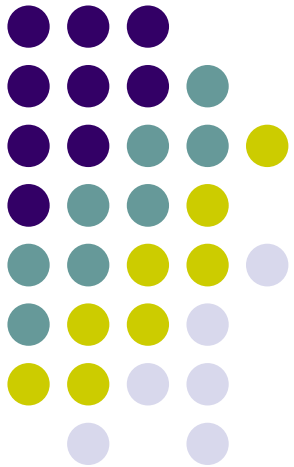
School of Computer Science
Carnegie Mellon

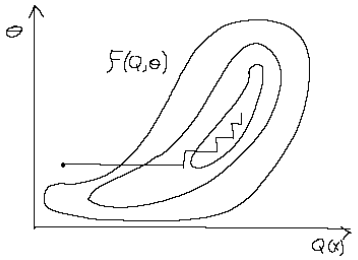
Probabilistic Graphical Models

Learning Partially Observed GM: the Expectation-Maximization algorithm



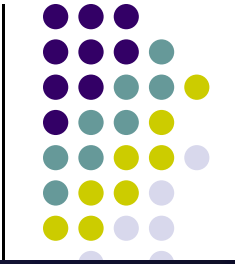
Eric Xing

Lecture 8, February 8, 2016



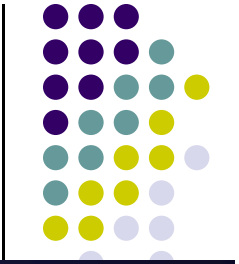
Reading: MJ Chap 9, and 11

Recall:
Learning Graphical Models



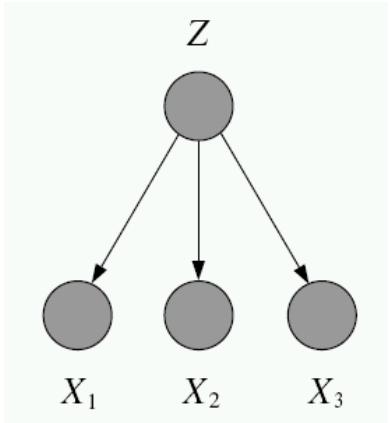
- Scenarios:
  - completely observed GMs
    - directed
    - undirected
  - partially or unobserved GMs
    - directed
    - undirected (an open research topic)
- Estimation principles:
  - Maximal likelihood estimation (MLE)
  - Bayesian estimation
  - Maximal conditional likelihood
  - Maximal "Margin"
  - Maximum entropy
- We use **learning** as a name for the process of estimating the parameters, and in some cases, the topology of the network, from data.

Inference is also a subroutine for Learning

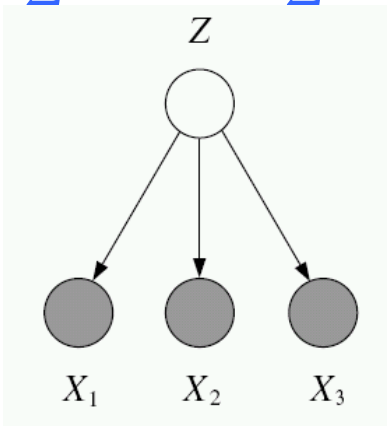


- Directed, but partially observed GM:

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



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

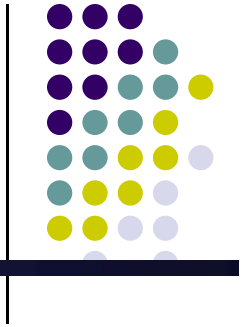


- Undirected, but fully observed GM:

$$\ell = \sum_c \sum_{\mathbf{x}_c} m(\mathbf{x}_c) \log \psi_c(\mathbf{x}_c) - N \log Z$$

$$\begin{aligned}
\frac{\partial \log Z}{\partial \psi_c(\mathbf{x}_c)} &= \frac{1}{Z} \frac{\partial}{\partial \psi_c(\mathbf{x}_c)} \left(\sum_{\tilde{\mathbf{x}}} \prod_d \psi_d(\tilde{\mathbf{x}}_d) \right) \\
&= \frac{1}{Z} \sum_{\tilde{\mathbf{x}}} \delta(\tilde{\mathbf{x}}_c, \mathbf{x}_c) \frac{\partial}{\partial \psi_c(\mathbf{x}_c)} \left(\prod_d \psi_d(\tilde{\mathbf{x}}_d) \right) \\
&= \sum_{\tilde{\mathbf{x}}} \delta(\tilde{\mathbf{x}}_c, \mathbf{x}_c) \frac{1}{\psi_c(\tilde{\mathbf{x}}_c)} \frac{1}{Z} \prod_d \psi_d(\tilde{\mathbf{x}}_d) \\
&= \frac{1}{\psi_c(\mathbf{x}_c)} \sum_{\tilde{\mathbf{x}}} \delta(\tilde{\mathbf{x}}_c, \mathbf{x}_c) p(\tilde{\mathbf{x}}) = \frac{p(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)}
\end{aligned}$$

Recall: Approaches to inference



- Exact inference algorithms
  - The elimination algorithm
  - Message-passing algorithm (sum-product, belief propagation)
  - The junction tree algorithms
- Approximate inference techniques
  - Stochastic simulation / sampling methods
  - Markov chain Monte Carlo methods
  - Variational algorithms

