UVA CS 6316 – Fall 2015 Graduate: Machine Learning

Lecture 23: EM

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Course Project

- Final project presentation
  - 10 mins per team
  - On Dec 3 and Dec 4
  - Template has been shared in Collab
- Final Report
  - Minimum 9 pages (excluding references)
  - Due at midnight Dec 15^{th}

Where are we ? ➔ major sections of this course

- ❑ Regression (supervised)
- ❑ Classification (supervised)
  - ❑ Feature selection
- ❑ Unsupervised models
  - ❑ Dimension Reduction (PCA)
  - ❑ Clustering (K-means, GMM/EM, Hierarchical)
- ❑ Learning theory
- ❑ Graphical models
  - ❑ (BN and HMM slides shared)

Today Outline

- Principles for Model Inference
  - Maximum Likelihood Estimation
  - ~~Bayesian Estimation~~
- Strategies for Model Inference
  - EM Algorithm – simplify difficult MLE
  - ~~MCMC – samples rather than maximizing~~

Model Inference through Maximum Likelihood Estimation (MLE)

Assumption: the data is coming from a known probability distribution

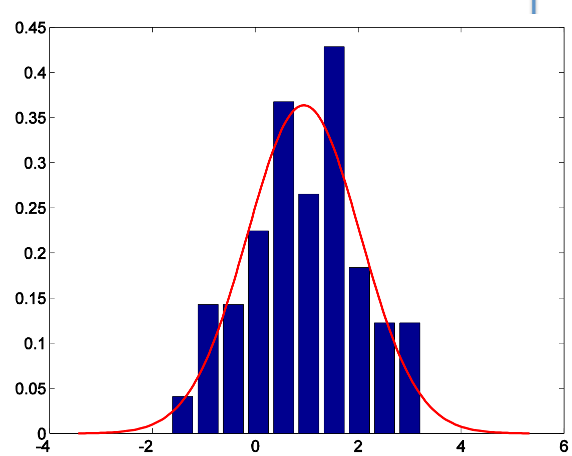
The probability distribution has some parameters that are unknown to you

Example: data is distributed as Gaussian $y_i = N(\mu, \sigma^2)$,
so the unknown parameters here are $\theta = (\mu, \sigma^2)$

MLE is a tool that estimates the unknown parameters of the probability distribution from data

MLE: e.g. Single Gaussian Model (when p=1)

- Need to adjust the parameters (➔ model inference)
- So that the resulting distribution fits the observed data well



Maximum Likelihood revisited

$$y_i = N(\mu, \sigma^2)$$

$$Y = \{y_1, y_2, \ldots, y_N\}$$

$$l(\theta) = \log(L(\theta;Y)) = \log \prod_{i=1}^{N} p(y_i)$$

Choose θ that maximizes $l(\theta)$ . . .

$$\frac{\partial l}{\partial \theta} = 0$$

MLE: e.g. Single Gaussian Model

- Assume observation data y_i are independent
- Form the Likelihood:

$$L(\theta;Y) = \prod_{i=1}^{N} p(y_i) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(y_i-\mu)^2}{2\sigma^2});$$

$$Y = \{y_1, y_2, \ldots, y_N\}$$

- Form the Log-likelihood:

$$l(\theta) = \log(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{(y_i-\mu)^2}{2\sigma^2})) = -\sum_{i=1}^{N} \frac{(y_i-\mu)^2}{2\sigma^2} - N\log(\sqrt{2\pi}\sigma)$$

MLE: e.g. Single Gaussian Model

- To find out the unknown parameter values, maximize the log-likelihood with respect to the unknown parameters:

Choose θ that maximizes $l(\theta)$ . . .

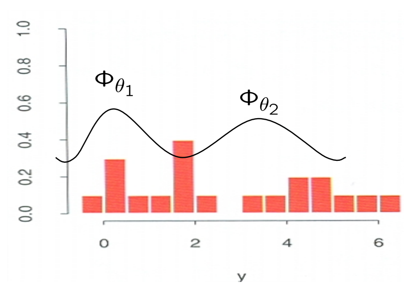
$$\frac{\partial l}{\partial \theta} = 0$$

$$\frac{\partial l}{\partial \mu} = 0 \Rightarrow \mu = \frac{\sum_{i=1}^{N} y_i}{N}; \quad \frac{\partial l}{\partial \sigma^2} = 0 \Rightarrow \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(y_i - \mu)^2$$

MLE: A Challenging Mixture Example

$$Y_1 \sim N(\mu_1, \sigma_1^2); \quad Y_2 \sim N(\mu_2, \sigma_2^2)$$
$$Y = (1-\Delta)Y_1 + \Delta Y_2; \quad \Delta \in \{0,1\}$$

Indicator variable



histogram

marginal prob $\Rightarrow p(y \mid \underbrace{\mu_1, \sigma_1, \mu_2, \sigma_2, \pi}_{\theta})$

Mixture model: $g_Y(y) = (1-\pi)\Phi_{\theta_1}(y) + \pi\Phi_{\theta_2}(y)$ $\quad (\pi = Pr(\Delta = 1))$

$$\theta_1 = (\mu_1, \sigma_1); \quad \theta_2 = (\mu_2, \sigma_2)$$

π *is the probability with which the observation is chosen from density model 2*

$(1-\pi)$ is the probability with which the observation is chosen from density 1

MLE: Gaussian Mixture Example

$p(y|\theta)$

$$g_Y(y) = (1-\pi)\Phi_{\theta_1}(y) + \pi\Phi_{\theta_2(y)} \qquad (\pi = Pr(\Delta=1))$$

$\{y_1, y_2, \cdots, y_n\}$

Maximum likelihood fitting for parameters: $\theta = (\pi, \mu_1, \mu_2, \sigma_1, \sigma_2)$

$$l(\theta) = \sum_{i=1}^{N} log[(1-\pi)\Phi_{\theta_1}(y_i) + \pi\Phi_{\theta_2(y_i)}]$$

$$\frac{\partial l}{\partial \theta} = 0$$

Numerically (and of course analytically, too) Challenging to solve!!

