

Statistical Models & Computing Methods

Lecture 10: Expectation Maximization



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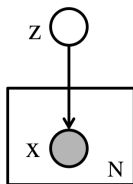
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- ▶ In this lecture, we discuss Expectation-Maximization (EM), which is an iterative optimization method dealing with missing or latent data.
- ▶ In such cases, we may assume the observed data x are generated from random variable X along with missing or unobserved data z from random variable Z . We envision complete data would have been $y = (x, z)$.
- ▶ Very often, the inclusion of the observed data z is a *data augmentation* strategy to ease computation. In this case, Z is often referred to as *latent* variable.

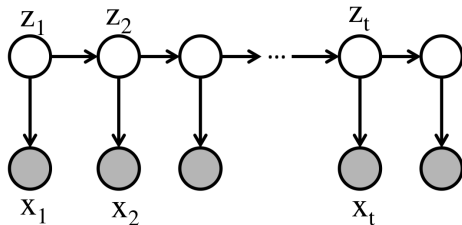


- ▶ Some of the variables in the model are not observed.
- ▶ Examples: mixture model, hidden Markov model (HMM), latent Dirichlet allocation (LDA), etc.
- ▶ We consider the learning problem of latent variable models

Mixture Model



Hidden Markov Model



- ▶ complete data likelihood $p(x, z|\theta)$, θ is model parameter
- ▶ When z is missing, we need to marginalize out z and use the marginal log-likelihood for learning

$$\log p(x|\theta) = \log \sum_z p(x, z|\theta)$$

- ▶ Examples: Gaussian mixture model. $z \sim \text{Discrete}(\pi)$,
 $\theta = (\pi, \mu, \Sigma)$

$$\begin{aligned} p(x|\theta) &= \sum_k p(z = k|\theta)p(x|z = k, \theta) \\ &= \sum_k \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \\ &= \sum_k \pi_k \frac{1}{(2\pi)^{d/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)\right) \end{aligned}$$



- ▶ For most of these latent variable models, when the missing components z are observed, the complete data likelihood often factorizes, and the maximum likelihood estimates hence have closed-form solutions.
- ▶ When z are not observed, marginalization destroys the factorizable structure and makes learning much more difficult.
- ▶ How to learn in this scenario?
 - ▶ **Idea 1:** simply take derivative and use gradient ascent directly
 - ▶ **Idea 2:** find appropriate estimates of z (e.g., using the current conditional distribution $p(z|x, \theta)$), fill them in and do complete data learning – This is **EM!**

- ▶ At each iteration, the EM algorithm involves two steps
 - ▶ based on the current $\theta^{(t)}$, fill in unobserved z to get *complete data* (x, z')
 - ▶ Update θ to maximize the complete data log-likelihood $\ell(x, z'|\theta) = \log p(x, z'|\theta)$
- ▶ How to choose z' ?
 - ▶ Use conditional distribution $p(z|x, \theta^{(t)})$
 - ▶ Take full advantage of the current estimates $\theta^{(t)}$

$$\mathbb{E}_{p(z|x, \theta^{(t)})} \ell(x, z|\theta) = \sum_z p(z|x, \theta^{(t)}) \ell(x, z|\theta)$$

In some sense, this is our best guess (as shown later).

More specifically, we start from some initial $\theta^{(0)}$. In each iteration, we follow the two steps below

- ▶ **Expectation (E-step)**: compute $p(z|x, \theta^{(t)})$ and form the expectation using the current estimate $\theta^{(t)}$

$$Q^{(t)}(\theta) = \mathbb{E}_{p(z|x, \theta^{(t)})} \ell(x, z|\theta)$$

- ▶ **Maximization (M-step)**: Find θ that maximizes the expected complete data log-likelihood

$$\theta^{(t+1)} = \arg \max_{\theta} Q^{(t)}(\theta)$$

In many cases, the expectation is easier to handle than the marginal log-likelihood.



