

Machine Learning

10-701/15-781, Fall 2006

Learning Graphical Models

Maximum Likelihood Estimation and
Expectation Maximization

Eric Xing

Lecture 14, October 31, 2006

Reading: Chap. 1&2, C.B book



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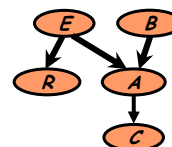
Learning Graphical Models

The goal:

Given set of independent samples (**assignments** of random variables), find the **best** (the most likely?) Bayesian Network (both DAG and CPDs)

E B
 R A
 C

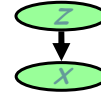
(B,E,A,C,R)=(T,F,F,T,F)
(B,E,A,C,R)=(T,F,T,T,F)
.....
(B,E,A,C,R)=(F,T,T,T,F)



E	B	$P(A E, B)$	
e	b	0.9	0.1
e	\bar{b}	0.2	0.8
\bar{e}	b	0.9	0.1
\bar{e}	\bar{b}	0.01	0.99

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Learning completely observed GMs

- The data:

$$\{(z^{(1)}, x^{(1)}), (z^{(2)}, x^{(2)}), (z^{(3)}, x^{(3)}), \dots, (z^{(N)}, x^{(N)})\}$$

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Review: the basic idea underlying MLE

- The completely observed model:

- Z is a class indicator vector

$$Z = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_M \end{bmatrix}, \quad \text{where } Z_m \in [0,1], \text{ and } \sum_m Z_m = 1$$

and a datum is in class i w.p. π_i

$$p(z_i = 1 | \pi) = \pi_i = \pi_1^{z_1} \times \pi_2^{z_2} \times \dots \times \pi_M^{z_M}$$

$$p(z) = \prod_m \pi_m^{z_m}$$

All except one of these terms will be one

- X is a conditional Gaussian variable with a class-specific mean

$$p(x | z_m = 1, \mu, \sigma) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x - \mu_m)^2\right\}$$

$$p(x | z, \mu, \sigma) = \prod_m N(x | \mu_m, \sigma)^{z_m}$$

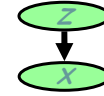
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Review: the basic idea underlying MLE

- Data log-likelihood

$$\begin{aligned}
 l(\theta | D) &= \log \prod_n p(z^{(n)}, x^{(n)}) = \log \prod_n p(z^{(n)} | \pi) p(x^{(n)} | z^{(n)}, \mu, \sigma) \\
 &= \sum_n \log p(z^{(n)} | \pi) + \sum_n \log p(x^{(n)} | z^{(n)}, \mu, \sigma) \\
 &= \sum_n \log \prod_m \pi_m^{z_m^{(n)}} + \sum_n \log \prod_m N(x^{(n)} | \mu_m, \sigma^2)^{z_m^{(n)}} \\
 &= \sum_n \sum_m z_m^{(n)} \log \pi_m - \sum_n \sum_m z_m^{(n)} \frac{1}{2\sigma^2} (x^{(n)} - \mu_m)^2 + C
 \end{aligned}$$



- MLE

$$\pi_m^* = \arg \max l(\theta | D), \quad \Rightarrow \frac{\partial}{\partial \pi_m} l(\theta | D) = 0, \forall m, \quad \text{s.t. } \sum_m \pi_m = 1$$

$$\Rightarrow \pi_m^* = \frac{\sum_n z_m^{(n)}}{N} = \frac{n_m}{N} \quad \text{the fraction of samples of class } m$$

$$\mu_m^* = \arg \max l(\theta | D), \quad \Rightarrow \mu_m^* = \frac{\sum_n z_m^{(n)} x^{(n)}}{\sum_n z_m^{(n)}} = \frac{\sum_n z_m^{(n)} x^{(n)}}{n_m} \quad \text{the average of samples of class } m$$

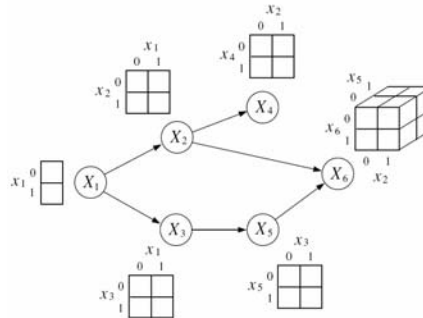
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MLE for general BNs