Bayesian Methods & Maximum Likelihood

- Bayesian
  Pr(model|data) i.e. posterior
  =>Pr(data|model) Pr(model)
  => Likelihood * prior

  θ as random variable

- Assume prior is uniform, equal to MLE
  argmax$_{_model}$ Pr(data | model) Pr(model)
  = argmax$_{_model}$ Pr(data | model)

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  - ~~Bayesian Estimation~~

- Strategies for Model Inference
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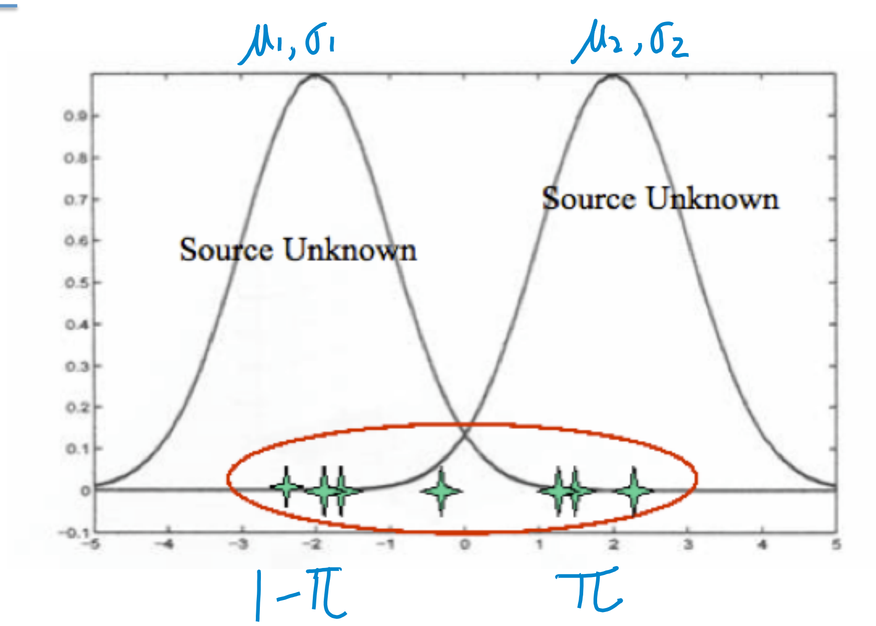
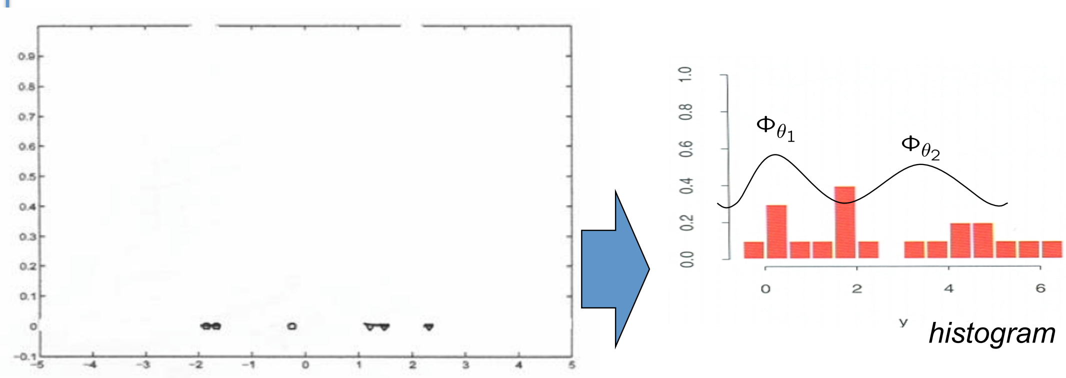
    - Algorithm
    - Application
    - Theory
  - ~~MCMC – samples rather than maximizing~~

Here is the problem



All we have is



From which we need to infer the likelihood function which generate the observations

Expectation Maximization: add latent variable Δ → latent data Δ_i

EM augments the data space– assumes with latent data

$\Delta_i \in 0, 1$ (latent data)

if($\Delta_i = 0$)

y_i was generated from first component

if($\Delta_i = 1$)

y_i was generated from second component

$\{y_1, y_2, \cdots, y_n\}$

$\{\Delta_1, \Delta_2, \cdots, \Delta_n\}$

Complete data: $t_i = (y_i, \Delta_i)$

$$p(t_i|\theta) = p(y_i, \Delta_i|\theta) = p(y_i|\Delta_i, \theta)Pr(\Delta_i)$$

$$p(t_i|\theta) = [\Phi_{\theta_1}(y_i)(1-\pi)]^{(1-\Delta_i)}[\Phi_{\theta_2}(y_i)\pi]^{\Delta_i}$$

Computing log-likelihood based on complete data

$$p(t_i|\theta) = [\Phi_{\theta_1}(y_i)(1-\pi)]^{(1-\Delta_i)}[\pi\Phi_{\theta_2}(y_i)\pi]^{\Delta_i}$$

$l_0(\theta; \mathbf{T})$ $\quad T = \{t_i = (y_i, \Delta_i), i = 1...N\}$

$$= \sum_{i=1}^{N}(1-\Delta_i)log[(1-\pi)\Phi_{\theta_1}(y_i)] + \Delta_i log[\pi\Phi_{\theta_2}(y_i)]$$

$$= \sum_{i=1}^{N}(1-\Delta_i)log\Phi_{\theta_1}(y_i) + \Delta_i log\Phi_{\theta_2}(y_i)]$$
$$+ \sum_{i=1}^{N}[(1-\Delta_i)log(1-\pi) + \Delta_i log\pi \quad (8.40)$$

only about π

Maximizing this form of log-likelihood is now tractable

Note that we cannot analytically maximize the previous log-likelihood with only observed Y={y_1, y_2, …, y_n}

EM: The Complete Data Likelihood

By simple differentiations we have:

$$\frac{\partial l_0}{\partial \mu_1} = 0 \Rightarrow \mu_1 = \frac{\sum_{i=1}^{N}(1-\Delta_i)y_i}{\sum_{i=1}^{N}(1-\Delta_i)};$$

$$\frac{\partial l_0}{\partial \sigma_1^2} = 0 \Rightarrow \sigma_1^2 = \frac{\sum_{i=1}^{N}(1-\Delta_i)(y_i-\mu_1)^2}{\sum_{i=1}^{N}(1-\Delta_i)};$$

So, maximization of the complete data likelihood is much easier!