Partially observed GMs

- Speech recognition

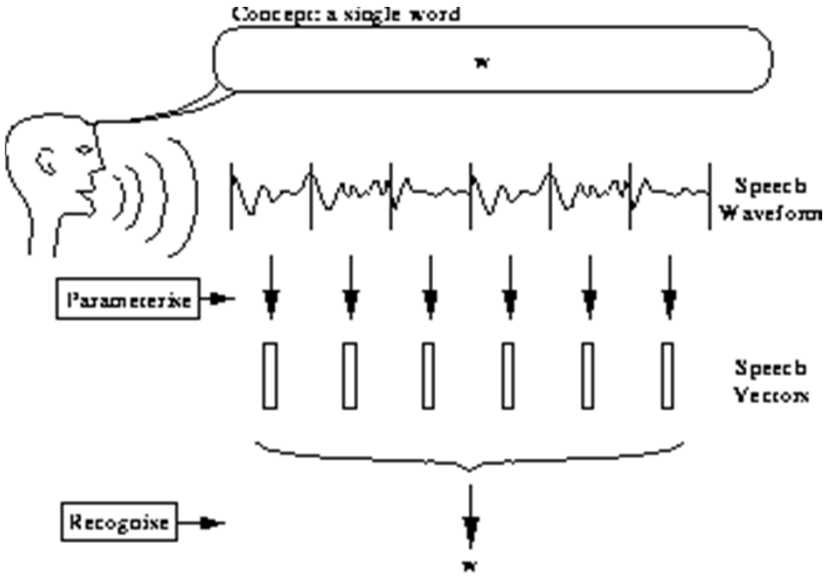
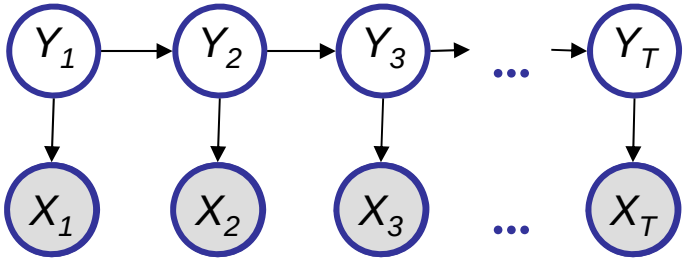
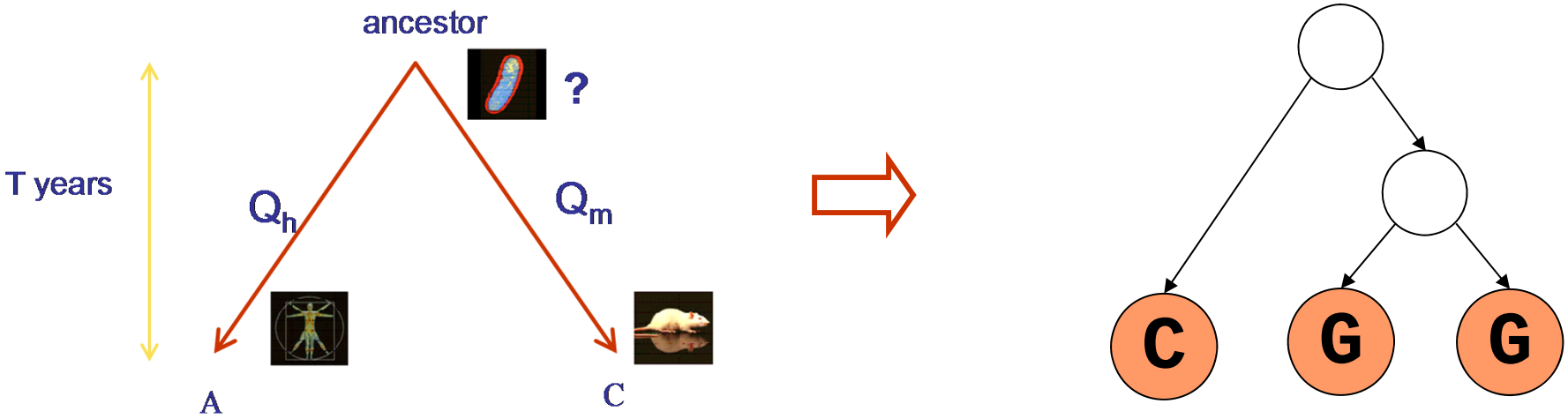


Fig. 1.2 Isolated Word Problem

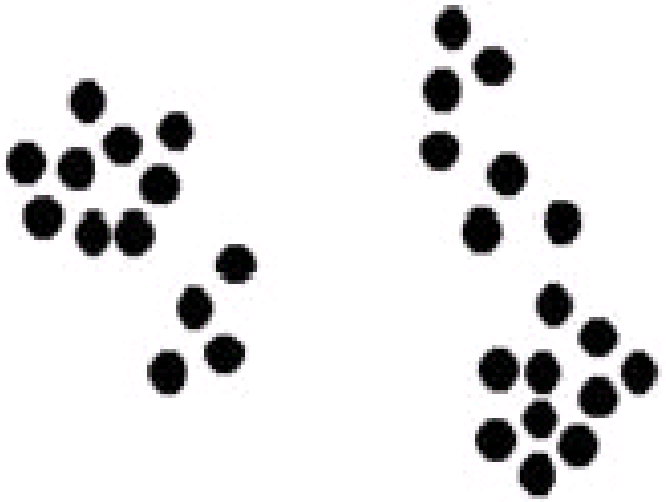


Partially observed GM

- Biological Evolution

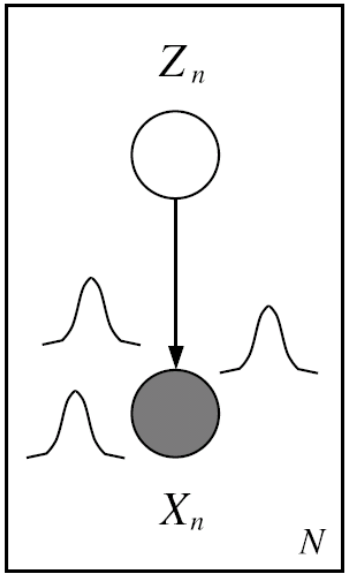


Mixture Models

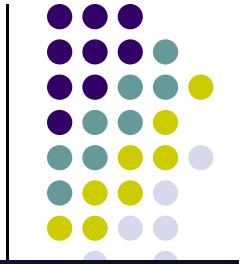


Mixture Models, con'd

- 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).

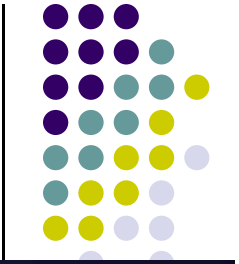


Unobserved Variables



- 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, etc.
- Discrete latent variables can be used to partition/cluster data into sub-groups.
- Continuous latent variables (factors) can be used for dimensionality reduction (factor analysis, etc).

