

# Expectation Maximization

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# Preliminary [2]

- Convex Functions:-

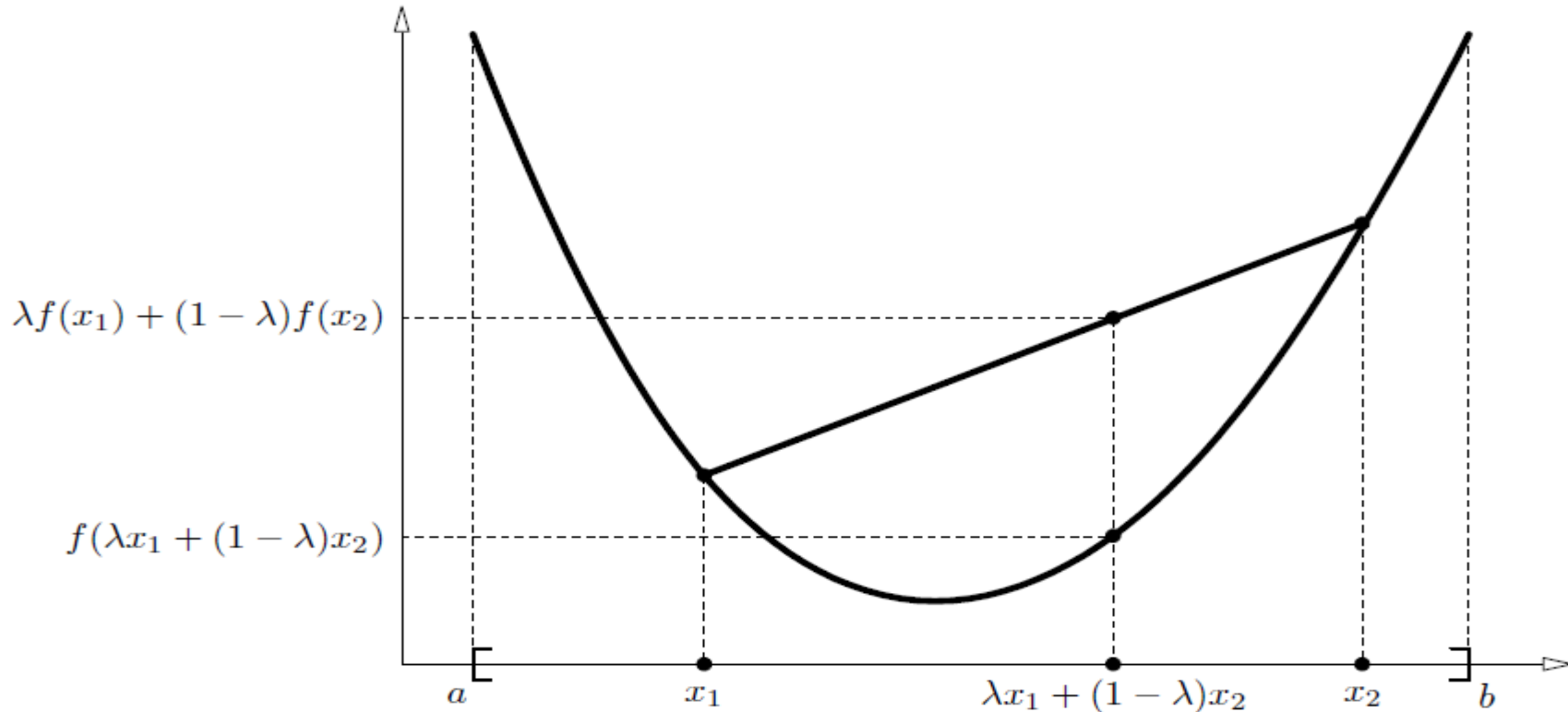
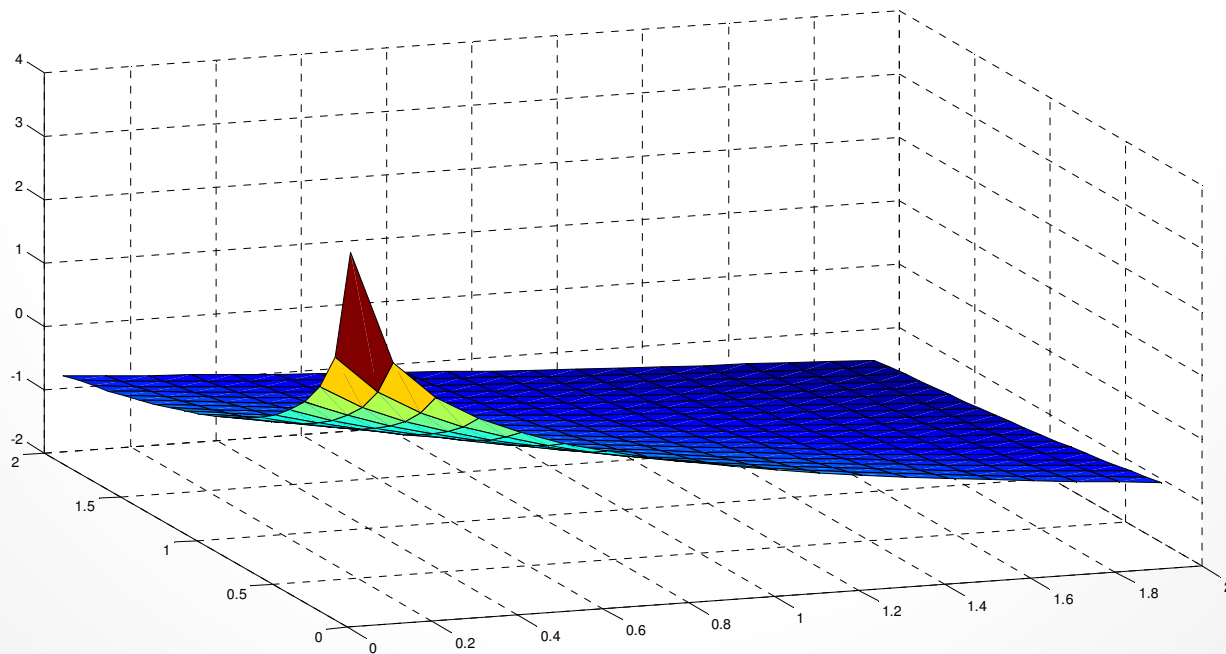