How do we get the latent variables?

EM: The Complete Data Likelihood

By simple differentiations we have:

$$\frac{\partial l_0}{\partial \mu_2} = 0 \Rightarrow \mu_2 = \frac{\sum_{i=1}^{N} \Delta_i y_i}{\sum_{i=1}^{N} \Delta_i};$$

$$\frac{\partial l_0}{\partial \sigma_2^2} = 0 \Rightarrow \sigma_2^2 = \frac{\sum_{i=1}^{N} \Delta_i (y_i - \mu_2)^2}{\sum_{i=1}^{N} \Delta_i};$$

So, maximization of the complete data likelihood is much easier!

$$\frac{\partial l_0}{\partial \pi} = 0 \Rightarrow \pi = \frac{\sum_{i=1}^{N} \Delta_i}{N};$$

How do we get the latent variables?

Obtaining Latent Variables

The latent variables are computed as expected values given the data and parameters:

$$\Delta_i \rightarrow \quad \gamma_i(\theta) = E(\Delta_i \mid \theta, y_i) = \Pr(\Delta_i = 1 \mid \theta, y_i)$$

Apply Bayes' rule:

$$\gamma_i(\theta) = \Pr(\Delta_i = 1 \mid \theta, y_i) = \frac{\Pr(y_i \mid \Delta_i = 1, \theta)\Pr(\Delta_i = 1 \mid \theta)}{\Pr(y_i \mid \Delta_i = 1, \theta)\Pr(\Delta_i = 1 \mid \theta) + \Pr(y_i \mid \Delta_i = 0, \theta)\Pr(\Delta_i = 0 \mid \theta)}$$

$$= \frac{\Phi_{\theta_2}(y_i)\pi}{\Phi_{\theta_1}(y_i)(1-\pi) + \Phi_{\theta_2}(y_i)\pi}$$

$$(y_i, \theta^{(t)}) \rightarrow E(\Delta_i)^{(t)}$$

Dilemma Situation

- We need to know latent variable / data to maximize the complete log-likelihood to get the parameters
- We need to know the parameters to calculate the expected values of latent variable / data
- ➔ Solve through iterations

So we iterate ➔ EM for Gaussian Mixtures…

1. Initialize parameters $\hat{\mu_1}, \hat{\sigma_1^2}, \hat{\mu_2}, \hat{\sigma_2^2}, \hat{\pi}$
2. Expectation Step:

$\{\theta^{(t)}, Y\} \Rightarrow E^{(t)}(\Delta_i)$

$$\gamma_i(\theta) = E(\Delta_i|\theta, Y) = Pr(\Delta_i = 1|\theta, Y)$$

By Bayes' theroem:

$$Pr(\Delta_i = 1|\theta, y_i) = \frac{p(y_i|\Delta_i=1,\theta).P(\Delta_i=1|\theta)}{p(y_i|\theta)}$$

$$= \frac{\Phi_{\hat{\theta_2}}(y_i).\hat{\pi}}{(1-\hat{\pi})\Phi_{\hat{\theta_1}}(y_i)+\hat{\pi}\Phi_{\hat{\theta_2}}(y_i)}$$

$$E[l_0(\theta; \mathbf{T}|Y, \hat{\theta}^{(j)})] = \sum_{i=1}^{N}[(1-\hat{\gamma_i})log\Phi_{\theta_1}(y_i) + \hat{\gamma_i}log\Phi_{\theta_2}(y_i)] + \sum_{i=1}^{N}[(1-\hat{\gamma_i})log(1-\pi) + \hat{\gamma_i}log\pi]$$

EM for Gaussian Mixtures…

3. Maximization Step:

$\{Y, E^{(t)}(\Delta_i)\} \Rightarrow \theta^{(t+1)}$

$$Q(\theta', \widehat{\theta}^{(j)}) = E[l_0(\theta'; \mathbf{T}|Y, \widehat{\theta}^{(j)})]$$

$$= \sum_{i=1}^{N}[(1-\widehat{\gamma}_i)log\Phi_{\theta_1}(y_i) + \widehat{\gamma}_i log\Phi_{\theta_2}(y_i)]$$
$$+ \sum_{i=1}^{N}[(1-\widehat{\gamma}_i)log(1-\pi) + \widehat{\gamma}_i log\pi]$$

Find θ' that maximizes $Q(\theta', \widehat{\theta}^{(j)}) \ldots$

Set $\frac{\partial Q}{\partial \widehat{\mu}_1}, \frac{\partial Q}{\partial \widehat{\mu}_2}, \frac{\partial Q}{\partial \widehat{\sigma}_1}, \frac{\partial Q}{\partial \widehat{\sigma}_2}, \frac{\partial Q}{\partial \widehat{\pi}} = 0$

to get $\widehat{\theta}^{(j+1)}$

4. Use this $\widehat{\theta}^{j+1}$ to compute the expected values $\widehat{\gamma}_i$ and repeat…until convergence

EM for Two-component Gaussian Mixture

- Initialize $\mu_1, \sigma_1, \mu_2, \sigma_2, \pi$
- Iterate until convergence
  - Expectation of latent variables Δ

$$\gamma_i(\theta) = \frac{\Phi_{\theta_2}(y_i)\pi}{\Phi_{\theta_1}(y_i)(1-\pi) + \Phi_{\theta_2}(y_i)\pi} = \frac{1}{1 + \frac{1-\pi}{\pi}\frac{\sigma_2}{\sigma_1}\exp(-\frac{(y_i-\mu_1)^2}{2\sigma_1^2} + \frac{(y_i-\mu_2)^2}{2\sigma_2^2})}$$

  - Maximization for finding parameters θ

$$\mu_1 = \frac{\sum_{i=1}^{N}(1-\gamma_i)y_i}{\sum_{i=1}^{N}(1-\gamma_i)}; \quad \mu_2 = \frac{\sum_{i=1}^{N}\gamma_i y_i}{\sum_{i=1}^{N}\gamma_i}; \quad \sigma_1^2 = \frac{\sum_{i=1}^{N}(1-\gamma_i)(y_i-\mu_1)^2}{\sum_{i=1}^{N}(1-\gamma_i)}; \quad \sigma_2^2 = \frac{\sum_{i=1}^{N}\gamma_i(y_i-\mu_2)^2}{\sum_{i=1}^{N}\gamma_i}; \quad \pi = \frac{\sum_{i=1}^{N}\gamma_i}{N};$$