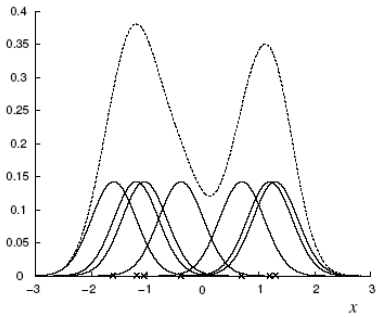
Gaussian Mixture Models (GMMs)

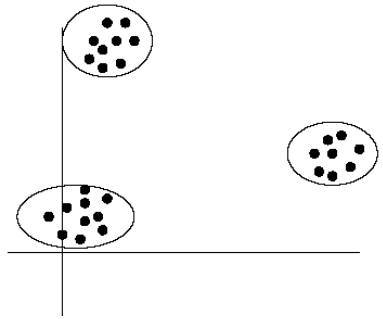


- Consider a mixture of *K* Gaussian components:

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

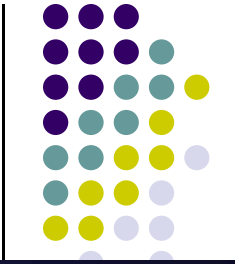
mixture proportion mixture component





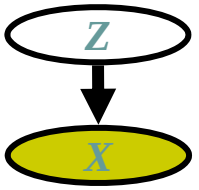
- This model can be used for unsupervised clustering.
  - This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

Gaussian Mixture Models (GMMs)



- Consider a mixture of *K* Gaussian components:
  - *Z* is a latent class indicator vector:

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



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

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

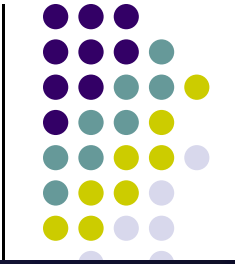
  - The likelihood of a sample:

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

mixture component

mixture proportion

Why is Learning Harder?

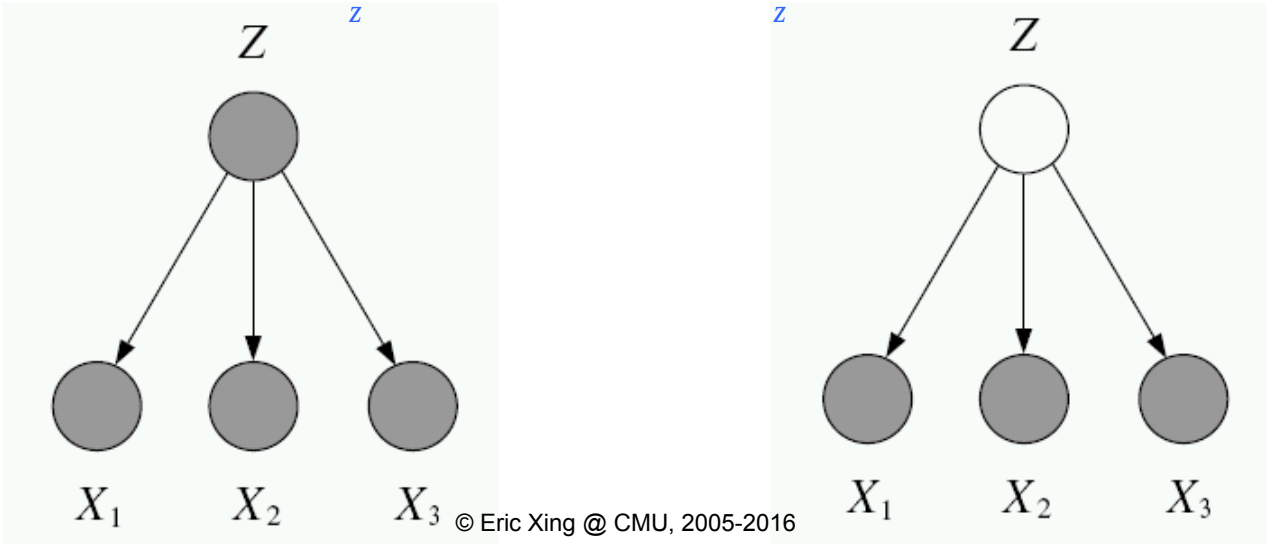


- In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models).

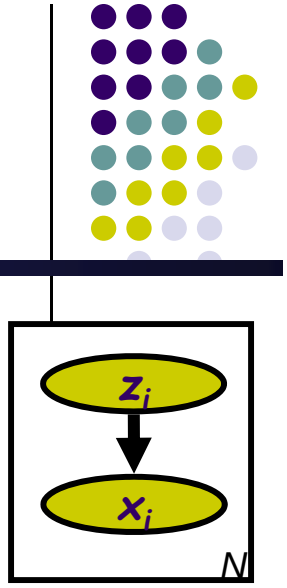
$$\ell_c(\theta; D) = \log p(x, z \mid \theta) = \log p(z \mid \theta_z) + \log p(x \mid z, \theta_x)$$

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

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



Toward the EM algorithm



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

$$\ell(\boldsymbol{\theta}; D) = \log \prod_n p(z_n, x_n) = \log \prod_n p(z_n \mid \pi) p(x_n \mid z_n, \mu, \sigma)$$

$$= \sum_n \log \prod_k \pi_k^{z_n^k} + \sum_n \log \prod_k N(x_n; \mu_k, \sigma)^{z_n^k}$$

$$= \sum_n \sum_k z_n^k \log \pi_k - \sum_n \sum_k z_n^k \frac{1}{2\sigma^2}(x_n - \mu_k)^2 + C$$

- MLE

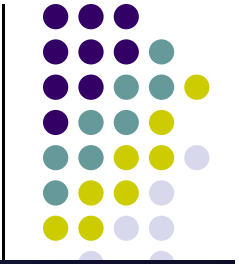
$$\hat{\pi}_{k,MLE} = \arg\max_\pi \ell(\boldsymbol{\theta}; D),$$

$$\hat{\mu}_{k,MLE} = \arg\max_\mu \ell(\boldsymbol{\theta}; D) \quad \Rightarrow \quad \hat{\mu}_{k,MLE} = \frac{\sum_n z_n^k x_n}{\sum_n z_n^k}$$

$$\hat{\sigma}_{k,MLE} = \arg\max_\sigma \ell(\boldsymbol{\theta}; D)$$

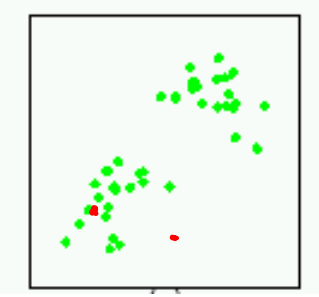
- What if we do not know z_n?