- ▶ EM algorithm can be viewed as optimizing a lower bound on the marginal log-likelihood $\mathcal{L}(\theta) = \log p(x|\theta)$
- ▶ A class of lower bounds

$$\begin{aligned}\mathcal{L}(\theta) &= \log \sum_z p(x, z|\theta) = \log \sum_z q(z) \frac{p(x, z|\theta)}{q(z)} \\ &\geq \sum_z q(z) \log \frac{p(x, z|\theta)}{q(z)} \quad - \text{Jensen's inequality} \\ &= \sum_z q(z) \log p(x, z|\theta) - \sum_z q(z) \log q(z), \quad \forall q(z)\end{aligned}$$

- ▶ The term in the last equation is often called *Free-energy*

$$\mathcal{F}(q, \theta) = \sum_z q(z) \log p(x, z|\theta) - \sum_z q(z) \log q(z)$$



- ▶ Free-energy is a lower bound of the true log-likelihood

$$\mathcal{L}(\theta) \geq \mathcal{F}(q, \theta)$$

- ▶ EM is simply doing **coordinate ascent** on $\mathcal{F}(q, \theta)$
 - ▶ E-step: Find $q^{(t)}$ that maximizes $\mathcal{F}(q, \theta^{(t)})$
 - ▶ M-step: Find $\theta^{(t+1)}$ that maximizes $\mathcal{F}(q^{(t)}, \theta)$
- ▶ Properties:
 - ▶ Each iteration improves \mathcal{F}

$$\mathcal{F}(q^{(t+1)}, \theta^{(t+1)}) \geq \mathcal{F}(q^{(t)}, \theta^{(t)})$$

- ▶ Each iteration improves \mathcal{L} as well

$$\mathcal{L}(\theta^{(t+1)}) \geq \mathcal{L}(\theta^{(t)})$$

will show later



- Find q that maximizes $\mathcal{F}(q, \theta^{(t)})$

$$\begin{aligned}\mathcal{F}(q, \theta) &= \sum_z q(z) \log p(x, z|\theta) - \sum_z q(z) \log q(z) \\ &= \sum_z q(z) \log \frac{p(z|x, \theta)p(x|\theta)}{q(z)} \\ &= \sum_z q(z) \log \frac{p(z|x, \theta)}{q(z)} + \log p(x|\theta) \\ &= \mathcal{L}(\theta) - D_{\text{KL}}(q(z) \| p(z|x, \theta)) \\ &\leq \mathcal{L}(\theta)\end{aligned}$$



$$\mathcal{F}(q, \theta^{(t)}) = \mathcal{L}(\theta^{(t)}) - D_{\text{KL}}(q(z) \| p(z|x, \theta^{(t)}))$$

- ▶ KL divergence is non-negative and is minimized (equals to 0) iff the two distributions are identical.
- ▶ Therefore, $\mathcal{F}(q, \theta^{(t)})$ is maximized at $q^{(t)}(z) = p(z|x, \theta^{(t)})$.
- ▶ So when we are computing $p(z|x, \theta^{(t)})$, we are actually computing $\arg \max_q \mathcal{F}(q, \theta^{(t)})$
- ▶ Moreover,

$$\mathcal{F}(q^{(t)}, \theta^{(t)}) = \mathcal{L}(\theta^{(t)})$$

this means **the lower bound matches the true log-likelihood at $\theta^{(t)}$** , which is crucial for the improvement on \mathcal{L} .

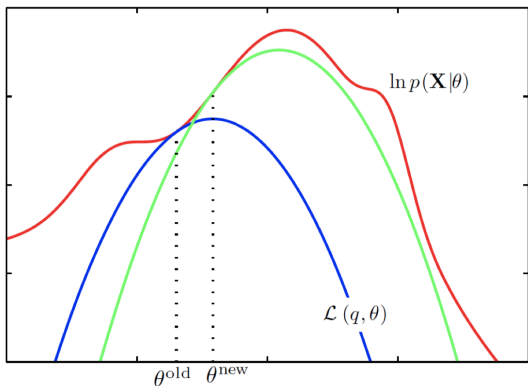


- Find $\theta^{(t+1)}$ that maximizes $\mathcal{F}(q^{(t)}, \theta)$

$$\begin{aligned}\theta^{(t+1)} &= \arg \max_{\theta} \mathcal{F}(q^{(t)}, \theta) \\ &= \arg \max_{\theta} \sum_z p(z|x, \theta^{(t)}) \log p(x, z|\theta) + H(p(z|x, \theta^{(t)})) \\ &= \arg \max_{\theta} \mathbb{E}_{p(z|x, \theta^{(t)})} \ell(x, z|\theta)\end{aligned}$$

