{aligned}
p(\theta \mid x) &= p(x \mid \theta)p(\theta)/p(x) \\
\log p(\theta \mid x) &= \log p(x \mid \theta) + \log p(\theta) - \log p(x)
\end{aligned}
$$

.

- Still can use our lower bound on $\log p(x, \theta)$.

$$
J(\theta) := \mathcal{L}(q^*, \theta) = \sum_z q^*(z) \log\left(\frac{p(x, z \mid \theta)}{q^*(z)}\right)
$$

- Maximization step becomes

$$
\theta^{\text{new}} = \arg\max_\theta \left[J(\theta) + \log p(\theta)\right]
$$

- Homework: Convince yourself our lower bound is still tight at θ.

Summer Homework: Gaussian Mixture Model (Hints)

Homework: Derive EM for GMM from General EM Algorithm

- Subsequent slides may help set things up.
- Key skills:
  - MLE for multivariate Gaussian distributions.
  - Lagrange multipliers

Gaussian Mixture Model (k Components)

- GMM Parameters

$$\begin{aligned} \text{Cluster probabilities :} \quad & \pi = (\pi_1, \ldots, \pi_k) \\ \text{Cluster means :} \quad & \mu = (\mu_1, \ldots, \mu_k) \\ \text{Cluster covariance matrices:} \quad & \Sigma = (\Sigma_1, \ldots \Sigma_k) \end{aligned}$$

- Let $\theta = (\pi, \mu, \Sigma)$.
- Marginal log-likelihood

$$\log p(x \mid \theta) = \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}(x \mid \mu_z, \Sigma_z) \right\}$$

$q^*(z)$ are "Soft Assignments"

- Suppose we observe n points: $X = (x_1, \ldots, x_n) \in \mathbf{R}^{n \times d}$.
- Let $z_1, \ldots, z_n \in \{1, \ldots, k\}$ be corresponding hidden variables.
- Optimal distribution q^* is:

$$q^*(z) \quad = \quad p(z \mid x, \theta).$$

- Convenient to define the conditional distribution for z_i given x_i as

$$\begin{aligned} \gamma_i^j &:= p(z = j \mid x_i) \\ &= \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_{c=1}^k \pi_c \mathcal{N}(x_i \mid \mu_c, \Sigma_c)} \end{aligned}$$

Expectation Step

- The complete log-likelihood is

$$\begin{aligned}\log p(x,z \mid \theta) &= \sum_{i=1}^{n} \log\left[\pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z)\right] \\ &= \sum_{i=1}^{n}\left(\log \pi_z + \underbrace{\log \mathcal{N}(x_i \mid \mu_z, \Sigma_z)}_{\text{simplifies nicely}}\right)\end{aligned}$$

- Take the expected complete log-likelihood w.r.t. q^*:

$$\begin{aligned}J(\theta) &= \sum_{z} q^*(z) \log p(x,z \mid \theta) \\ &= \sum_{i=1}^{n}\sum_{j=1}^{k} \gamma_i^j \left[\log \pi_j + \log \mathcal{N}(x_i \mid \mu_j, \Sigma_j)\right]\end{aligned}$$

Maximization Step

- Find θ^* maximizing $J(\theta)$:

$$
\begin{aligned}
\mu_c^{\text{new}} &= \frac{1}{n_c}\sum_{i=1}^{n}\gamma_i^c x_i \\
\Sigma_c^{\text{new}} &= \frac{1}{n_c}\sum_{i=1}^{n}\gamma_i^c \left(x_i-\mu_{\text{MLE}}\right)\left(x_i-\mu_{\text{MLE}}\right)^T \\
\pi_c^{\text{new}} &= \frac{n_c}{n},
\end{aligned}
$$

for each $c = 1,\ldots,k$.