School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Learning Partially Observed GM: the Expectation-Maximization algorithm

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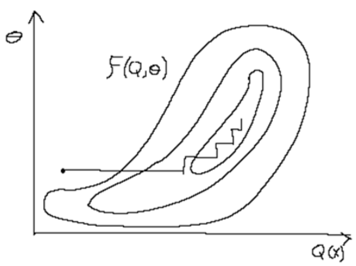
Lecture 8, February 9, 2015



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.

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

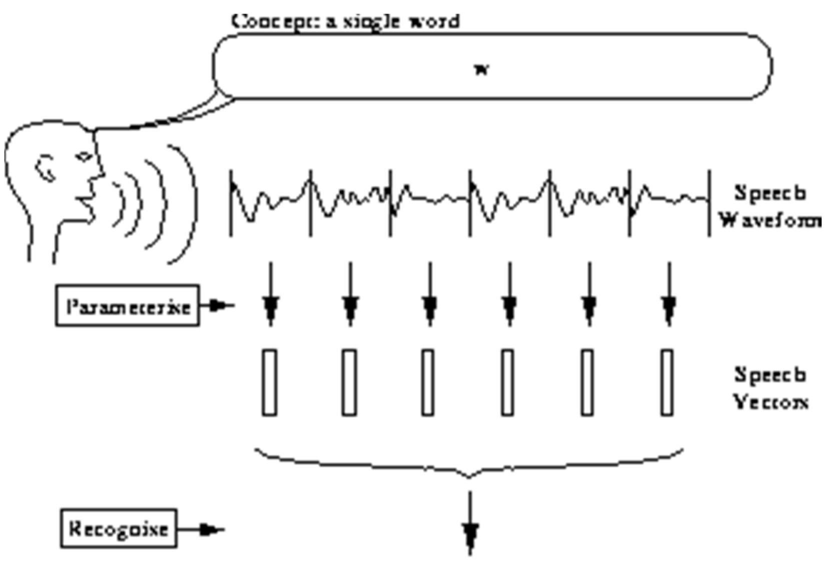
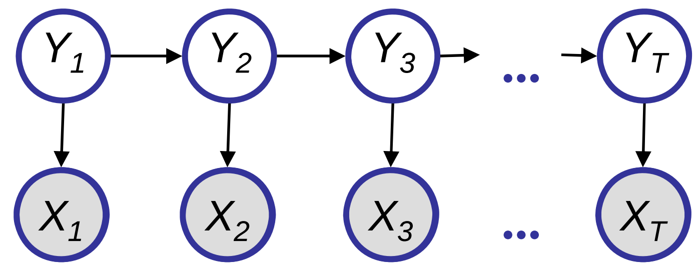
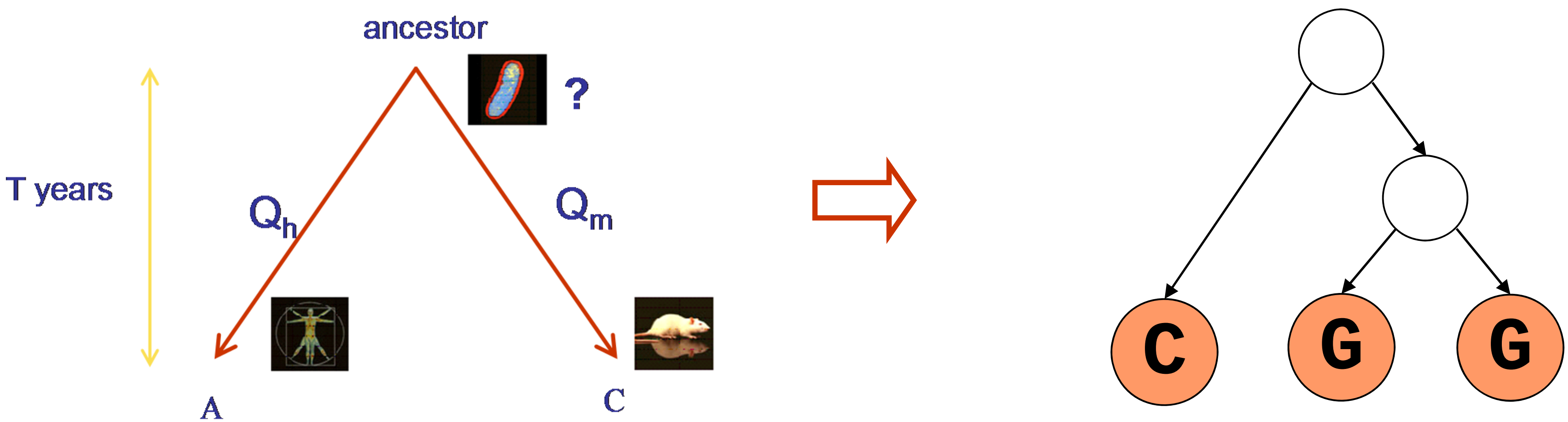