- The expected complete data log-likelihood usually can be solved in the same manner (closed-form solutions) as the fully-observed model.

$$\begin{aligned}\mathcal{L}(\theta^{(t+1)}) &\geq \mathcal{F}(q^{(t)}, \theta^{(t+1)}) \\ &\geq \mathcal{F}(q^{(t)}, \theta^{(t)}) = \mathcal{L}(\theta^{(t)})\end{aligned}$$



- ▶ When the complete data follow an exponential family distribution (in canonical form), the density is

$$p(x, z|\theta) = h(x, z) \exp(\theta \cdot T(x, z) - A(\theta))$$

- ▶ E-step

$$\begin{aligned} Q^{(t)}(\theta) &= \mathbb{E}_{p(z|x, \theta^{(t)})} \log p(x, z|\theta) \\ &= \theta \cdot \mathbb{E}_{p(z|x, \theta^{(t)})} T(x, z) - A(\theta) + \text{Const} \end{aligned}$$

- ▶ M-step

$$\nabla_{\theta} Q^{(t)}(\theta) = 0 \Rightarrow \mathbb{E}_{p(z|x, \theta^{(t)})} T(x, z) = \nabla_{\theta} A(\theta) = \mathbb{E}_{p(x, z|\theta)} T(x, z)$$

- ▶ In survival analyses, we often have to terminate our study before observing the real survival times, leading to censored survival data.
- ▶ Suppose the observed data are $Y = \{(t_1, \delta_1), \dots, (t_n, \delta_n)\}$, where $T_j \sim \text{Exp}(\mu)$ and δ_j is the indicator of a censored sample. WLOG, assume $\delta_i = 0, i \leq r, \quad \delta_i = 1, i > r$
- ▶ The log-likelihood function is

$$\begin{aligned}\log p(Y|\mu) &= \sum_{i=1}^r \log p(t_i|\mu) + \sum_{i>r} \log p(T_i > t_i|\mu) \\ &= -r \log \mu - \sum_{i=1}^n t_i/\mu\end{aligned}$$

- ▶ The MLE of μ : $\hat{\mu} = \sum_{i=1}^n t_i/r$



- ▶ Let us see how EM works in this simple case.
- ▶ Let $t = (T_1, \dots, T_n) = (T_1, \dots, T_r, z)$ be the complete data vector, where $z = (T_{r+1}, \dots, T_n)$ are the unobserved $n - r$ censored random variables.
- ▶ Natural parameter $1/\mu$, sufficient statistics $\sum_{i=1}^n T_i$, and $\mathbb{E}_\mu \sum_{i=1}^n T_i = n\mu$
- ▶ By the lack of memory, $T_i | T_i > t_i \sim t_i + \text{Exp}(\mu)$, $\forall i > r$.

$$\mathbb{E}_{p(z|Y, \mu^{(k)})} \sum_{i=1}^n T_i = \sum_{i=1}^r t_i + \sum_{i>r} t_i + (n-r)\mu^{(k)}$$

- ▶ Update formula

$$\mu^{(k+1)} = \frac{\sum_{i=1}^n t_i + (n-r)\mu^{(k)}}{n}$$



- ▶ Consider clustering of data $X = \{x_1, \dots, x_N\}$ using a finite mixture of Gaussians.

$$z \sim \text{Discrete}(\pi), \quad x|z = k \sim \mathcal{N}(\mu_k, \Sigma_k)$$

$\theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ are model parameters

- ▶ Complete data log-likelihood

$$\begin{aligned} \log p(x, z|\theta) &= \log \prod_{k=1}^K (p(z = k)p(x|z = k))^{1_{z=k}} \\ &= \sum_{k=1}^K 1_{z=k} (\log \pi_k + \log \mathcal{N}(x|\mu_k, \Sigma_k)) \end{aligned}$$