- If we assume the parameters for each CPD are globally independent, and all nodes are fully observed, then the log-likelihood function decomposes into a sum of local terms, one per node:

$$\mathcal{L}(\theta; D) = \log p(D | \theta) = \log \prod_n \left(\prod_i p(x_{n,i} | \mathbf{x}_{n,\pi_i}, \theta_i) \right) = \sum_i \left(\sum_n \log p(x_{n,i} | \mathbf{x}_{n,\pi_i}, \theta_i) \right)$$



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MLE for BNs with tabular CPDs

- Assume each CPD is represented as a table (multinomial) where

$$\theta_{ijk} \stackrel{\text{def}}{=} p(X_i = j \mid X_{\pi_i} = k)$$

- Note that in case of multiple parents, X_{π_i} will have a composite state, a CPD will be a high-dimensional table
- The sufficient statistics are counts of family configurations



$$n_{ijk} \stackrel{\text{def}}{=} \sum_n x_{n,i}^j x_{n,\pi_i}^k$$

- The log-likelihood is

$$\ell(\theta; \mathcal{D}) = \log \prod_{i,j,k} \theta_{ijk}^{n_{ijk}} = \sum_{i,j,k} n_{ijk} \log \theta_{ijk}$$

- Using a Lagrange multiplier to enforce so $\sum_j \theta_{ijk} = 1$ we get

$$\theta_{ijk}^{ML} = \frac{n_{ijk}}{\sum_{j'} n_{ij'k}}$$

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Partially observed GMs

- Speech recognition

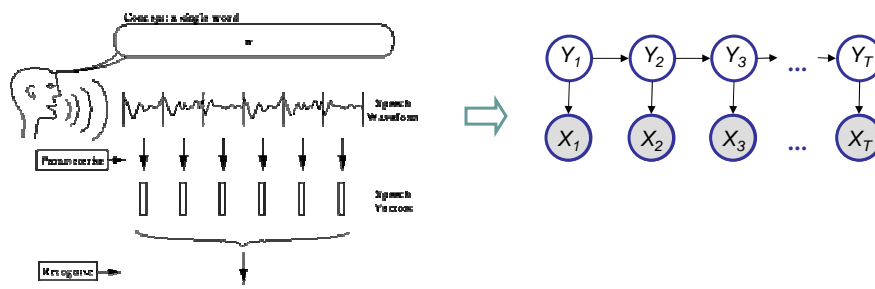


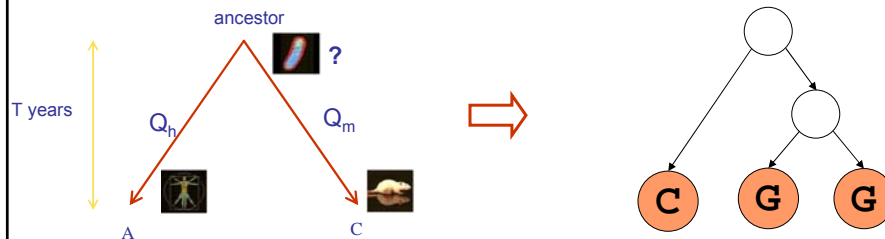
Fig. 1.2 Isolated Word Problem

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Partially observed GM

- Biological Evolution



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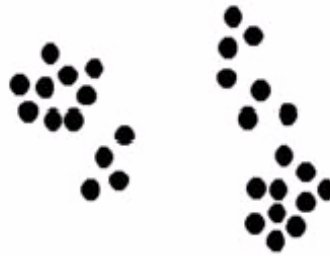
Unobserved Variables

- A variable can be unobserved (latent) because:
 - it is an imaginary quantity meant to provide some simplified and abstractive view of the data generation process
 - e.g., speech recognition models, mixture models ...
 - it is a real-world object and/or phenomena, but difficult or impossible to measure
 - e.g., the temperature of a star, causes of a disease, evolutionary ancestors ...
 - it is a real-world object and/or phenomena, but sometimes wasn't measured, because of faulty sensors; or was measure with a noisy channel, etc.
 - e.g., traffic radio, aircraft signal on a radar screen,
- Discrete latent variables can be used to partition/cluster data into sub-groups (mixture models, forthcoming).
- Continuous latent variables (factors) can be used for dimensionality reduction (factor analysis, etc., later lectures).