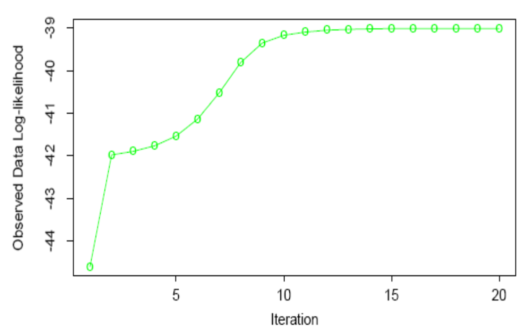
EM in….simple words

- Given observed data, you need to come up with a generative model
- You choose a model that comprises of some hidden variables Δ_i (this is your belief!)
- Problem: To estimate the parameters of model
  - Assume some initial values parameters
  - Replace values of hidden variable with their expectation (given the old parameters)
  - Recompute new values of parameters (given Δ_i)
  - Check for convergence using log-likelihood

① stationary

② until parameters stabalize ☆☆

EM – Example (cont'd)



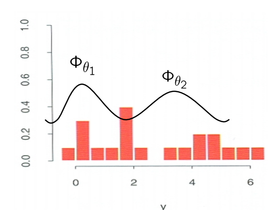


Figure 8.6: *EM algorithm: observed data log-likelihood as a function of the iteration number.*

Selected iterations of the EM algorithm For mixture example

Iteration	π
1	0.485
5	0.493
10	0.523
15	0.544
20	0.546

EM Summary

- An iterative approach for MLE
- Good idea when you have missing or latent data
- Has a nice property of convergence
- Can get stuck in local minima (try different starting points)
- Generally hard to calculate expectation over all possible values of hidden variables
- Still not much known about the rate of convergence

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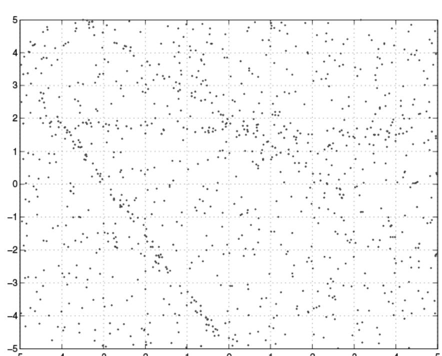
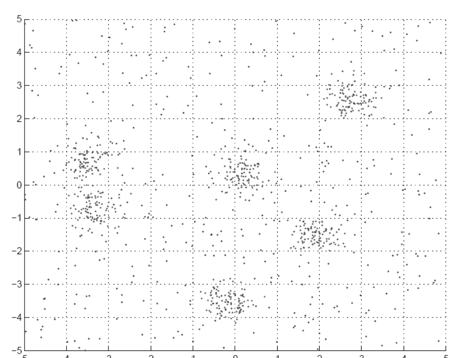
Applications of EM

- Mixture models
- HMMs
- Latent variable models
- Missing data problems
- …

Applications of EM (1)

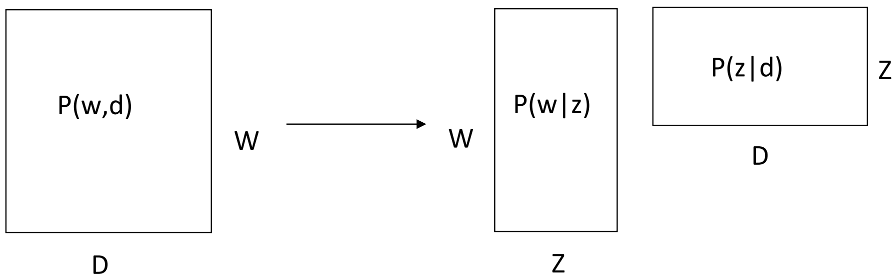
- Fitting mixture models





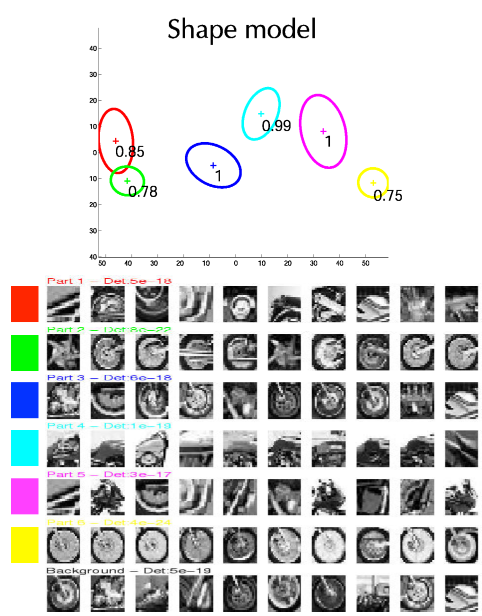
Applications of EM (2)

- Probabilistic Latent Semantic Analysis (pLSA)
  - Technique from text for topic modeling



Applications of EM (3)

- Learning parts and structure models



Applications of EM (4)

- Automatic segmentation of layers in video

http://www.psi.toronto.edu/images/figures/cutouts_vid.gif

Expectation Maximization (EM)

- Old idea (late 50's) but formalized by Dempster, Laird and Rubin in 1977

- Subject of much investigation. See McLachlan & Krishnan book 1997.

single-variable

+

two-cluster case

⊛ page 10 / $\pi = P(\Delta = 1)$

⊛ Joint Prob. Model:

① $P(y_i, \Delta_i | \theta) = P(y_i | \Delta_i, \theta)\, P(\Delta_i)$ $\begin{cases} \Delta_i = 1 \\ \Delta_i = 0 \end{cases}$

$$= [N(y_i|\mu_1, \sigma_1)(1-\pi)]^{1-\Delta_i} [N(y_i|\mu_2, \sigma_2)\, \pi]^{\Delta_i}$$

② $\boxed{\text{Marginal}}$ Prob.