- ▶ Compute the conditional probability $p(z_n|x_n, \theta^{(t)})$ via Bayes' theorem

$$p(z_n|x_n, \theta) = \frac{p(z_n, x_n|\theta)}{\sum_{z_n} p(z_n, x_n|\theta)}$$

$$p(z_n = k|x_n, \theta^{(t)}) = \frac{\pi_k^{(t)} \mathcal{N}(x_n|\mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_k \pi_k^{(t)} \mathcal{N}(x_n|\mu_k^{(t)}, \Sigma_k^{(t)})}$$

- ▶ Denote $\gamma_{n,k}^{(t)} \triangleq p(z_n = k|x_n, \theta^{(t)})$, which can be viewed as a *soft clustering* of x_n

$$\sum_k \gamma_{n,k}^{(t)} = 1$$



- ▶ Expected complete-data log-likelihood

$$\begin{aligned} Q^{(t)}(\theta) &= \sum_n \sum_{z_n} p(z_n | x_n, \theta^{(t)}) \log p(x_n, z_n | \theta) \\ &= \sum_n \sum_k \gamma_{n,k}^{(t)} (\log \pi_k + \log \mathcal{N}(x_n | \mu_k, \Sigma_k)) \\ &= \sum_k \sum_n \gamma_{n,k}^{(t)} (\log \pi_k + \log \mathcal{N}(x_n | \mu_k, \Sigma_k)) \end{aligned}$$

Substitute $\mathcal{N}(x_n | \mu_k, \Sigma_k)$ in

$$\begin{aligned} Q^{(t)}(\theta) &= \sum_k \sum_n \gamma_{n,k}^{(t)} \left(\log \pi_k - \frac{d}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma_k| \right. \\ &\quad \left. - \frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right) \end{aligned}$$



- ▶ Maximize $Q^{(t)}(\theta)$ with respect to π using Lagrange multipliers

$$\pi_k^{(t+1)} \propto \sum_n \gamma_{n,k}^{(t)}$$

Therefore

$$\pi_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)}}{\sum_k \sum_n \gamma_{n,k}^{(t)}} = \frac{\sum_n \gamma_{n,k}^{(t)}}{\sum_n \sum_k \gamma_{n,k}^{(t)}} = \frac{\sum_n \gamma_{n,k}^{(t)}}{N}$$

- ▶ Note that $\sum_n \gamma_{n,k}^{(t)}$ can be viewed as the weighted number of data points in mixture component k , and $\pi_k^{(t+1)}$ is the fraction of data that belongs to mixture component k .



- ▶ Compute the derivative w.r.t μ_k

$$\frac{\partial Q^{(t)}(\theta)}{\partial \mu_k} = \sum_n \gamma_{n,k}^{(t)} \Sigma_k^{-1} (x_n - \mu_k) = \Sigma_k^{-1} \sum_n \gamma_{n,k}^{(t)} (x_n - \mu_k)$$

- ▶ Therefore,

$$\mu_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)} x_n}{\sum_n \gamma_{n,k}^{(t)}}$$

$\mu_k^{(t+1)}$ is the weighted mean of data points assigned to mixture component k

- ▶ Similarly, we can get

$$\Sigma_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \gamma_{n,k}^{(t)}}$$



- ▶ **E-step:** Compute the soft clustering probabilities

$$\gamma_{n,k}^{(t)} = \frac{\pi_k^{(t)} \mathcal{N}(x_n | \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_k \pi_k^{(t)} \mathcal{N}(x_n | \mu_k^{(t)}, \Sigma_k^{(t)})}$$

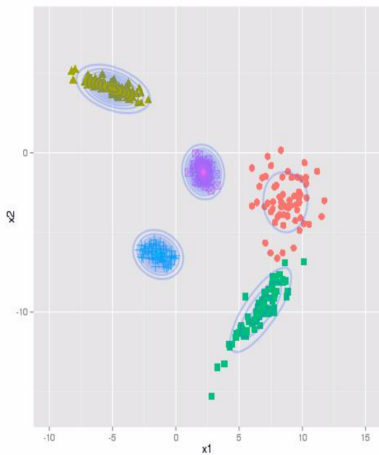
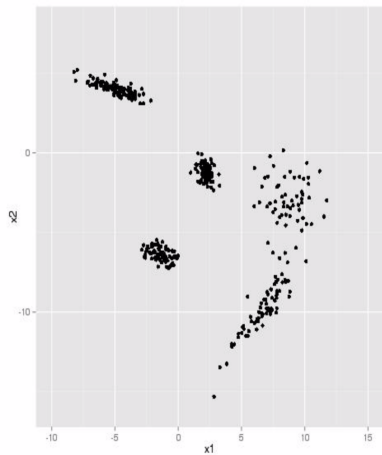
- ▶ **M-step:** Update parameters