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Mixture Models



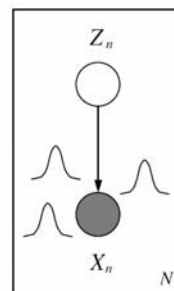
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Mixture Models, con'd



- A density model $p(x)$ may be multi-modal.
- We may be able to model it as a mixture of uni-modal distributions (e.g., Gaussians).
- Each mode may correspond to a different sub-population (e.g., male and female).



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Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

- Z is a latent class indicator vector:

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

- 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:

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

mixture proportion mixture component

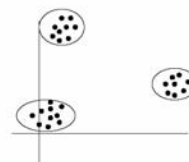
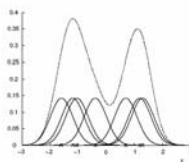
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Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

$$p(x_n | \mu, \Sigma) = \sum_k \pi_k \mathcal{N}(x, | \mu_k, \Sigma_k)$$



- This model can be used for unsupervised clustering.

- This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

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Why is Learning Harder?

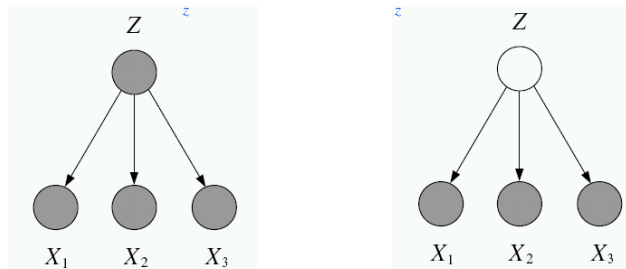


- In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models).

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

- With latent variables, all the parameters become coupled together via marginalization

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



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Toward the EM algorithm



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

- Z is a latent class indicator vector

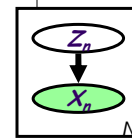
$$p(z_n) = \text{multi}(z_n : \pi) = \sum_k (\pi_k)^{z_n^k}$$

- 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:

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



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Toward the EM algorithm

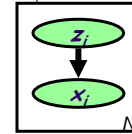


- Recall MLE for completely observed data
- Data log-likelihood

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

- MLE

$$\begin{aligned}\hat{\pi}_{k,MLE} &= \arg \max_{\pi} \mathcal{L}(\theta; D), \\ \hat{\mu}_{k,MLE} &= \arg \max_{\mu} \mathcal{L}(\theta; D) \\ \hat{\sigma}_{k,MLE} &= \arg \max_{\sigma} \mathcal{L}(\theta; D)\end{aligned} \quad \Rightarrow \quad \hat{\mu}_{k,MLE} = \frac{\sum_n z_n^k x_n}{\sum_n z_n^k}$$
- What if we do not know z_n ?



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Expectation-Maximization (EM) Algorithm



- EM is an optimization strategy for objective functions that can be interpreted as likelihoods in the presence of missing data.
- It is much simpler than gradient methods:
 - No need to choose step size.
 - Enforces constraints automatically.
 - Calls inference and fully observed learning as subroutines.
- EM is an Iterative algorithm with two linked steps:
 - E-step: fill-in hidden values using inference, $p(z|x, \theta)$.
 - M-step: update parameters $t+1$ 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.