Figure 1:  $f$  is *convex* on  $[a, b]$  if  $f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda)f(x_2)$   $\forall x_1, x_2 \in [a, b], \lambda \in [0, 1]$ .

# Convex Fn properties

- $f$  is concave if  $-f$  is convex
- If  $f(x)$  is twice differentiable and  $f''(x) \geq 0$  then  $f(x)$  is convex
- $-\ln(x)$  is convex on the interval  $(0, \infty)$



# Contd

- Jensen's inequality

**Theorem 2 (Jensen's inequality)** *Let  $f$  be a convex function defined on an interval  $I$ . If  $x_1, x_2, \dots, x_n \in I$  and  $\lambda_1, \lambda_2, \dots, \lambda_n \geq 0$  with  $\sum_{i=1}^n \lambda_i = 1$ ,*

$$f\left(\sum_{i=1}^n \lambda_i x_i\right) \leq \sum_{i=1}^n \lambda_i f(x_i)$$

$$\begin{aligned} f\left(\sum_{i=1}^{n+1} \lambda_i x_i\right) &= f\left(\lambda_{n+1} x_{n+1} + \sum_{i=1}^n \lambda_i x_i\right) \\ &= f\left(\lambda_{n+1} x_{n+1} + (1 - \lambda_{n+1}) \frac{1}{1 - \lambda_{n+1}} \sum_{i=1}^n \lambda_i x_i\right) \end{aligned}$$

# Contd

$$\begin{aligned} &\leq \lambda_{n+1}f(x_{n+1}) + (1 - \lambda_{n+1})f\left(\frac{1}{1 - \lambda_{n+1}} \sum_{i=1}^n \lambda_i x_i\right) \\ &= \lambda_{n+1}f(x_{n+1}) + (1 - \lambda_{n+1})f\left(\sum_{i=1}^n \frac{\lambda_i}{1 - \lambda_{n+1}} x_i\right) \\ &\leq \lambda_{n+1}f(x_{n+1}) + (1 - \lambda_{n+1}) \sum_{i=1}^n \frac{\lambda_i}{1 - \lambda_{n+1}} f(x_i) \\ &= \lambda_{n+1}f(x_{n+1}) + \sum_{i=1}^n \lambda_i f(x_i) \\ &= \sum_{i=1}^{n+1} \lambda_i f(x_i) \end{aligned}$$

- Note that since  $-\ln(x)$  is convex we have

$$\ln \sum_{i=1}^n \lambda_i x_i \geq \sum_{i=1}^n \lambda_i \ln(x_i).$$

# Three coin Example <sup>[1]</sup>

- We observe a series of coin tosses generated in the following way:
- A person has three coins.
  - Coin 0: probability of Head is  $\lambda$
  - Coin 1: probability of Head  $p$
  - Coin 2: probability of Head  $q$
- Consider the following coin-tossing scenarios:

# Estimation Problems

- Scenario I: Toss one of the coins six times.

Observing HHHTHT

Which coin is more likely to produce this sequence? Suppose we know the probability of H for each coin.

- Scenario II: Toss coin 0. If Head – toss coin 1; o/w – toss coin 2

Observing the sequence HHHHT, THTHT, HHHT, HHTTH produced by Coin 0, Coin1 and Coin2

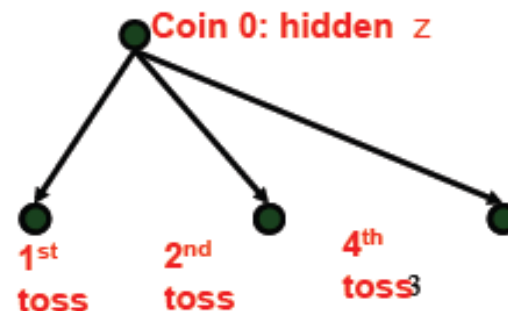
Estimate most likely values for  $p$ ,  $q$ ,  $\lambda$  (the probability of H in each coin)

- Scenario III: Toss coin 0. If Head – toss coin 1; o/w – toss coin 2

Observing the sequence HHHT, HTHT, HHHT, HHTH produced by Coin 1 and/or Coin 2

Estimate most likely values for  $\lambda$ ,  $p$ ,  $q$ .

The label of the first toss ( $z$ ) is hidden, we want to estimate the most likely hypothesis  $\theta = (\lambda, p, q)$  under hidden  $z$ .



# Key Intuition

- If we knew which of the data points (HHHT), (HTHT), (HTTH) came from Coin1 and which from Coin2, there was no problem.
- Recall that the “simple” estimation is the ML estimation:
- Assume that you toss a  $(p, 1-p)$  coin  $m$  times and get  $k$  Heads  $m-k$  Tails.

$$\log[P(D|p)] = \log [ p^k (1-p)^{m-k} ] = k \log p + (m-k) \log (1-p)$$

- To maximize, set the derivative w.r.t.  $p$  equal to 0:

$$d/dp \{ \log P(D|p) \} = k/p - (m-k)/(1-p) = 0$$

- Solving this for  $p$ , gives:  $p=k/m$



# Key Intuition

- Since we do not know which of the data points (HHHT), (HTHT), (HTTH) came from Coin1 and which from Coin2, we use an iterative approach for estimating  $(\lambda, p, q)$ .