$$p(y_i|\theta) = \sum_{\Delta_i} p(y_i|\Delta_i, \theta)\, p(\Delta_i)$$

$$= N(y_i|\mu_1, \sigma_1)(1-\pi) + N(y_i|\mu_2, \sigma_2)\, \pi$$

③ $\boxed{\text{conditional}}$

$$\Rightarrow p(y_i|\Delta_i, \theta) = \begin{cases} \Delta_i = 1 & N(y_i|\mu_1, \sigma_1) \\ \Delta_i = 0 & N(y_2|\mu_2, \sigma_2) \end{cases}$$

E step ⇒

$$\Rightarrow p(\Delta_i = 1 | y_i, \theta) = \frac{Pr(y_i|\Delta_i = 1)\, Pr(\Delta_i = 1|\theta)}{P(y_i|\theta)}$$

$=$

multi-variable

+

multi-cluster case

multi-variate ⇒ Given $(x_1, x_2, \cdots, x_n)$

multi-cluster ⇒ complete $(\vec{z}_1, \vec{z}_2, \cdots, \vec{z}_n)$

with

each vector $\vec{z}_i = (0, 0, 0, 0, \cdots, 1, 0, 0, 0)_K$ jth position

$z_i^{(j)} = 1$ ⇒ Basis Vector $z_i^{(j)} = 1$

⇒ parameters $\vec{\theta}$ includes

$$\begin{cases} \{\mu_j, \Sigma_j\}, \quad j = 1, 2, \cdots, K \\ \vec{\pi} \text{ vector}, \quad \pi_j = p(z^{(j)} = 1) \\ \quad \text{s.t. } \sum_{j=1}^{K} \pi_j = 1 \end{cases}$$

① Joint Prob.

$$p(x_i, \vec{z}_i | \theta) = \prod_{j=1}^{K} [\pi_j N(x_i|\mu_j, \Sigma_j)]^{z_i^{(j)}}$$

$$p(x_i, z_i^{(j)} = 1 | \theta) = \pi_j N(x_i|\mu_j, \Sigma_j)$$

② Marginal

$$p(x_i|\theta) = \sum_{j=1}^{K} \pi_j N(x_i|\mu_j, \Sigma_j)$$

③ Conditional

$$p(z_i^{(j)} = 1 | x_i, \mu_j, \Sigma_j) \overset{\text{Bayes Rule}}{=\!=} \frac{\pi_j N(x_i|\mu_j, \Sigma_j)}{\sum_{k=1}^{K} \pi_k N(x_i|\mu_k, \Sigma_k)}$$

Detour for HW5:
In L21: Learning a Gaussian Mixture

(with known covariance and single-variable and multi-cluster case)

- Probability $p(x = x_i)$ $\nearrow$ $p(x_i, z_i^{(j)}=1)$

marginal $p(x=x_i) = \sum_{\mu_j} p(x=x_i, \mu=\mu_j) = \sum_{\mu_j} p(\mu=\mu_j)\underbrace{p(x=x_i \mid \mu=\mu_j)}_{N(x_i \mid \mu_j, \Sigma)}$

$$= \sum_{\mu_j} \underbrace{p(\mu=\mu_j)}_{\pi_j} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{\|x_i - \mu_j\|_2}{2\sigma^2}\right)$$

Assuming

- Log-likelihood of data $logp(x_1, x_2, x_3, ..., x_n) =$

$$\sum_{i=1}^{n} \log p(x=x_i) = \sum_i \log\left[\sum_{\mu_j} p(\mu=\mu_j)\frac{1}{(2\pi\sigma^2)^{d/2}}\exp\left(-\frac{\|x_i-\mu_j\|_2}{2\sigma^2}\right)\right]$$

- Apply MLE to find optimal parameters $\{\underbrace{p(\mu=\mu_j)}_{\pi_j}, \mu_j\}_j$ $j=1,\cdots,K$

In HW5: with known covariance and multi-variable and multi-cluster case

- We assume in HW5, K clusters shared the same known covariance matrix (to reduce the total number of estimated parameters)
- We just use the sample covariance calculating from all samples
  - Full case:

$$\widehat{\Sigma} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^T(x_i - \bar{x})$$

  - Diagonal case: to simply use the diagonal of the above sample covariance

In L21: Learning a Gaussian Mixture
(with known covariance and single-variable and multi-cluster case)

m_{ij} – k means → $E[z_i^{(j)}=1 | X, \theta]$

E-Step $E[z_{ij}] = p(\mu = \mu_j \mid x = x_i)$ conditional

membership of data x_i to cluster j

$$= \frac{p(x = x_i \mid \mu = \mu_j)p(\mu = \mu_j)}{\sum_{n=1}^{k} p(x = x_i \mid \mu = \mu_n)p(\mu = \mu_j)}$$

$$= \frac{e^{-\frac{1}{2\sigma^2}(x_i-\mu_j)^2} p(\mu = \mu_j)}{\sum_{n=1}^{k} e^{-\frac{1}{2\sigma^2}(x_i-\mu_n)^2} p(\mu = \mu_n)}$$

→ π_j

In HW5 – E step
(with known covariance and multi-variable and multi-cluster case)

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$$\underline{p(x = x_i|\mu = \mu_j)} = \frac{1}{\sqrt{(2\pi)^p det(\Sigma)}} exp(-\frac{1}{2}(x_i - \mu_j)^T\Sigma^{-1}(x_i - \mu_j))$$

Conditional $p(x_i | z_i^{(j)}=1, \theta)$

$$\mathbb{E}[z_{ij}] = \frac{\frac{1}{\sqrt{(2\pi)^p det(\Sigma)}} exp(-\frac{1}{2}(x_i - \mu_j)^T\Sigma^{-1}(x_i - \mu_j))p(\mu = \mu_j)}{\sum_{s=1}^{k} \frac{1}{\sqrt{(2\pi)^p det(\Sigma)}} exp(-\frac{1}{2}(x_i - \mu_s)^T\Sigma^{-1}(x_i - \mu_s))p(\mu = \mu_s)}$$

$\{x_i, \theta\} \to E[\vec{z}_i]$

In L21: Learning a Gaussian Mixture

(almost the same for HW5)

k mean => centroid $\frac{1}{N_j}\sum_{i=1} m_{ij} X_i$

M-Step

$$\mu_j \leftarrow \frac{1}{\sum_{i=1}^{n} E[z_{ij}]} \sum_{i=1}^{n} E[z_{ij}] x_i$$

$\{X_i, E[\vec{z}_i]\}$

$\Rightarrow \theta^{(t+1)}$

$$\pi_j = p(\mu = \mu_j) \leftarrow \frac{1}{n}\sum_{i=1}^{n} E[z_{ij}]$$

Two-clusters

$$\mu_1 = \frac{\sum_{i=1}^{N}(1-\gamma_i)y_i}{\sum_{i=1}^{N}(1-\gamma_i)};$$

$$\mu_2 = \frac{\sum_{i=1}^{N}\gamma_i y_i}{\sum_{i=1}^{N}\gamma_i};$$

$$\pi = \frac{\sum_{i=1}^{N}\gamma_i}{N};$$

Covariance: Σ_j (j: 1 to K) could also be derived in the M-step under a full setting

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Why is Learning Harder?