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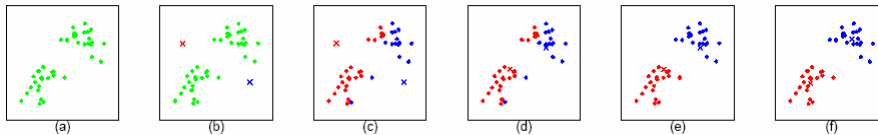
K-means

- Start:
 - "Guess" the centroid μ_k and covariance Σ_k of each of the K clusters
- Loop
 - For each point $n=1$ to N ,
compute its cluster label:

$$z_n^{(t)} = \arg \max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

- For each cluster $k=1:K$

$$\mu_k^{(t+1)} = \frac{\sum_n \delta(z_n^{(t)}, k) x_n}{\sum_n \delta(z_n^{(t)}, k)} \quad \Sigma_k^{(t+1)} = \dots$$

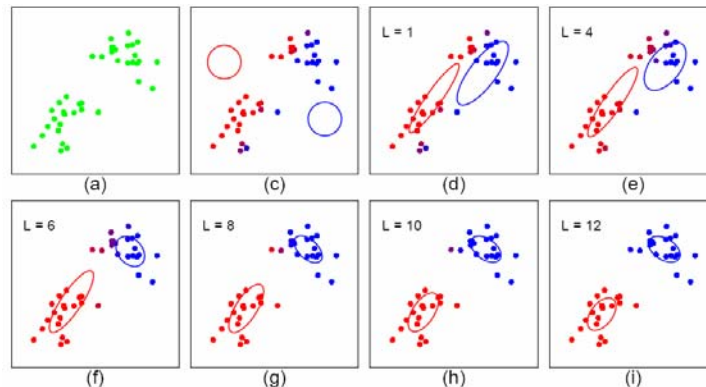


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Expectation-Maximization

- Start:
 - "Guess" the centroid μ_k and covariance Σ_k of each of the K clusters
- Loop



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Example: Gaussian mixture model



- A mixture of K Gaussians:

- Z is a latent class indicator vector
- $$p(z_n) = \text{multi}(z_n : \pi) = \sum_k (\pi_k)^{z_n^k}$$

- 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:

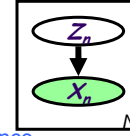
$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z_n^k = 1 | \pi) p(x_n | z_n^k = 1, \mu, \Sigma) \\ &= \sum_k \pi_k \prod_k (\pi_k)^{z_n^k} \mathcal{N}(x_n : \mu_k, \Sigma_k)^{z_n^k} = \sum_k \pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k) \end{aligned}$$

- The expected complete log likelihood

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

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E-step

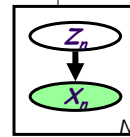


- We maximize $\langle \ell_c(\theta) \rangle$ iteratively using the following iterative procedure:

- **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., π and μ).

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

- Here we are essentially doing **inference**



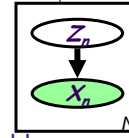
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M-step

- 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



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

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

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

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

Fact:

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

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

- 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**")

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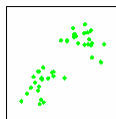
Compare: K-means

- The EM algorithm for mixtures of Gaussians is like a "soft version" of the K-means algorithm.
- In the K-means "E-step" we do hard assignment:

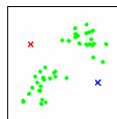
$$z_n^{(t)} = \arg \max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

- In the K-means "M-step" we update the means as the weighted sum of the data, but now the weights are 0 or 1:

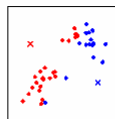
$$\mu_k^{(t+1)} = \frac{\sum_n \delta(z_n^{(t)}, k) x_n}{\sum_n \delta(z_n^{(t)}, k)}$$



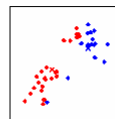
(a)



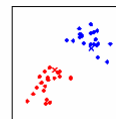
(b)



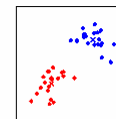
(c)



(d)



(e)



(f)

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EM for general BNs



```

while not converged
  % E-step
  for each node  $i$ 
     $ESS_i = 0$       % reset expected sufficient statistics
  for each data sample  $n$ 
    do inference with  $X_{n,H}$ 
    for each node  $i$ 
       $ESS_i += \langle SS_i(x_{n,i}, x_{n,\pi_i}) \rangle_{p(x_{n,H} | x_{n,-H})}$ 
  % M-step
  for each node  $i$ 
     $\theta_i := \text{MLE}(ESS_i)$ 
  