# Derivation [2]

- Log likelihood:-  $L(\theta) = \ln \mathcal{P}(\mathbf{X}|\theta)$ .  
$$\mathcal{P}(\mathbf{X}|\theta) = \sum_{\mathbf{z}} \mathcal{P}(\mathbf{X}|\mathbf{z}, \theta)\mathcal{P}(\mathbf{z}|\theta).$$
- We wish to find  $\theta$  iterative such that  $L(\theta) > L(\theta_n)$   
Where  $\theta_n$  is previous iterations  $\theta$  value.
- The difference can be written as

$$\begin{aligned} L(\theta) - L(\theta_n) &= \ln \mathcal{P}(\mathbf{X}|\theta) - \ln \mathcal{P}(\mathbf{X}|\theta_n). \\ &= \ln \left( \sum_{\mathbf{z}} \mathcal{P}(\mathbf{X}|\mathbf{z}, \theta)\mathcal{P}(\mathbf{z}|\theta) \right) - \ln \mathcal{P}(\mathbf{X}|\theta_n). \end{aligned}$$

# Derivation

- Note that  $\ln \sum_{i=1}^n \lambda_i x_i \geq \sum_{i=1}^n \lambda_i \ln(x_i)$

$$\begin{aligned} L(\theta) - L(\theta_n) &= \ln \left( \sum_{\mathbf{z}} \mathcal{P}(\mathbf{X}|\mathbf{z}, \theta) \mathcal{P}(\mathbf{z}|\theta) \right) - \ln \mathcal{P}(\mathbf{X}|\theta_n) \\ &= \ln \left( \sum_{\mathbf{z}} \mathcal{P}(\mathbf{X}|\mathbf{z}, \theta) \mathcal{P}(\mathbf{z}|\theta) \cdot \frac{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n)}{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n)} \right) - \ln \mathcal{P}(\mathbf{X}|\theta_n) \\ &= \ln \left( \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \frac{\mathcal{P}(\mathbf{X}|\mathbf{z}, \theta) \mathcal{P}(\mathbf{z}|\theta)}{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n)} \right) - \ln \mathcal{P}(\mathbf{X}|\theta_n) \\ &\geq \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \left( \frac{\mathcal{P}(\mathbf{X}|\mathbf{z}, \theta) \mathcal{P}(\mathbf{z}|\theta)}{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n)} \right) - \ln \mathcal{P}(\mathbf{X}|\theta_n) \\ &= \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \left( \frac{\mathcal{P}(\mathbf{X}|\mathbf{z}, \theta) \mathcal{P}(\mathbf{z}|\theta)}{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \mathcal{P}(\mathbf{X}|\theta_n)} \right) \\ &\triangleq \Delta(\theta|\theta_n). \end{aligned}$$

# Derivation

- So far  $L(\theta) \geq \underbrace{L(\theta_n) + \Delta(\theta|\theta_n)}$

$$l(\theta|\theta_n) \quad \longrightarrow \quad L(\theta) \geq l(\theta|\theta_n)$$

$$\begin{aligned} l(\theta_n|\theta_n) &= L(\theta_n) + \Delta(\theta_n|\theta_n) \\ &= L(\theta_n) + \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \frac{\mathcal{P}(\mathbf{X}|\mathbf{z}, \theta_n) \mathcal{P}(\mathbf{z}|\theta_n)}{\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \mathcal{P}(\mathbf{X}|\theta_n)} \\ &= L(\theta_n) + \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \frac{\mathcal{P}(\mathbf{X}, \mathbf{z}|\theta_n)}{\mathcal{P}(\mathbf{X}, \mathbf{z}|\theta_n)} \\ &= L(\theta_n) + \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln 1 \\ &= L(\theta_n), \end{aligned}$$