Fig. 1.2 Isolated Word Problem



Partially observed GM

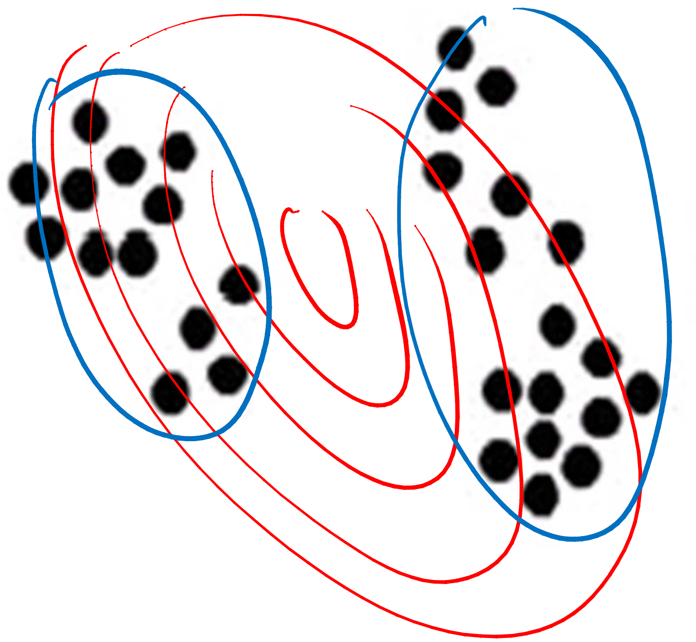
- Biological Evolution



Mixture Models

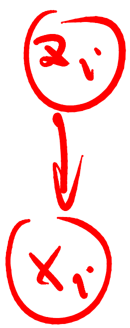
$P(x)$?

$= \pi_1 P(x \mid \mu_1, \Sigma_1)$
$+ \pi_2 P(x \mid \mu_2, \Sigma_2)$

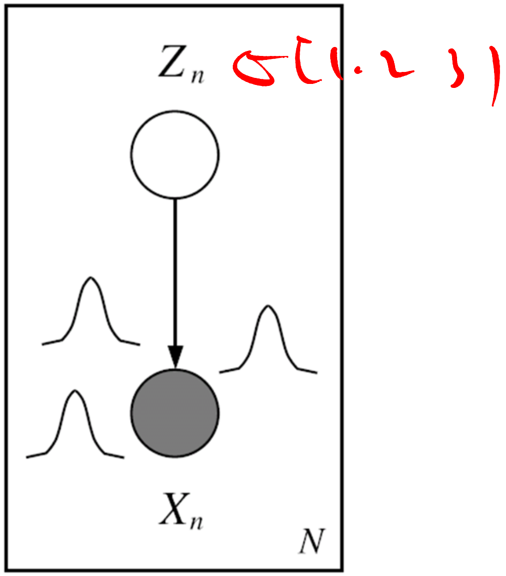


Mixture Models, con'd

- 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).



$\Rightarrow$



Unobserved Variables

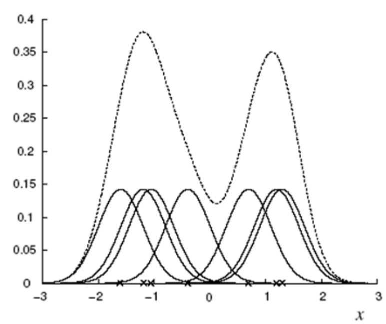
- A variable can be unobserved (latent) because:
  - it is an imaginary quantity meant to provide some simplified and abstractive view of the data generation process
    - e.g., speech recognition models, mixture models …
  - it is a real-world object and/or phenomena, but difficult or impossible to 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).