```

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Partially Hidden Data



- Of course, we can learn when there are missing (hidden) variables on some cases and not on others.
- In this case the cost function is:

$$\ell_c(\theta; D) = \sum_{n \in \text{Complete}} \log p(x_n, y_n | \theta) + \sum_{m \in \text{Missing}} \log \sum_{y_m} p(x_m, y_m | \theta)$$

- Note that y_m do not have to be the same in each case --- the data can have different missing values in each different sample
- Now you can think of this in a new way: in the E-step we estimate the hidden variables on the incomplete cases only.
- The M-step optimizes the log likelihood on the complete data plus the expected likelihood on the incomplete data using the E-step.

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Optional Material!

-- Theory underlying EM

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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

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

is difficult!

- What shall we do?

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Complete & Incomplete Log Likelihoods



- Complete log likelihood

Let \mathcal{X} denote the observable variable(s), and \mathcal{Z} denote the latent variable(s).

If \mathcal{Z} could be observed, then

$$\ell_c(\theta; \mathcal{X}, \mathcal{Z}) \stackrel{\text{def}}{=} \log p(\mathcal{X}, \mathcal{Z} | \theta)$$

- Usually, optimizing $\ell_c()$ given both \mathcal{Z} and \mathcal{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 \mathcal{Z} is not observed, $\ell_c()$ is a random quantity, cannot be maximized directly.**

- Incomplete log likelihood

With \mathcal{Z} unobserved, our objective becomes the log of a marginal probability:

$$\ell_c(\theta; \mathcal{X}) = \log p(\mathcal{X} | \theta) = \log \sum_{\mathcal{Z}} p(\mathcal{X}, \mathcal{Z} | \theta)$$

- This objective won't decouple**

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Expected Complete Log Likelihood



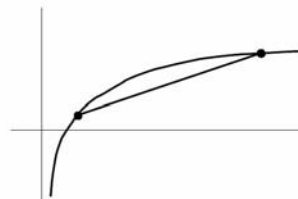
- For **any** distribution $q(\mathcal{Z})$, define **expected complete log likelihood**:

$$\langle \ell_c(\theta; \mathcal{X}, \mathcal{Z}) \rangle_q \stackrel{\text{def}}{=} \sum_{\mathcal{Z}} q(\mathcal{Z} | \mathcal{X}, \theta) \log p(\mathcal{X}, \mathcal{Z} | \theta)$$

- A deterministic function of θ
- Linear in $\ell_c()$ --- inherit its factorizability
- Does maximizing this surrogate yield a maximizer of the likelihood?

- Jensen's inequality

$$\begin{aligned} \ell(\theta; \mathcal{X}) &= \log p(\mathcal{X} | \theta) \\ &= \log \sum_{\mathcal{Z}} p(\mathcal{X}, \mathcal{Z} | \theta) \\ &= \log \sum_{\mathcal{Z}} q(\mathcal{Z} | \mathcal{X}) \frac{p(\mathcal{X}, \mathcal{Z} | \theta)}{q(\mathcal{Z} | \mathcal{X})} \\ &\geq \sum_{\mathcal{Z}} q(\mathcal{Z} | \mathcal{X}) \log \frac{p(\mathcal{X}, \mathcal{Z} | \theta)}{q(\mathcal{Z} | \mathcal{X})} \Rightarrow \ell(\theta; \mathcal{X}) \geq \langle \ell_c(\theta; \mathcal{X}, \mathcal{Z}) \rangle_q + H_q \end{aligned}$$



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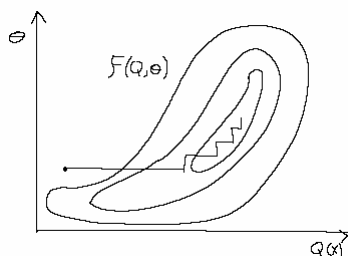
Lower Bounds and Free Energy

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

$$F(q, \theta) \stackrel{\text{def}}{=} \sum_z q(z | x) \log \frac{p(x, z | \theta)}{q(z | x)} \leq \ell(\theta; x)$$

- The EM algorithm is coordinate-ascent on F :

- E-step:** $q^{t+1} = \arg \max_q F(q, \theta^t)$
- M-step:** $\theta^{t+1} = \arg \max_{\theta} F(q^{t+1}, \theta)$



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

- Claim: $q^{t+1} = \arg \max_q F(q, \theta^t) = p(z | x, \theta^t)$
 - 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 classification).