- In fully observed iid settings, the complete log likelihood decomposes into a sum of local terms.

$$\ell_c(\theta;D) = \log p(\underbrace{x,z}|\theta) = \log p\underbrace{(z|\theta_z)}_{\theta_z} + \log p\underbrace{(x|z,\theta_x)}_{\theta_x}$$

- When with latent variables, all the parameters become coupled together via *marginalization*

$$l(\theta;D) = \log p(x|\theta) = \log \sum_z p(z|\underbrace{\theta_z}_{\pi})p(x|z,\underbrace{\theta_x}_{\mu_i,\ \sigma_i})$$

Gradient Learning for mixture models

- We can learn mixture densities using gradient descent on the observed log likelihood. The gradients are quite interesting:

$$\ell(\theta) = \log p(\mathrm{x}|\theta) = \underbrace{\log \sum_k \pi_k p_k(\mathrm{x}|\theta_k)}$$

$$\frac{\partial \ell}{\partial \theta} = \frac{1}{p(\mathrm{x}|\theta)} \sum_k \pi_k \frac{\partial p_k(\mathrm{x}|\theta_k)}{\partial \theta}$$

$$= \sum_k \frac{\pi_k}{p(\mathrm{x}|\theta)} p_k(\mathrm{x}|\theta_k) \frac{\partial \log p_k(\mathrm{x}|\theta_k)}{\partial \theta}$$

$$= \sum_k \pi_k \underbrace{\frac{p_k(\mathrm{x}|\theta_k)}{p(\mathrm{x}|\theta)}} \frac{\partial \log p_k(\mathrm{x}|\theta_k)}{\partial \theta_k} = \boxed{\sum_k r_k \frac{\partial \ell_k}{\partial \theta_k}}$$

- In other words, the gradient is the responsibility weighted sum of the individual log likelihood gradients.
- Can pass this to a conjugate gradient routine.

Parameter Constraints

- Often we have constraints on the parameters, e.g. Σ_k being symmetric positive definite.
- We can use constrained optimization, or we can re-parameterize in terms of unconstrained values.
  - For normalized weights, softmax to e.g. $\sum_{j=1}^{K} \pi_j = 1$
  - For covariance matrices, use the Cholesky decomposition:

$$\Sigma^{-1} = \mathbf{A}^T \mathbf{A}$$

where A is upper diagonal with positive diagonal:

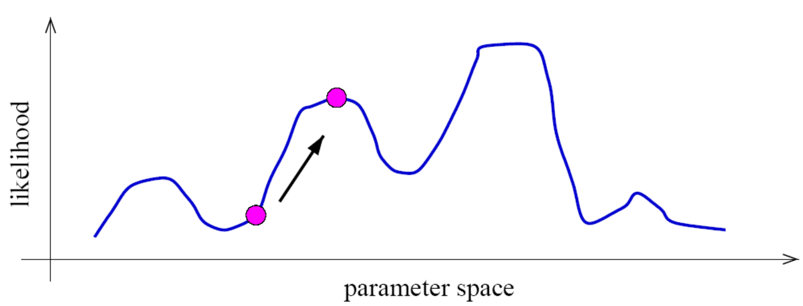
$$\mathbf{A}_{ii} = \exp(\lambda_i) > 0 \quad \mathbf{A}_{ij} = \eta_{ij} \ (j > i) \quad \mathbf{A}_{ij} = 0 \ (j < i)$$

  - Use chain rule to compute

$$\frac{\partial \ell}{\partial \pi}, \frac{\partial \ell}{\partial \mathbf{A}}.$$

Identifiability

- A mixture model induces a multi-modal likelihood.
- Hence gradient ascent can only find a local maximum.
- Mixture models are unidentifiable, since we can always switch the hidden labels without affecting the likelihood.
- Hence we should be careful in trying to interpret the "meaning" of latent variables.



Expectation-Maximization (EM) Algorithm

- EM is an Iterative algorithm with two linked steps:
  - E-step: fill-in hidden values using inference: $p(z|x, \theta^t)$.
  - M-step: update parameters (t+1) rounds using standard MLE/MAP method applied to completed data
- We will prove that this procedure monotonically improves (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.

Theory underlying EM

- What are we doing?
- Recall that according to MLE, we intend to learn the model parameter that would have maximize the likelihood of the data.
- But we do not observe z, so computing

$$\ell_c(\theta; D) = \log \sum_z p(x, z \mid \theta) = \log \sum_z p(z \mid \theta_z) p(x \mid z, \theta_x)$$

  is difficult!

- What shall we do?

(1) Incomplete Log Likelihoods

- Incomplete log likelihood

With z unobserved, our objective becomes the log of a marginal probability:

– **This objective won't decouple**

$$l(\theta;x)=\log \underbrace{p(x|\theta)}_{\text{marginal given observed } x}=\log\sum_z p(x,z|\theta) \quad \in \text{[one sample]}$$

(2) Complete Log Likelihoods

[a random quantity]

- Complete log likelihood

Let X denote the observable variable(s), and Z denote the latent variable(s).
If Z could be observed, then

Joint Prob.

$$l_c(\theta;x,z)\overset{\text{def}}{=}\underbrace{\log p(x,z|\theta)}=\log p(z|\theta_z)p(x|z,\theta_x)$$

– Usually, optimizing $l_c()$ given both z and x is straightforward (c.f. MLE for fully observed models).

– Recalled that in this case the objective for, e.g., MLE, decomposes into a sum of factors, the parameter for each factor can be estimated separately.