Question



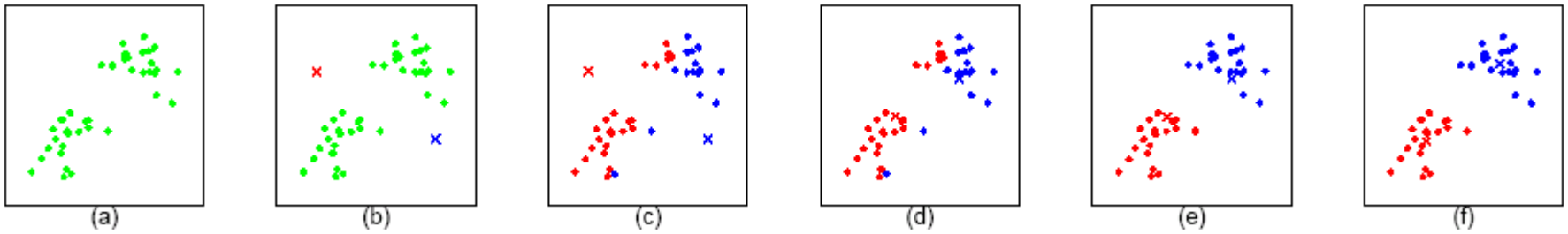
- " … We solve problem X using Expectation-Maximization …"
  - What does it mean?
- E
  - What do we take expectation with?
  - What do we take expectation over?
- M
  - What do we maximize?
  - What do we maximize with respect to?

Recall: K-means

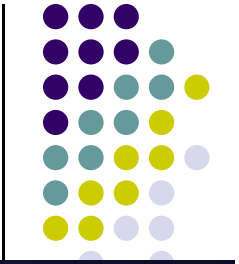


$$z_n^{(t)} = \arg\max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

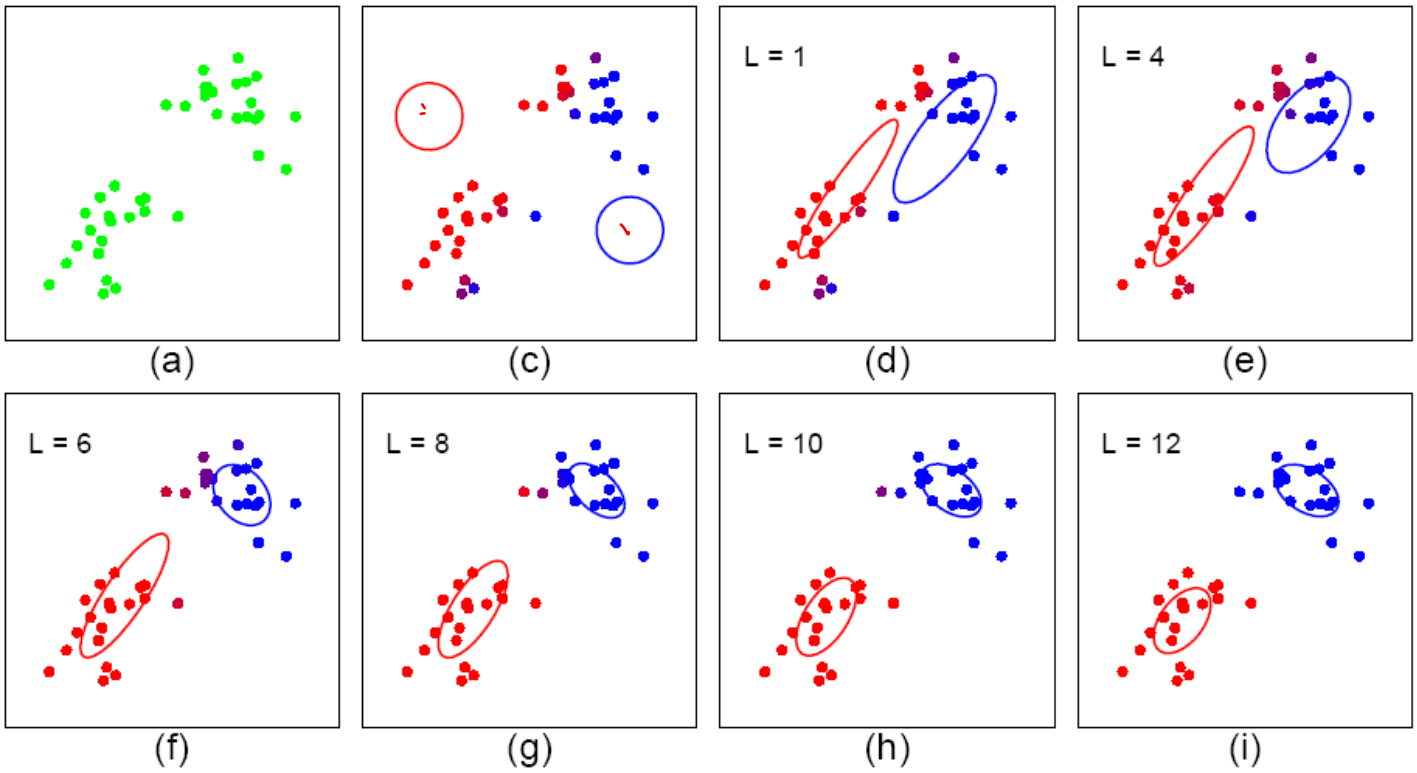
$$\mu_k^{(t+1)} = \frac{\sum_n \delta(z_n^{(t)}, k) x_n}{\sum_n \delta(z_n^{(t)}, k)}$$



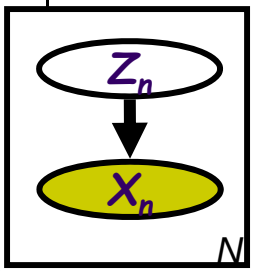
Expectation-Maximization



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



Example: Gaussian mixture model



- 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 class-specific mean/covariance

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

  - The likelihood of a sample:

$$p(x_n \mid \mu, \Sigma) = \sum_k p(z^k = 1 \mid \pi) p(x, \mid z^k = 1, \mu, \Sigma)$$

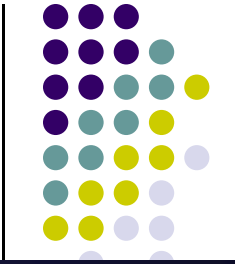
$$= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k}\right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k)$$

- The expected complete log likelihood

$$\left\langle \ell_c(\theta; x, z) \right\rangle = \sum_n \left\langle \log p(z_n \mid \pi) \right\rangle_{p(z|x)} + \sum_n \left\langle \log p(x_n \mid z_n, \mu, \Sigma) \right\rangle_{p(z|x)}$$

$$= \sum_n \sum_k \left\langle z_n^k \right\rangle \log \pi_k - \frac{1}{2} \sum_n \sum_k \left\langle z_n^k \right\rangle \left((x_n - \mu_k)^T \Sigma_k^{-1}(x_n - \mu_k) + \log|\Sigma_k| + C\right)$$

E-step



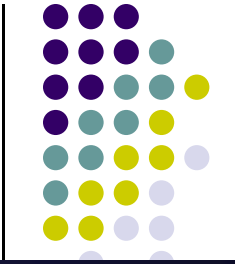
- We maximize $\langle l_c(\theta) \rangle$ iteratively using the following iterative procedure:

  – 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., π and μ).