# Intuition

- In EM we optimize  $l(\theta|\theta_n)$

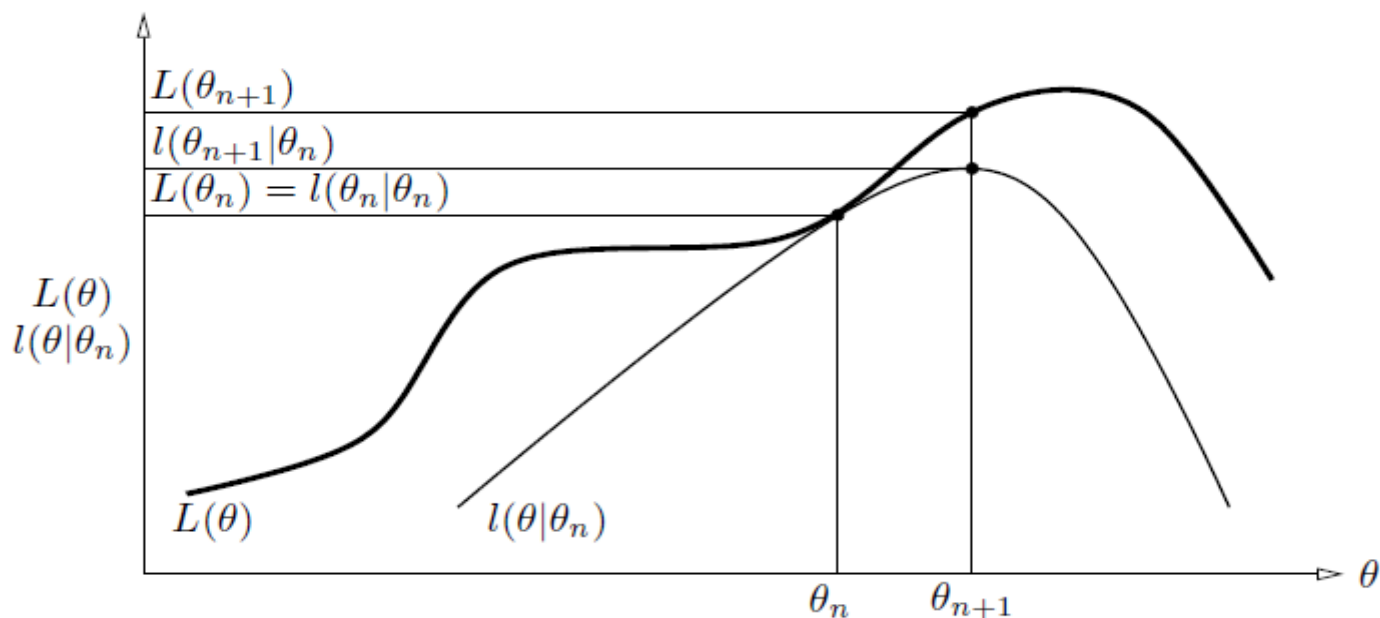


Figure 2: Graphical interpretation of a single iteration of the EM algorithm: The function  $l(\theta|\theta_n)$  is bounded above by the likelihood function  $L(\theta)$ . The functions are equal at  $\theta = \theta_n$ . The EM algorithm chooses  $\theta_{n+1}$  as the value of  $\theta$  for which  $l(\theta|\theta_n)$  is a maximum. Since  $L(\theta) \geq l(\theta|\theta_n)$  increasing  $l(\theta|\theta_n)$  ensures that the value of the likelihood function  $L(\theta)$  is increased at each step.

# Derivation

- Formally we have

$$\begin{aligned}\theta_{n+1} &= \arg \max_{\theta} \{l(\theta|\theta_n)\} \\ &= \arg \max_{\theta} \left\{ L(\theta_n) + \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \frac{\mathcal{P}(\mathbf{X}|\mathbf{z}, \theta)\mathcal{P}(\mathbf{z}|\theta)}{\mathcal{P}(\mathbf{X}|\theta_n)\mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n)} \right\} \\ &\quad \text{Now drop terms which are constant w.r.t. } \theta \\ &= \arg \max_{\theta} \left\{ \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \mathcal{P}(\mathbf{X}|\mathbf{z}, \theta)\mathcal{P}(\mathbf{z}|\theta) \right\} \\ &= \arg \max_{\theta} \left\{ \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \frac{\mathcal{P}(\mathbf{X}, \mathbf{z}, \theta)}{\mathcal{P}(\mathbf{z}, \theta)} \frac{\mathcal{P}(\mathbf{z}, \theta)}{\mathcal{P}(\theta)} \right\} \\ &= \arg \max_{\theta} \left\{ \sum_{\mathbf{z}} \mathcal{P}(\mathbf{z}|\mathbf{X}, \theta_n) \ln \mathcal{P}(\mathbf{X}, \mathbf{z}|\theta) \right\} \\ &= \arg \max_{\theta} \{E_{\mathbf{Z}|\mathbf{X}, \theta_n} \{\ln \mathcal{P}(\mathbf{X}, \mathbf{z}|\theta)\}\}\end{aligned}$$

# Algorithm

- E-step Find the conditional expectation,

$$E_{\mathbf{z}|\mathbf{X},\theta_n} \{\ln \mathcal{P}(\mathbf{X}, \mathbf{z}|\theta)\}$$

- Maximize wrt  $\theta$

# Convergence

- Intuition
  - At each iteration the objective is non-decreasing
  - The log-likelihood is bounded above
- It should converge but at a local minima



# Three Coin Estimation Problems

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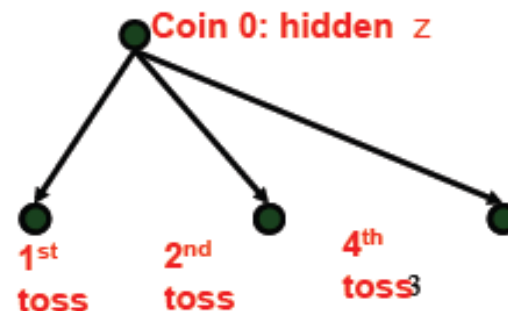
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Estimate most likely values for  $\lambda$ ,  $p$ ,  $q$ .

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# EM

$$P(D^i, 1 | \lambda, p, q) = \lambda p^{h_i} (1-p)^{m-h_i}$$

$$P(D^i, 0 | \lambda, p, q) = (1-\lambda) q^{h_i} (1-q)^{m-h_i}$$

$z_i$  is an indicator variable

$$\begin{aligned} P(D^i, z_i | \lambda, p, q) &= [\lambda p^{h_i} (1-p)^{m-h_i}]^{z_i} [(1-\lambda) q^{h_i} (1-q)^{m-h_i}]^{(1-z_i)} \\ &= \lambda^{z_i} p^{z_i h_i} (1-p)^{z_i(m-h_i)} (1-\lambda)^{1-z_i} q^{(1-z_i)h_i} (1-q)^{(1-z_i)(m-h_i)} \end{aligned}$$