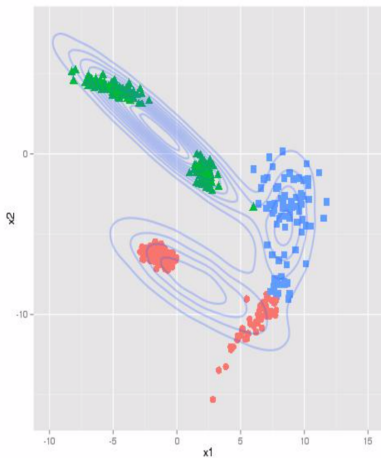
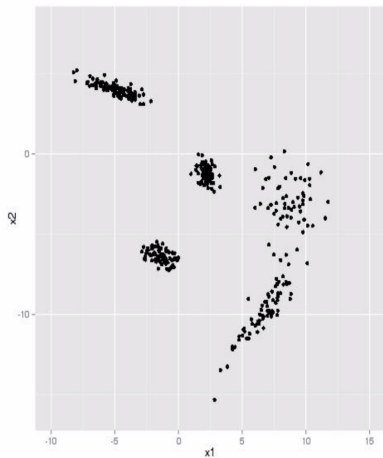
$$\pi_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)}}{N}$$

$$\mu_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)} x_n}{\sum_n \gamma_{n,k}^{(t)}}$$

$$\Sigma_k^{(t+1)} = \frac{\sum_n \gamma_{n,k}^{(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \gamma_{n,k}^{(t)}}$$







- ▶ The k -means algorithm follows two steps
 - ▶ Assignment step: assign data to the nearest cluster

$$\gamma_{n,k} = \begin{cases} 1, & k = \arg \min_{k'} \|x_n - \mu_{k'}\| \\ 0, & \text{otherwise} \end{cases}$$

- ▶ Update step: set μ_k to the mean of data points assigned to the k -th cluster

$$\mu_k = \frac{\sum_n \gamma_{n,k}^{(t)} x_n}{\sum_n \gamma_{n,k}^{(t)}} = \frac{1}{N_k} \sum_{n:\gamma_{n,k}=1} x_n$$

N_k is the number of data points assigned to the k -th cluster.

- ▶ Therefore, k -means can be viewed as a special case of EM for Gaussian mixture models where $\Sigma_k = I$ and $\gamma_{n,k}$ are hard assignments instead of soft clustering probabilities.

- ▶ Sequence data x_1, x_2, \dots, x_T , each $x_n \in \mathbb{R}^d$
- ▶ Hidden variables z_1, z_2, \dots, z_T , each $z_t \in \{1, 2, \dots, K\}$
- ▶ Joint probability

$$p(x, z) = p(z_1) \prod_{t=1}^{T-1} p(z_{t+1}|z_t) \prod_{t=1}^T p(x_t|z_t)$$

- ▶ $p(x_t|z_t)$ is the *emission probability*, could be a Gaussian

$$p(x_t|z_t = k) = \mathcal{N}(x_t|\mu_k, \Sigma_k)$$

- ▶ $p(z_{t+1}|z_t)$ is the *transition probability*, a $K \times K$ matrix
 $a_{ij} = p(z_{t+1} = j|z_t = i)$, $\sum_j a_{ij} = 1$
- ▶ $p(z_1) \sim \text{Discrete}(\pi)$ is the prior for the first hidden state



- ▶ The expected complete data log-likelihood is

$$\begin{aligned} Q &= \mathbb{E}_{p(z|x)} \log p(x, z) \\ &= \sum_z p(z|x) \left(\log p(z_1) + \sum_{t=1}^{T-1} \log p(z_{t+1}|z_t) + \sum_{t=1}^T \log p(x_t|z_t) \right) \\ &= \sum_{z_1} p(z_1|x) \log p(z_1) + \sum_{t=1}^{T-1} \sum_{z_t, z_{t+1}} p(z_t, z_{t+1}|x) \log p(z_{t+1}|z_t) \\ &\quad + \sum_{t=1}^T \sum_{z_t} p(z_t|x) \log p(x_t|z_t) \end{aligned}$$

- ▶ Therefore, in the E-step, we need to compute unary and pairwise marginal probabilities $p(z_t|x)$ and $p(z_t, z_{t+1}|x)$.