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

  - Here we are essentially doing **inference**

M-step



- We maximize $\langle l_c(\theta) \rangle$ iteratively using the following iterative procudure:
  - Maximization step: compute the parameters under current results of the expected value of the hidden variables

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

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

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

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

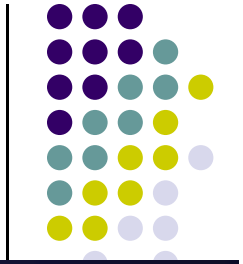
Fact :

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

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

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

Compare: K-means and EM



The EM algorithm for mixtures of Gaussians is like a "soft version" of the K-means algorithm.

- K-means
  - 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:

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

- EM
  - E-step

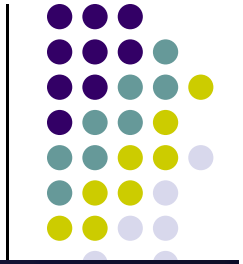
$$\tau_n^{k(t)} = \left\langle z_n^k \right\rangle_{q^{(t)}}$$

$$= p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} N(x_n, \mid \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} N(x_n, \mid \mu_i^{(t)}, \Sigma_i^{(t)})}$$

  - M-step

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

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.

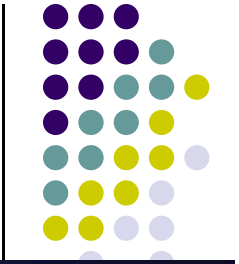
- But we do not observe z, so computing

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

  is difficult!

- What shall we do?

Complete & Incomplete Log Likelihoods



- Complete log likelihood

  Let X denote the observable variable(s), and Z denote the latent variable(s).

  If Z could be observed, then

$$\ell_c(\theta; x, z) \overset{\text{def}}{=} \log p(x, z \mid \theta)$$

  - Usually, optimizing $\ell_c()$ 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, $\ell_c()$ is a random quantity, cannot be maximized directly**.

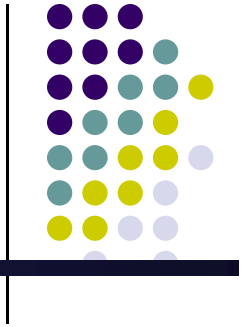
- Incomplete log likelihood

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

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

  - **This objective won't decouple**

Expected Complete Log Likelihood



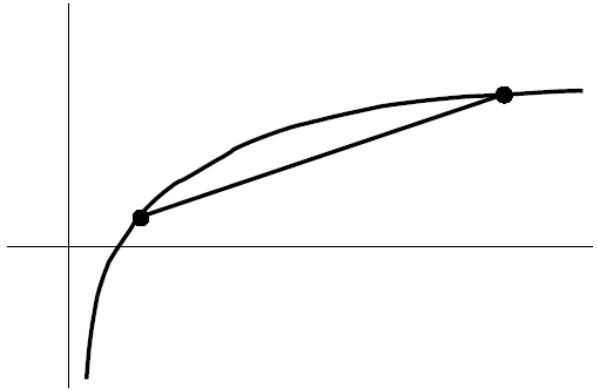
- For ***any*** distribution $q(z)$, define *expected complete log likelihood*:

$$\left\langle \ell_c(\theta; x, z) \right\rangle_q \stackrel{\text{def}}{=} \sum_z q(z \mid x, \theta) \log p(x, z \mid \theta)$$

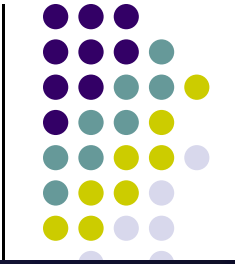
  - A deterministic function of θ
  - Linear in $\ell_c()$ --- inherit its factorizabiility
  - Does maximizing this surrogate yield a maximizer of the likelihood?

- Jensen's inequality

$$\begin{aligned}
\ell(\theta; x) &= \log p(x \mid \theta) \\
&= \log \sum_z p(x, z \mid \theta) \\
&= \log \sum_z q(z \mid x) \frac{p(x, z \mid \theta)}{q(z \mid x)} \\
&\geq \sum_z q(z \mid x) \log \frac{p(x, z \mid \theta)}{q(z \mid x)} \qquad \Rightarrow \quad \ell(\theta; x) \geq \left\langle \ell_c(\theta; x, z) \right\rangle_q + H_q
\end{aligned}$$



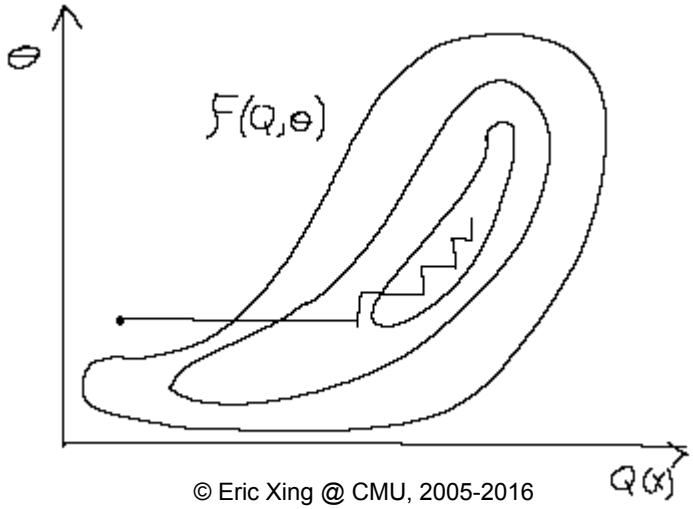
Lower Bounds and Free Energy



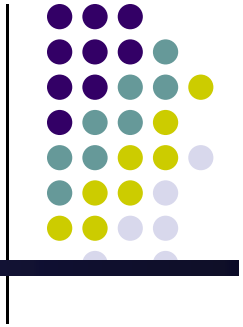
- For fixed data x, define a functional called the free energy:

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

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



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



- Claim:

$$q^{t+1} = \arg\max_q F(q, \theta^t) = p(z \mid x, \theta^t)$$

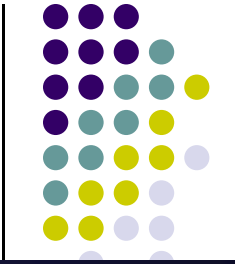
  - This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform classification).