$$\begin{aligned} \log P(D^i, z_i | \lambda, p, q) &= z_i \log \lambda + z_i h_i \log p + z_i (m - h_i) \log(1-p) + \\ &\quad (1-z_i) \log(1-\lambda) + (1-z_i) h_i \log q + (1-z_i)(m-h_i) \log(1-q) \end{aligned}$$

$$P(D, z | \lambda, p, q) = \prod_i P(D^i, z_i | \lambda, p, q)$$

$$\log P(D, z | \lambda, p, q) = \sum_i \log P(D^i, z_i | \lambda, p, q)$$

$$E[X + Y] = E[X] + E[Y]$$

$$E[\log P(D, z | \lambda, p, q)] = E\left[\sum_i \log P(D^i, z_i | \lambda, p, q)\right] = \sum_i E[\log P(D^i, z_i | \lambda, p, q)]$$

$$E[z_i] = P_i$$

$$= \sum_i E[z_i \log \lambda + z_i h_i \log p + z_i (m - h_i) \log(1-p) + (1-z_i) \log(1-\lambda) + (1-z_i) h_i \log q + (1-z_i)(m-h_i) \log(1-q)]$$

$$= \sum_i P_i \log \lambda + P_i h_i \log p + P_i (m - h_i) \log(1-p) + (1-P_i) \log(1-\lambda) + (1-P_i) h_i \log q + (1-P_i)(m-h_i) \log(1-q)$$

# EM

- Suppose  $(\tilde{\lambda}, \tilde{p}, \tilde{q})$  is the current estimate of parameters.
- What is the probability  $P(z)$  given  $(\tilde{\lambda}, \tilde{p}, \tilde{q})$  and  $D$ ?
- Suppose there were  $m$  coin tosses and  $h$  heads in  $D^i$ . Given the current parameters,

$$P_i = P(z_i = 1 | D^i) = P(\text{Coin1} | D^i) = \frac{P(D^i | \text{Coin1}) P(\text{Coin1})}{P(D^i)} =$$

$$= \frac{\tilde{\lambda} \tilde{p}^{h_i} (1 - \tilde{p})^{m - h_i}}{\tilde{\lambda} \tilde{p}^{h_i} (1 - \tilde{p})^{m - h_i} + (1 - \tilde{\lambda}) \tilde{q}^{h_i} (1 - \tilde{q})^{m - h_i}}$$

$$E[Y] = \sum_{y_i} y_i P(Y = y_i)$$

$$E[z_i] = 1 \times P(D_i \text{ was obtained from Coin 1}) + \\ 0 \times P(D_i \text{ was obtained from Coin 2}) = P_i$$

# EM

$$\frac{dE}{d\lambda} = \sum \left( \frac{P_i}{\lambda} - \frac{1-P_i}{1-\lambda} \right) = 0$$

$$\lambda = \frac{\sum P_i}{n}$$

$$\frac{dE}{dp} = \sum P_i \left( \frac{h_i}{p} - \frac{m-h_i}{1-p} \right) = 0$$

$\Rightarrow$

$$p = \frac{\sum P_i \frac{h_i}{m}}{\sum P_i}$$

$$\frac{dE}{dq} = \sum_{i=1}^n (1-P_i) \left( \frac{h_i}{q} - \frac{m-h_i}{1-q} \right) = 0$$

$\Rightarrow$

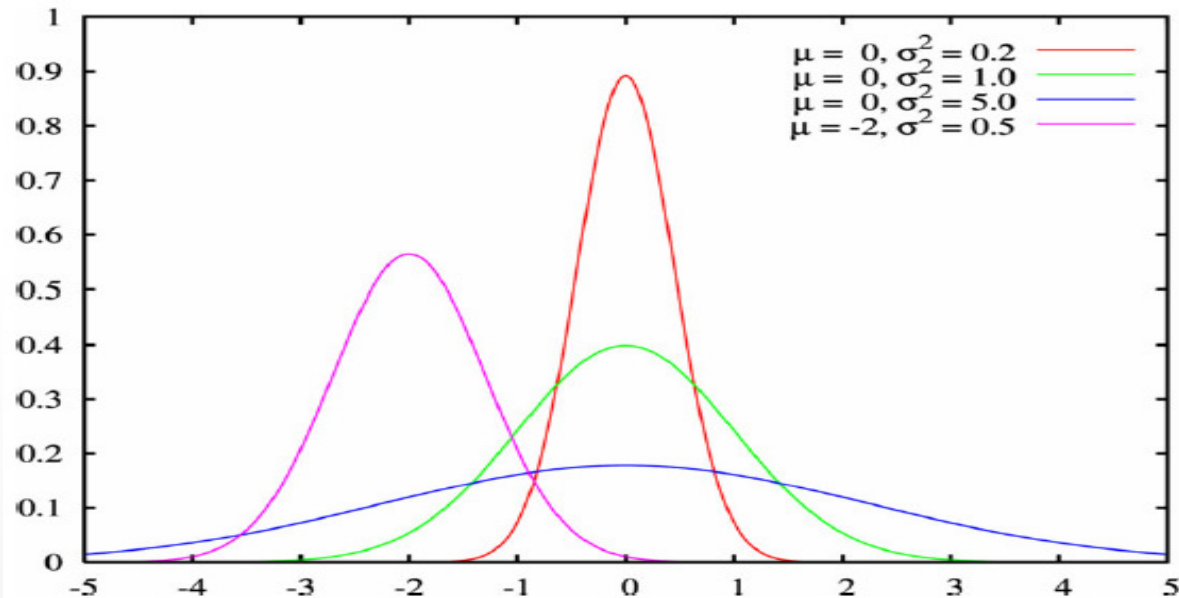
$$q = \frac{\sum (1-P_i) \frac{h_i}{m}}{\sum (1-P_i)}$$