- Proof (easy): this setting attains the bound $\ell(\theta, x) \geq F(q, \theta)$

$$\begin{aligned} F(p(z | x, \theta^t), \theta^t) &= \sum_z p(z | x, \theta^t) \log \frac{p(x, z | \theta^t)}{p(z | x, \theta^t)} \\ &= \sum_z q(z | x) \log p(x | \theta^t) \\ &= \log p(x | \theta^t) = \ell(\theta^t; x) \end{aligned}$$

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

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

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E-step \equiv plug in posterior expectation of latent variables



- Without loss of generality: assume that $p(\mathbf{x}, \mathbf{z} | \theta)$ is a generalized exponential family distribution:

$$p(\mathbf{x}, \mathbf{z} | \theta) = \frac{1}{Z(\theta)} h(\mathbf{x}, \mathbf{z}) \exp \left\{ \sum_i \theta_i f_i(\mathbf{x}, \mathbf{z}) \right\}$$

- Special cases: if $p(\mathbf{x} | \mathbf{z})$ are GLIMs, then $f_i(\mathbf{x}, \mathbf{z}) = \eta_i^T(\mathbf{z}) \xi_i(\mathbf{x})$

- The expected complete log likelihood under $q^{t+1} = p(\mathbf{z} | \mathbf{x}, \theta^t)$ is

$$\begin{aligned} \langle \ell_c(\theta^t; \mathbf{x}, \mathbf{z}) \rangle_{q^{t+1}} &= \sum_{\mathbf{z}} q(\mathbf{z} | \mathbf{x}, \theta^t) \log p(\mathbf{x}, \mathbf{z} | \theta^t) - A(\theta) \\ &= \sum_i \theta_i^t \langle f_i(\mathbf{x}, \mathbf{z}) \rangle_{q(\mathbf{z} | \mathbf{x}, \theta^t)} - A(\theta) \\ &\stackrel{p\text{-GLIM}}{=} \sum_i \theta_i^t \langle \eta_i(\mathbf{z}) \rangle_{q(\mathbf{z} | \mathbf{x}, \theta^t)} \xi_i(\mathbf{x}) - A(\theta) \end{aligned}$$

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M-step: maximization of expected ℓ_c w.r.t. θ



- Note that the free energy breaks into two terms:

$$\begin{aligned} F(q, \theta) &= \sum_{\mathbf{z}} q(\mathbf{z} | \mathbf{x}) \log \frac{p(\mathbf{x}, \mathbf{z} | \theta)}{q(\mathbf{z} | \mathbf{x})} \\ &= \sum_{\mathbf{z}} q(\mathbf{z} | \mathbf{x}) \log p(\mathbf{x}, \mathbf{z} | \theta) - \sum_{\mathbf{z}} q(\mathbf{z} | \mathbf{x}) \log q(\mathbf{z} | \mathbf{x}) \\ &= \langle \ell_c(\theta; \mathbf{x}, \mathbf{z}) \rangle_q + H_q \end{aligned}$$

- The first term is the expected complete log likelihood (energy) and the second term, which does not depend on θ , is the entropy.
- Thus, in the M-step, maximizing with respect to θ for fixed q we only need to consider the first term:

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

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

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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: $\theta^{t+1} = \arg \max_{\theta} F(q^{t+1}, \theta)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

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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
- Some bad things about EM:
 - can get stuck in local minima
 - can be slower than conjugate gradient (especially near convergence)
 - requires expensive inference step
 - is a maximum likelihood/MAP method

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