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

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

- Can also show this result using variational calculus or the fact that $\ell(\theta; x) - F(q, \theta) = \mathrm{KL}(q \,\|\, p(z \mid x, \theta))$

E-step ≡ plug in posterior expectation of latent variables



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

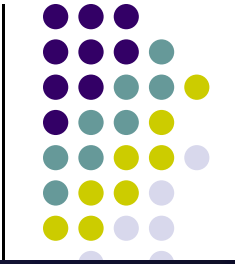
$$p(x,z|\theta) = \frac{1}{Z(\theta)} h(x,z) \exp\left\{\sum_i \theta_i f_i(x,z)\right\}$$

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

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

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

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



- Note that the free energy breaks into two terms:

$$\begin{aligned} F(q,\theta) &= \sum_z q(z \mid x) \log \frac{p(x,z \mid \theta)}{q(z \mid x)} \\ &= \sum_z q(z \mid x) \log p(x,z \mid \theta) - \sum_z q(z \mid x) \log q(z \mid x) \\ &= \left\langle \ell_c(\theta; x, z) \right\rangle_q + H_q \end{aligned}$$

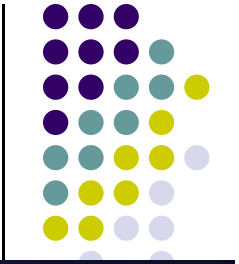
  - The first term is the expected complete log likelihood (energy) and the second term, which does not depend on θ, is the entropy.

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

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

  - 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. $p(z|x,\theta)$.

Example: HMM



- **Supervised learning**: estimation when the "right answer" is known
  - **Examples:**

    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands

    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls

- **Unsupervised learning**: estimation when the "right answer" is unknown
  - **Examples:**

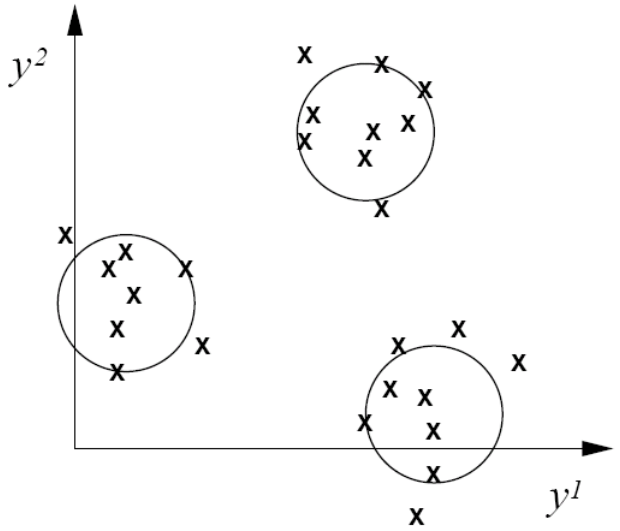
    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition

    GIVEN: 10,000 rolls of the casino player, but we don't see when he changes dice

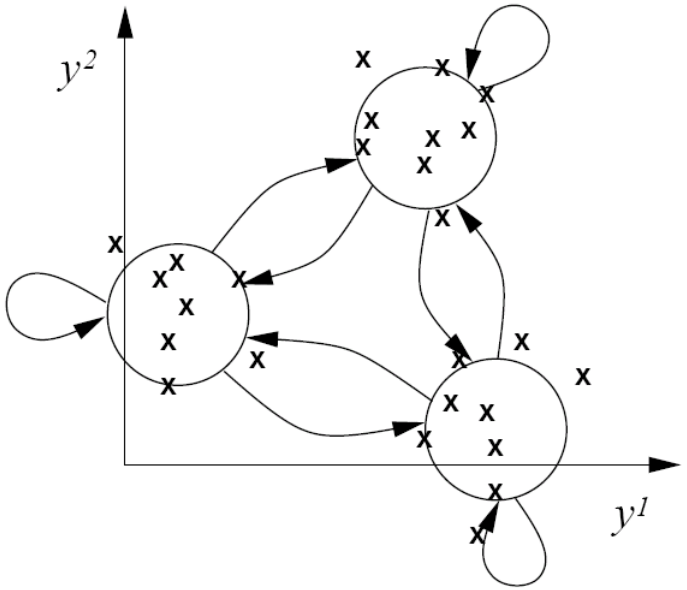
- **QUESTION:** Update the parameters θ of the model to maximize $P(x|\theta)$ --- Maximal likelihood (ML) estimation

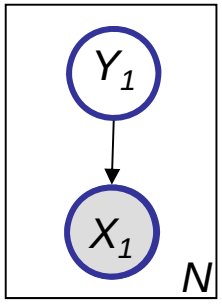
Hidden Markov Model:
from static to dynamic mixture models

Static mixture



Dynamic mixture





The underlying source:

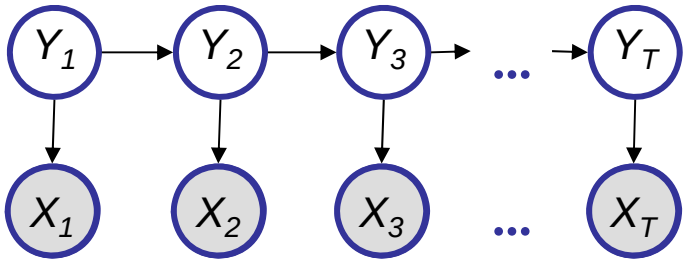
Speech signal,

dice,

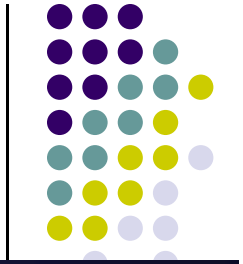
The sequence:

Phonemes,

sequence of rolls,



The Baum Welch algorithm



- The complete log likelihood

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

- The expected complete log likelihood

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

- EM
  - The **E** step

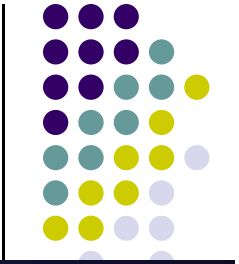
$$\gamma_{n,t}^i = \left\langle y_{n,t}^i \right\rangle = p(y_{n,t}^i = 1 \mid \mathbf{x}_n)$$

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

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

$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N} \qquad a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i} \qquad b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^{T} \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

Unsupervised ML estimation



- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is unknown,

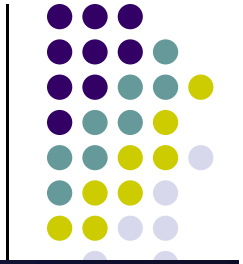
  - **EXPECTATION MAXIMIZATION**

  0. Starting with our best guess of a model M, parameters θ:
  1. Estimate A_{ij} , B_{ik} in the training data
     - How? $A_{ij} = \sum_{n,t} \left\langle y^i_{n,t-1} y^j_{n,t} \right\rangle$, $B_{ik} = \sum_{n,t} \left\langle y^i_{n,t} \right\rangle x^k_{n,t}$,
  2. Update θ according to A_{ij} , B_{ik}
     - Now a "supervised learning" problem
  3. Repeat 1 & 2, until convergence

  This is called the Baum-Welch Algorithm

  We can get to a provably more (or equally) likely parameter set θ each iteration

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

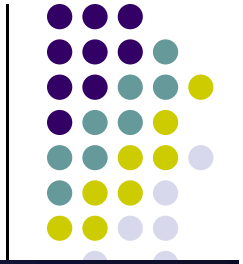
$$ESS_i \mathrel{+}= \left\langle SS_i(x_{n,i}, x_{n,\pi_i}) \right\rangle_{p(x_{n,H} | x_{n,-H})}$$

% M-step

for each node i

θ_i := MLE(ESS_i)

Summary: EM Algorithm



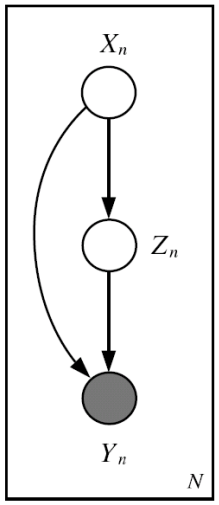
- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:
  1. Estimate some "missing" or "unobserved" data from observed data and current parameters.
  2. Using this "complete" data, find the maximum likelihood parameter estimates.

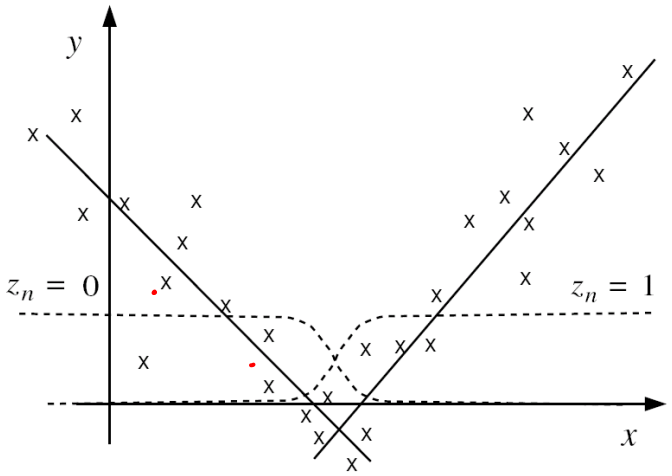
- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:

  - 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.

Conditional mixture model: Mixture of experts





- We will model $p(Y|X)$ using different experts, each responsible for different regions of the input space.
  - Latent variable Z chooses expert using softmax gating function:

$$P(z^k = 1|x) = \text{Softmax}\left(\xi^T x\right)$$

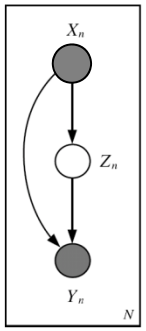
  - Each expert can be a linear regression model:

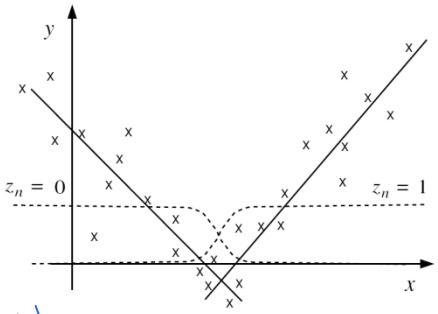
$$P(y|x, z^k = 1) = \mathcal{N}\left(y; \theta_k^T x, \sigma_k^2\right)$$

  - The posterior expert responsibilities are

$$P(z^k = 1|x, y, \theta) = \frac{p(z^k = 1|x)\, p_k(y|x, \theta_k, \sigma_k^2)}{\sum_j p(z^j = 1|x)\, p_j(y|x, \theta_j, \sigma_j^2)}$$

EM for conditional mixture model





- Model:

$$P(y|x) = \sum_k p(z^k = 1 \mid x, \xi) p(y \mid z^k = 1, x, \theta_i, \sigma)$$