# Example 2 GMM [3]

- Gaussian Distribution

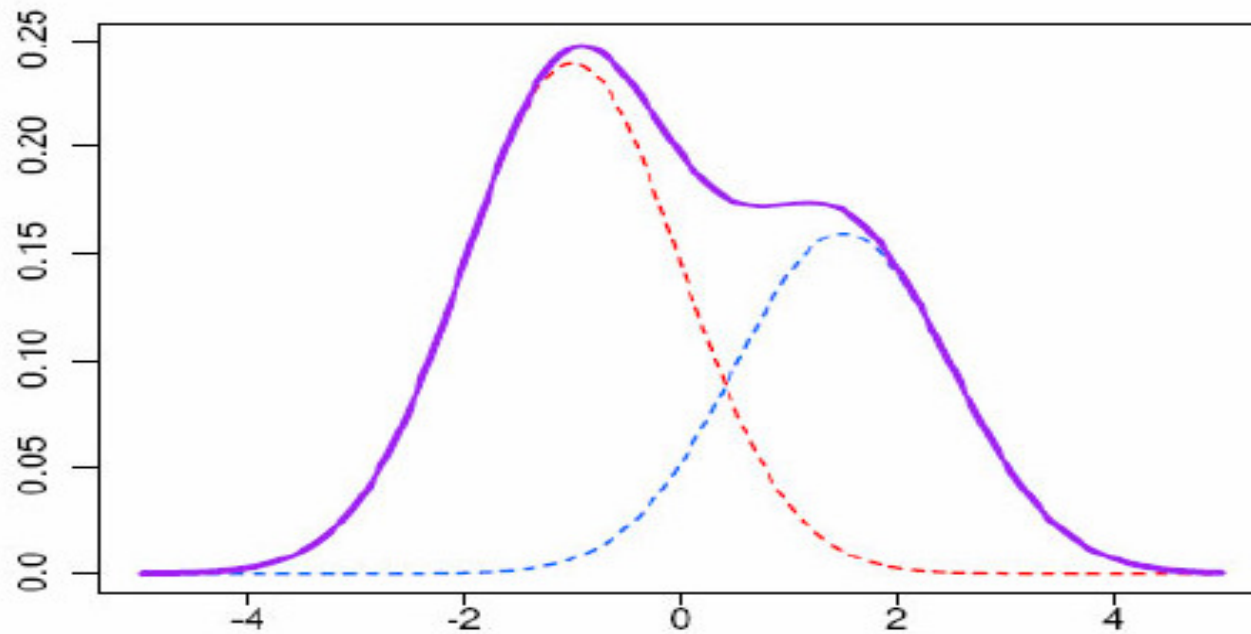
$$G_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Mixture of Gaussian can model arbitrary distributions

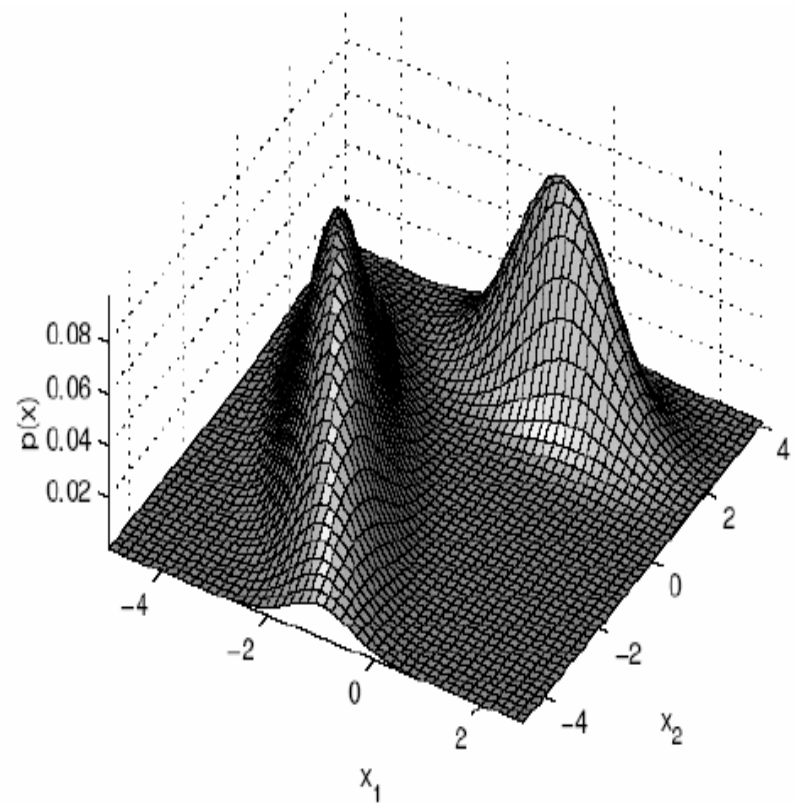
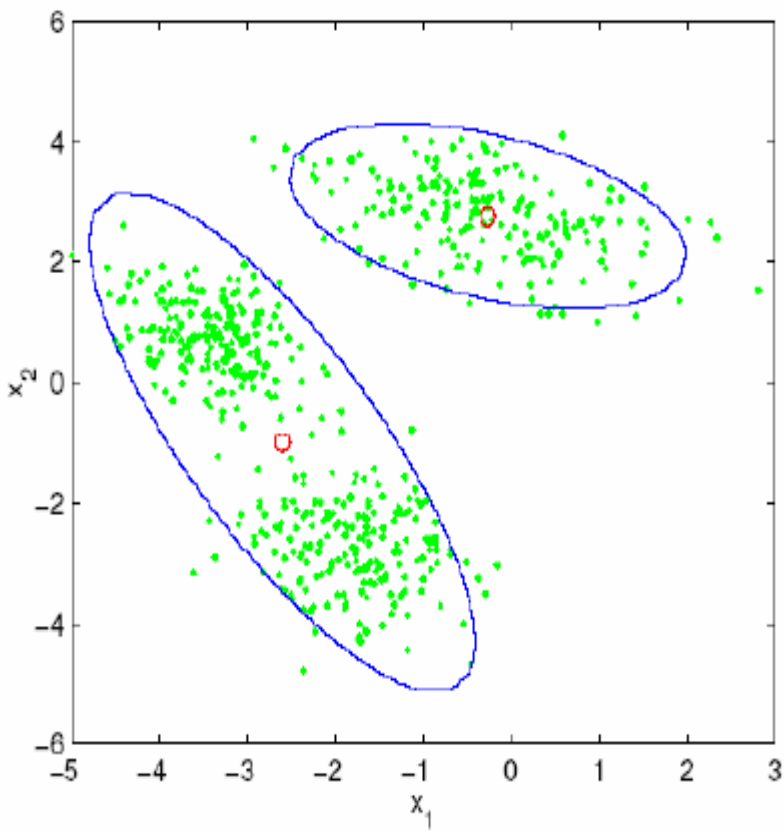