– **But given that Z is not observed, $l_c()$ is a random quantity, cannot be maximized directly**.

Three types of log-likelihood
over multiple observed samples (x_1, x_2, …, x_N)

Observed data	x	$= \boxed{(x_1, x_2, \ldots, x_N)}$
Latent variables	z	$= (z_1, z_2, \ldots, z_N)$
Iteration index	t	

$E_q[f(z)] = \sum_z q(z) f(z)$

Log-likelihood [Incomplete log-likelihood (ILL)]

$$l(\theta; x) = log\, p(x|\theta) = log\, \prod_x p(x|\theta)$$
$$= \sum_x log\, \sum_z p(x, z|\theta)$$

Complete log-likelihood (CLL)

$$l_c(\theta; x, z) \triangleq \sum_x \log p(x, z \mid \theta)$$

$z \sim q(z|x, \theta)$

Expected complete log-likelihood (ECLL)

$$E_q[f(z)] = \langle l_c(\theta; x, z)\rangle_q \triangleq \sum_{\substack{x \\ x_1, x_2, \ldots, x_n}} \sum_z \underbrace{q(z \mid x, \theta)} \underbrace{\log p(x, z \mid \theta)}$$

(3) Expected Complete Log Likelihood

- For ***any*** distribution $q(z)$, define *expected complete log likelihood (ECLL)*:
  - CLL is random variable ➔ ECLL is a deterministic function of *q*
  - Linear in CLL() --- inherit its factorizabiility
  - Does maximizing this surrogate yield a maximizer of the likelihood?

$$ECLL = \langle l_c(\theta; x, z)\rangle_q \stackrel{\text{def}}{=} \sum_z q(z|x, \theta) \log p(x, z|\theta)$$

Jensen's inequality

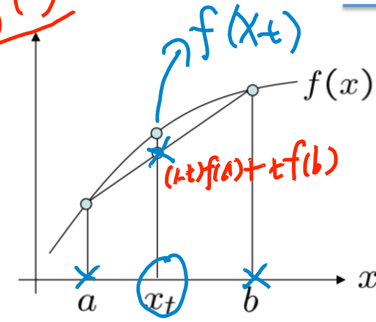
Concave func $f(x)$ e.g. log( )

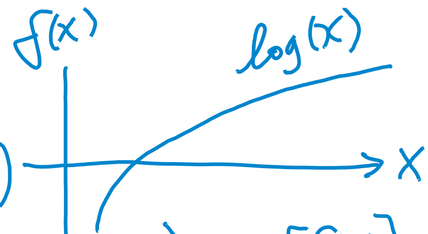
$x_t = (1-t)a + tb$

$\Rightarrow f(x_t) \geq (1-t) f(a) + t f(b)$

$\Rightarrow f(\sum_{j=1}^{M} \lambda_j x_j) \geq \sum_{j=1}^{M} \lambda_j f(x_j)$

$\sum_j \lambda_j = 1$





$f(E[X]) \geq E[f(X)]$

Jensen's inequality

- Jensen's inequality

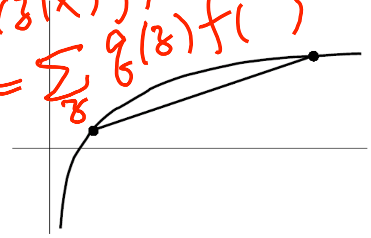
$$ECLL = \langle l_c(\theta; x, z) \rangle_q \overset{\text{def}}{=} \sum_z q(z|x,\theta) \log p(x,z|\theta)$$

$$ILL = l(\theta; x) = \log p(x|\theta)$$
$$= \log \sum_z p(x,z|\theta)$$
$$= \log \sum_z q(z|x) \frac{p(x,z|\theta)}{q(z|x)}$$

$z \sim q(z|x)$ $\quad f = \log(\ )$

$\Rightarrow f(E_q[\frac{p(x,z|\theta)}{q(z|x)}])$

Jensen's $\geq \sum_z q(z|x) \log \frac{p(x,z|\theta)}{q(z|x)}$ $\Rightarrow E_q[f(\ )] = \sum_z q(z) f(\ )$



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

Entropy term

$$= ECLL + H_q$$

$$\Rightarrow \ell(\theta; x) \geq \langle \ell_c(\theta; x, z) \rangle_q + H_q$$

ILL $\geq$ ECLL + H_q

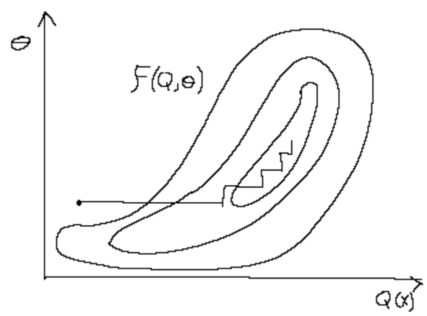
Lower Bounds and Free Energy

- For fixed data x, define a functional called the free energy:

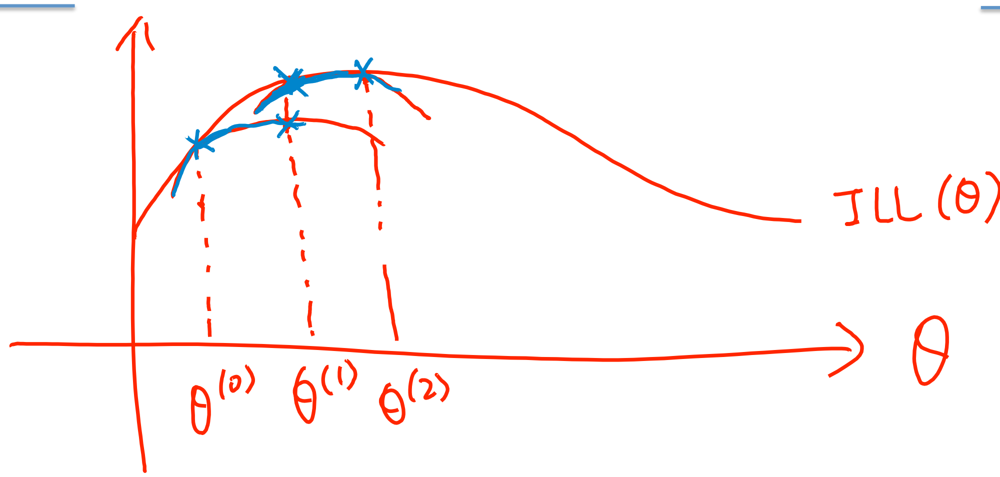
$E_{q(z)} f((z))$

$$F(q,\theta) \overset{\text{def}}{=} \sum_z q(z \mid x) \log \frac{p(x,z \mid \theta)}{q(z \mid x)} \le \ell(\theta; x)$$

- The EM algorithm is coordinate-ascent on F :
  - **E-step:** $q^{t+1} = \arg\max_q F(q, \theta^t)$
  - **M-step:** $\theta^{t+1} = \arg\max_\theta F(q^{t+1}, \theta^t)$



How EM optimize ILL ?