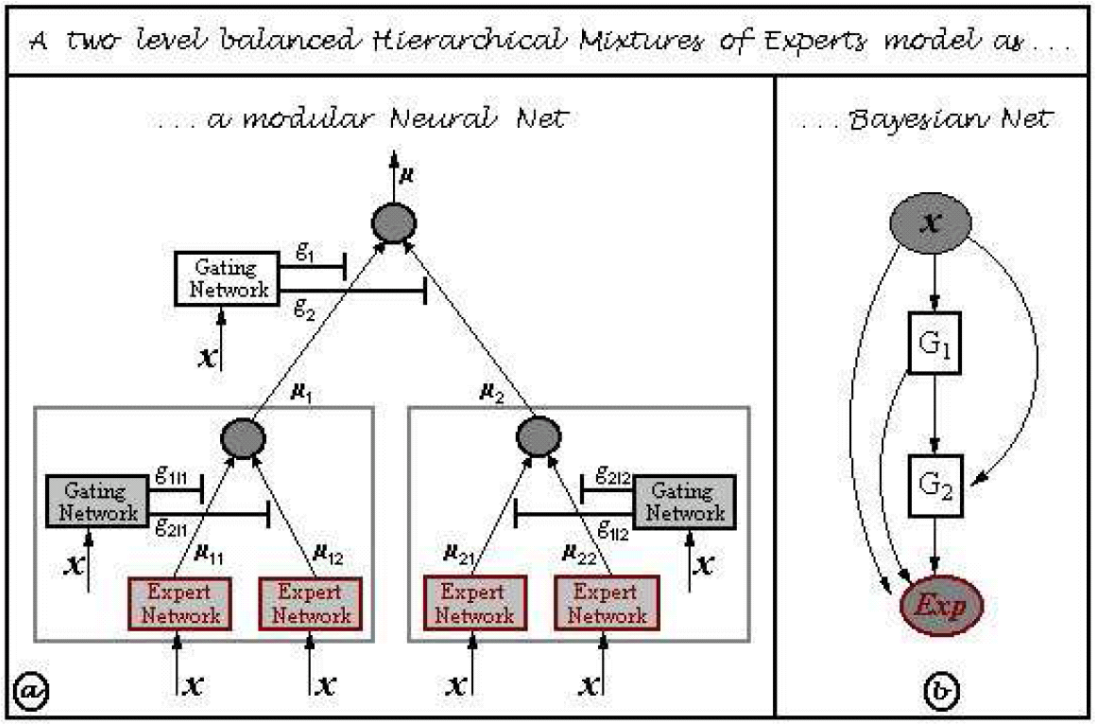
- The objective function

$$\langle \ell_c(\theta; x, y, z) \rangle = \sum_n \langle \log p(z_n \mid x_n, \xi) \rangle_{p(z|x,y)} + \sum_n \langle \log p(y_n \mid x_n, z_n, \theta, \sigma) \rangle_{p(z|x,y)}$$

$$= \sum_n \sum_k \langle z_n^k \rangle \log\left(\text{softmax}(\xi_k^T x_n)\right) - \frac{1}{2} \sum_n \sum_k \langle z_n^k \rangle \left(\frac{(y_n - \theta_k^T x_n)}{\sigma_k^2} + \log \sigma_k^2 + C \right)$$

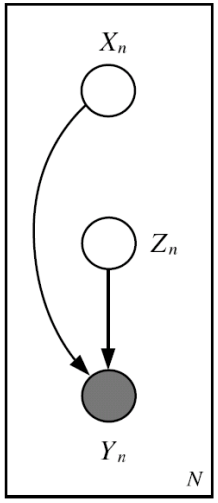
- EM:
  - E-step: $\tau_n^{k(t)} = P(z_n^k = 1 | x_n, y_n, \theta) = \frac{p(z_n^k = 1 | x_n) p_k(y_n | x_n, \theta_k, \sigma_k^2)}{\sum_j p(z_n^j = 1 | x_n) p_j(y_n | x_n, \theta_j, \sigma_j^2)}$
  - M-step:
    - using the normal equation for standard LR $\theta = (X^T X)^{-1} X^T y$, but with the data re-weighted by τ (homework)
    - IRLS and/or weighted IRLS algorithm to update $\{\xi_k, \theta_k, \sigma_k\}$ based on data pair (x_n, y_n), with weights $\tau_n^{k(t)}$ (homework?)

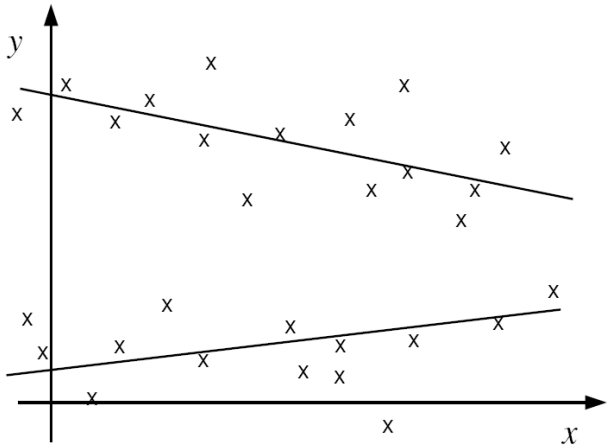
Hierarchical mixture of experts



- This is like a soft version of a depth-2 classification/regression tree.
- $P(Y|X,G_1,G_2)$ can be modeled as a GLIM, with parameters dependent on the values of G_1 and G_2 (which specify a "conditional path" to a given leaf in the tree).

Mixture of overlapping experts

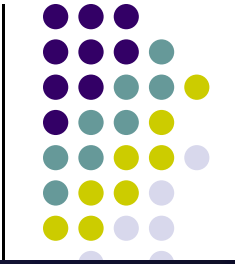




- By removing the $X \rightarrow Z$ arc, we can make the partitions independent of the input, thus allowing overlap.
- This is a mixture of linear regressors; each subpopulation has a different conditional mean.

$$P(z^k = 1 | x, y, \theta) = \frac{p(z^k = 1) p_k(y | x, \theta_k, \sigma_k^2)}{\sum_j p(z^j = 1) p_j(y | x, \theta_j, \sigma_j^2)}$$

Partially Hidden Data



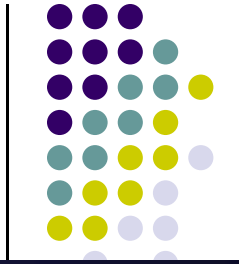
- Of course, we can learn when there are missing (hidden) variables on some cases and not on others.
- In this case the cost function is:

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

  - 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.

EM Variants



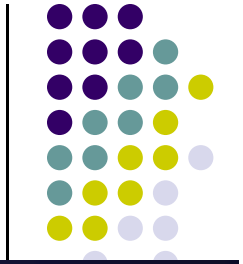
- Sparse EM:

  Do not re-compute exactly the posterior probability on each data point under all models, because it is almost zero. Instead keep an “active list” which you update every once in a while.

- Generalized (Incomplete) EM:

  It might be hard to find the ML parameters in the M-step, even given the completed data. We can still make progress by doing an M-step that improves the likelihood a bit (e.g. gradient step). Recall the IRLS step in the mixture of experts model.

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