# GMM

- An example of two mixtures:-



# GMM



# EM algorithm for GMM



- E.g., A mixture of K Gaussians:

- $Z$  is a latent class indicator vector

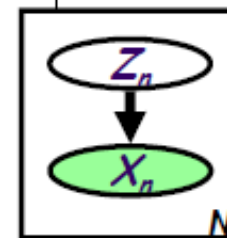
$$p(z_n) = \text{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$

- $X$  is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n | z_n^k = \mathbf{1}, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{-\frac{1}{2}(x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k)\right\}$$

- The likelihood of a sample:

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z^k = \mathbf{1} | \pi) p(x, | z^k = \mathbf{1}, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left( (\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, | \mu_k, \Sigma_k) \end{aligned}$$





# How is EM derived?



- A mixture of K Gaussians:

- $Z$  is a latent class indicator vector

$$p(\mathbf{z}_n) = \text{multi}(\mathbf{z}_n; \boldsymbol{\pi}) = \prod_k (\pi_k)^{z_n^k}$$

- $X$  is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n | z_n^k = 1, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{-\frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k)\right\}$$

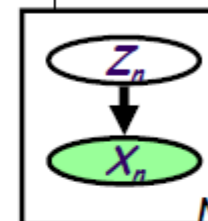
- The likelihood of a sample:

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z_n^k = 1 | \boldsymbol{\pi}) p(x_n | z_n^k = 1, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left( (\pi_k)^{z_n^k} N(x_n | \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x_n | \mu_k, \Sigma_k) \end{aligned}$$

- The “complete” likelihood

$$\begin{aligned} p(x_n, z_n^k = 1 | \mu, \Sigma) &= p(z_n^k = 1 | \boldsymbol{\pi}) p(x_n | z_n^k = 1, \mu, \Sigma) = \pi_k N(x_n | \mu_k, \Sigma_k) \\ p(x_n, z_n | \mu, \Sigma) &= \prod_k [\pi_k N(x_n | \mu_k, \Sigma_k)]^{z_n^k} \end{aligned}$$

**But this is itself a random variable! Not good as objective function**

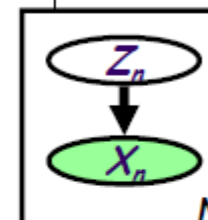


# How is EM derived?



- The complete log likelihood:

$$\begin{aligned}
 \ell(\theta; D) &= \log \prod_n p(z_n, x_n) = \log \prod_n p(z_n | \pi) p(x_n | z_n, \mu, \sigma) \\
 &= \sum_n \log \prod_k \pi_k^{z_n^k} + \sum_n \log \prod_k N(x_n; \mu_k, \sigma) \\
 &= \sum_n \sum_k z_n^k \log \pi_k - \sum_n \sum_k z_n^k \frac{1}{2\sigma^2} (x_n - \mu_k)^2 + C
 \end{aligned}$$



- The expected complete log likelihood

$$\begin{aligned}
 \langle \ell_c(\theta; \mathbf{x}, \mathbf{z}) \rangle &= \sum_n \langle \log p(\mathbf{z}_n | \pi) \rangle_{p(\mathbf{z}|\mathbf{x})} + \sum_n \langle \log p(x_n | \mathbf{z}_n, \mu, \Sigma) \rangle_{p(\mathbf{z}|\mathbf{x})} \\
 &= \sum_n \sum_k \langle z_n^k \rangle \log \pi_k - \frac{1}{2} \sum_n \sum_k \langle z_n^k \rangle ((x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) + \log |\Sigma_k| + C)
 \end{aligned}$$

# E-step



- We maximize  $\langle l_c(\theta) \rangle$  iteratively using the following iterative procedure:

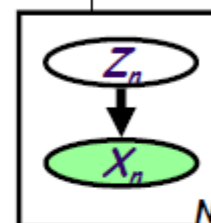


- **Expectation step**: computing the expected value of the sufficient statistics of the hidden variables (i.e.,  $z$ ) given current est. of the parameters (i.e.,  $\pi$  and  $\mu$ ).

$$\tau_n^{k(t)} = \langle z_n^k \rangle_{q^{(t)}} = p(z_n^k = 1 | \mathcal{X}, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} \mathcal{N}(x_n, | \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} \mathcal{N}(x_n, | \mu_i^{(t)}, \Sigma_i^{(t)})}$$