- ▶ Using the sequential structure of HMM, we can compute these marginal probabilities via **dynamic programming**.
- ▶ The **forward algorithm**

$$\begin{aligned}\alpha_{t+1}(j) &= p(z_{t+1} = j, x_1, \dots, x_{t+1}) \\ &= \sum_i p(z_{t+1} = j, z_t = i, x_1, \dots, x_{t+1}) \\ &= p(x_{t+1} | z_{t+1} = j) \sum_i p(z_{t+1} = j | z_t = i) p(z_t, x_1, \dots, x_t) \\ &= p(x_{t+1} | z_{t+1} = j) \sum_i a_{ij} p(z_t, x_1, \dots, x_t) \\ &= p(x_{t+1} | z_{t+1} = j) \sum_i a_{ij} \alpha_t(i)\end{aligned}$$



► The **backward algorithm**

$$\begin{aligned}\beta_t(i) &= p(x_{t+1}, \dots, x_T | z_t = i) \\ &= \sum_j p(x_{t+1}, \dots, x_T, z_{t+1} = j | z_t = i) \\ &= \sum_j a_{ij} p(x_{t+1} | z_{t+1} = j) \beta_{t+1}(j)\end{aligned}$$

► Unary marginal probability

$$p(z_t = j | x) \propto p(z_t = j, x) = \alpha_t(j) \beta_t(j)$$

► Pairwise marginal probability

$$\begin{aligned}p(z_{t+1} = j, z_t = i | x) &\propto p(z_{t+1} = j, z_t = i, x) \\ &= \alpha_t(i) a_{ij} p(x_{t+1} | z_{t+1} = j) \beta_{t+1}(j)\end{aligned}$$



- ▶ From the E-step, we have

$$\gamma_{t,k} = p(z_t = k|x) = \frac{\alpha_t(k)\beta_t(k)}{\sum_k \alpha_t(k)\beta_t(k)}$$
$$\xi_t(i, j) = p(z_{t+1} = j, z_t = i|x) = \frac{\alpha_t(i)a_{ij}p(x_{t+1}|z_{t+1} = j)\beta_{t+1}(j)}{\sum_k \alpha_t(k)\beta_t(k)}$$

- ▶ The expected complete data log-likelihood is

$$Q = \sum_k \gamma_{1,k} \log \pi_k + \sum_{t=1}^{T-1} \sum_{i,j} \xi_t(i, j) \log a_{ij}$$
$$+ \sum_{t=1}^T \sum_k \gamma_{t,k} \log \mathcal{N}(x_t | \mu_k, \Sigma_k)$$

- ▶ Closed form solution for M-step – just like in the Gaussian mixture model

EM algorithm finds MLE for models with missing/latent variables. Applicable if the following pieces are easy to solve

- ▶ Estimating missing data from observed data using current parameters (E-step)
- ▶ Find complete data MLE (M-step)

Pros

- ▶ No need for gradients, learning rates, etc.
- ▶ Fast convergence
- ▶ Monotonicity. Guaranteed to improve \mathcal{L} at every iteration

Cons

- ▶ Can get stuck at local optimal
- ▶ Requires conditional distribution $p(z|x, \theta)$ to be tractable

- ▶ A. P. Dempster, N. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society, Series B*, 39:1–38, 1977.
- ▶ R. M. Neal and G. E. Hinton. A view of the em algorithm that justifies incremental, sparse, and other variants. *Learning in Graphical Models*, 89:355–368, 1998.
- ▶ Baum, L. E. (1972). An inequality and associated maximization technique in statistical estimation for probabilistic functions of Markov processes. In Shisha, O. (Ed.), *Inequalities III: Proceedings of the 3rd Symposium on Inequalities*, 1–8. Academic Press.