E-step: maximization of w.r.t. q

- Claim: $$q^{t+1} = \arg\max_{q} F(q,\theta^t) = p(z \mid x,\theta^t)$$
  - This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform clustering).
- Proof (easy): this setting attains the bound of ILL

$$\boxed{F(p(z|x,\theta^t),\theta^t)} = \sum_z p(z|x,\theta^t)\log\frac{p(x,z\mid\theta^t)}{p(z|x,\theta^t)}$$

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

$$= \log p(x\mid\theta^t) = \boxed{\ell(\theta^t;x)} \quad \text{ILL}$$

- Can also show this result using variational calculus or the fact that

$$\ell(\theta;x) - F(q,\theta) = \mathrm{KL}\big(q \,\|\, p(z\mid x,\theta)\big)$$

E-step: Alternative derivation

$\Rightarrow \ell(\theta;x) \geq F(q,\theta)$

$$\ell(\theta;x) - F(q,\theta) = \mathrm{KL}\big(q \,\|\, p(z\mid x,\theta)\big)$$

$$= l(\theta;x) - \sum_z q(z\mid x)\log\frac{p(x,z\mid\theta)}{q(z\mid x)}$$

$p(z|x,\theta)p(x,\theta) \Rightarrow$

$$= \sum_z q(z\mid x)\log p(x\mid\theta) - \sum_z q(z\mid x)\log\frac{p(x,z\mid\theta)}{q(z\mid x)}$$

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

$$= D_{KL}(q(z\mid x)\,\|\,p(z\mid x,\theta)).$$

$\Rightarrow$ [$D_{KL} = 0$ iff $q = p$ almost everywhere]

M-step: maximization w.r.t. \theta

- Note that the free energy breaks into two terms:

$$F(q,\theta) = \sum_z q(z|x) \log \frac{p(x,z|\theta)}{q(z|x)}$$
$$= \sum_z q(z|x) \log p(x,z|\theta) - \sum_z q(z|x) \log q(z|x)$$
$$\boxed{= \langle \ell_c(\theta; x, z) \rangle_q + H_q}$$

ECLL + entropy

– The first term is the expected complete log likelihood (energy) and the second term, which does not depend on θ, is the entropy.

M-step: maximization w.r.t. \theta

- Thus, in the M-step, maximizing with respect to θ for fixed q we only need to consider the first term:

ECLL

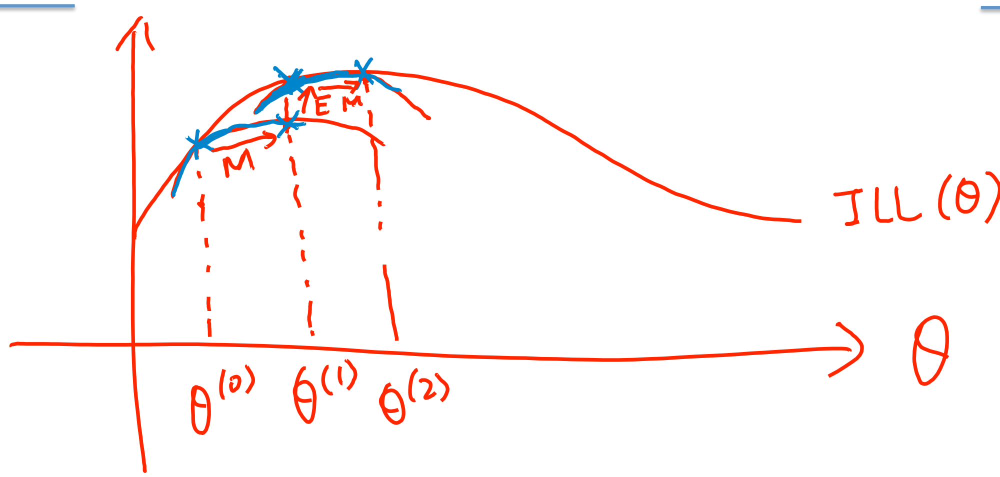
$$\theta^{t+1} = \arg\max_\theta \langle \ell_c(\theta; x, z) \rangle_{q^{t+1}} = \arg\max_\theta \sum_z q(z|x) \log p(x,z|\theta)$$

– Under optimal q^{t+1}, this is equivalent to solving a standard MLE of fully observed model $p(x,z|\theta)$, with the sufficient statistics involving z replaced by their expectations w.r.t. $p(z|x,\theta)$.

Summary: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:
    1. Estimate some "missing" or "unobserved" data from observed data and current parameters.
    2. Using this "complete" data, find the maximum likelihood parameter estimates.
- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:
    - E-step: $q^{t+1} = \arg\max_q F(q, \theta^t)$
    - M-step: $\theta^{t+1} = \arg\max_\theta F(q^{t+1}, \theta^t)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

How EM optimize ILL ?



A Report Card for EM

- Some good things about EM:
  - no learning rate (step-size) parameter
  - automatically enforces parameter constraints
  - very fast for low dimensions
  - each iteration guaranteed to improve likelihood
  - Calls inference and fully observed learning as subroutines.

- Some bad things about EM:
  - can get stuck in local minima
  - can be slower than conjugate gradient (especially near convergence)
  - requires expensive inference step $\Rightarrow P(z|x,\theta)$
  - is a maximum likelihood/MAP method

References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- **The EM Algorithm and Extensions** by Geoffrey J. MacLauchlan, Thriyambakam Krishnan