- Here we are essentially doing **inference**

# M-step



- We maximize  $\langle l_c(\theta) \rangle$  iteratively using the following iterative procedure:

- **Maximization step:** compute the parameters under current results of the expected value of the hidden variables

$$\pi_k^* = \arg \max \langle l_c(\theta) \rangle, \quad \Rightarrow \frac{\partial}{\partial \pi_k} \langle l_c(\theta) \rangle = 0, \forall k, \quad \text{s.t. } \sum_k \pi_k = 1$$

$$\Rightarrow \pi_k^* = \frac{\sum_n \langle z_n^k \rangle_{q^{(t)}}}{N} = \frac{\sum_n \tau_n^{k(t)}}{N} = \langle n_k \rangle / N$$

$$\mu_k^* = \arg \max \langle l(\theta) \rangle, \quad \Rightarrow \mu_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} X_n}{\sum_n \tau_n^{k(t)}}$$

$$\Sigma_k^* = \arg \max \langle l(\theta) \rangle, \quad \Rightarrow \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (X_n - \mu_k^{(t+1)})(X_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

Fact:

$$\frac{\partial \log |A^{-1}|}{\partial A^{-1}} = A^T$$

$$\frac{\partial x^T A x}{\partial A} = x x^T$$

- This is isomorphic to **MLE** except that the variables that are hidden are replaced by their expectations (in general they will be replaced by their corresponding "**sufficient statistics**")

# Example 3 HMM

- **Observation space**

Alphabetic set:

$$C = \{c_1, c_2, \dots, c_K\}$$

Euclidean space:

$$\mathbb{R}^d$$

- **Index set of hidden states**

$$I = \{1, 2, \dots, M\}$$

- **Transition probabilities between any two states**

$$p(y_t^j = 1 | y_{t-1}^i = 1) = a_{i,j},$$

or  $p(y_t | y_{t-1}^i = 1) \sim \text{Multinomial}(a_{i,1}, a_{i,2}, \dots, a_{i,M}), \forall i \in I.$

- **Start probabilities**

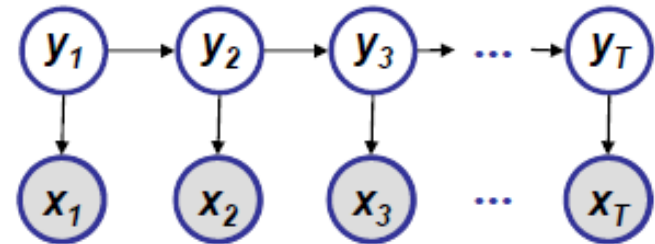
$$p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \dots, \pi_M).$$

- **Emission probabilities associated with each state**

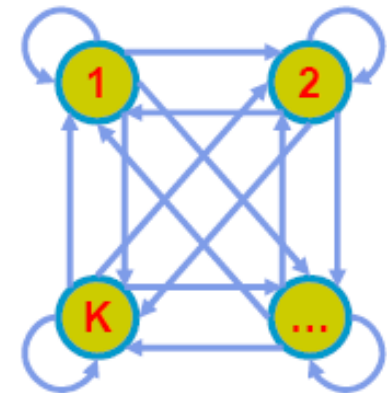
$$p(x_t | y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,2}, \dots, b_{i,K}), \forall i \in I.$$

or in general:

$$p(x_t | y_t^i = 1) \sim f(\cdot | \theta_i), \forall i \in I.$$



Graphical model



State automata



# The Baum Welch algorithm

- The complete log likelihood

$$\ell_c(\theta; \mathbf{x}, \mathbf{y}) = \log p(\mathbf{x}, \mathbf{y}) = \log \prod_n \left( p(y_{n,1}) \prod_{t=2}^T p(y_{n,t} | y_{n,t-1}) \prod_{t=1}^T p(x_{n,t} | x_{n,t}) \right)$$

- The expected complete log likelihood

$$\langle \ell_c(\theta; \mathbf{x}, \mathbf{y}) \rangle = \sum_n \left( \langle y_{n,1}^i \rangle_{p(y_{n,1} | \mathbf{x}_n)} \log \pi_i \right) + \sum_n \sum_{t=2}^T \left( \langle y_{n,t-1}^i y_{n,t}^j \rangle_{p(y_{n,t-1}, y_{n,t} | \mathbf{x}_n)} \log a_{i,j} \right) + \sum_n \sum_{t=1}^T \left( x_{n,t}^k \langle y_{n,t}^i \rangle_{p(y_{n,t} | \mathbf{x}_n)} \log b_{i,k} \right)$$

- EM

- The E step

$$\gamma_{n,t}^i = \langle y_{n,t}^i \rangle = p(y_{n,t}^i = 1 | \mathbf{x}_n)$$

$$\xi_{n,t}^{i,j} = \langle y_{n,t-1}^i y_{n,t}^j \rangle = p(y_{n,t-1}^i = 1, y_{n,t}^j = 1 | \mathbf{x}_n)$$

- The M step ("symbolically" identical to MLE)

$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N}$$

$$a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^T \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

$$b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^T \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

# EM summary

- Nice method to get to **local optimum solution**
- Guaranteed to converge, never decrease likelihood.
- Some problem may require time consuming inference.

- [1] <http://www.cs.ucsb.edu/~ambuj/Courses/bioinformatics/EM.pdf>
- [2] [http://www.seanborman.com/publications/EM\\_algorithm.pdf](http://www.seanborman.com/publications/EM_algorithm.pdf)
- [3] Class lecture notes