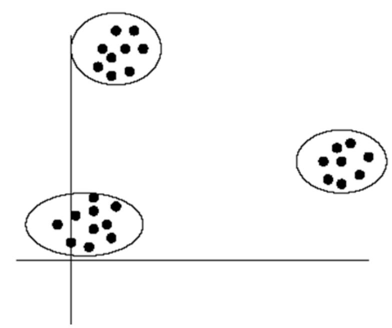
Gaussian Mixture Models (GMMs)

- 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.

$p(x|z) = N(u, \Sigma)$

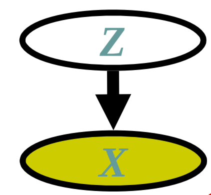
  - This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

Gaussian Mixture Models (GMMs)

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

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

$z_i : \begin{bmatrix} 0 \\ \vdots \end{bmatrix}$



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

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

$p(x,z) = p(x|z)\,p(z)$

  - The likelihood of a sample:

$= \sum_z p(z,x)$

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

$$= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \underbrace{\pi_k}_{\text{mixture proportion}} \underbrace{N(x, | \mu_k, \Sigma_k)}_{\text{mixture component}}$$

$\forall k$

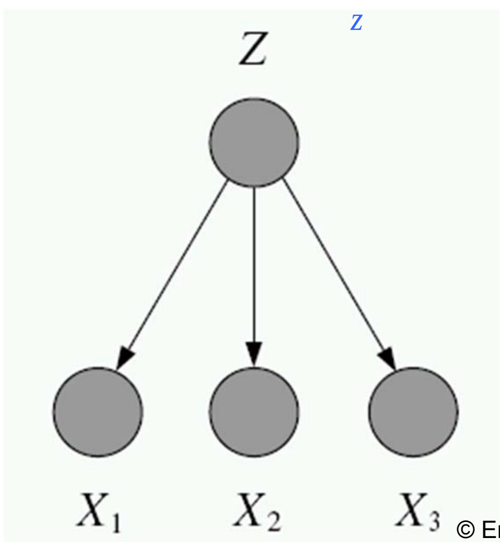
Why is Learning Harder?

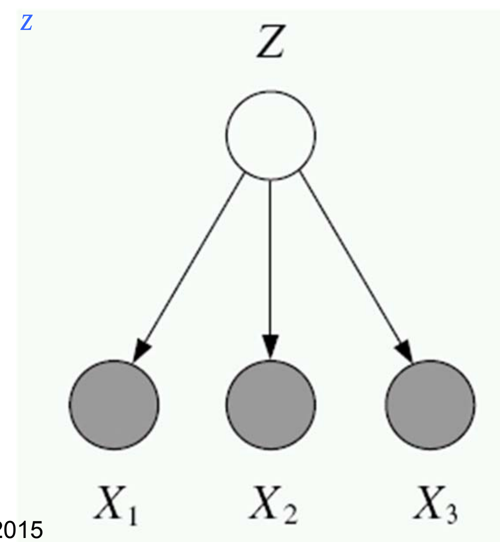
- In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models).

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

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

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





Gradient Learning for mixture models

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

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

$$\pi_k = \frac{N_k}{N}$$

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

$$\theta_k =$$

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

$$= \sum_k \pi_k \frac{p_k(\mathrm{x}|\theta_k)}{p(\mathrm{x} \mid \theta)} \frac{\partial \log p_k(\mathrm{x}|\theta_k)}{\partial \theta_k} = \sum_k r_k \frac{\partial \ell_k}{\partial \theta_k} = 0$$

- 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. $\Sigma_k \pi_k = 1$, Σ being symmetric positive definite (hence $\Sigma_{ii} > 0$).
- We can use constrained optimization, or we can reparameterize in terms of unconstrained values.
  - For normalized weights, use the softmax transform:
  - For covariance matrices, use the Cholesky decomposition:

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

where A is upper diagonal with positive diagonal:

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

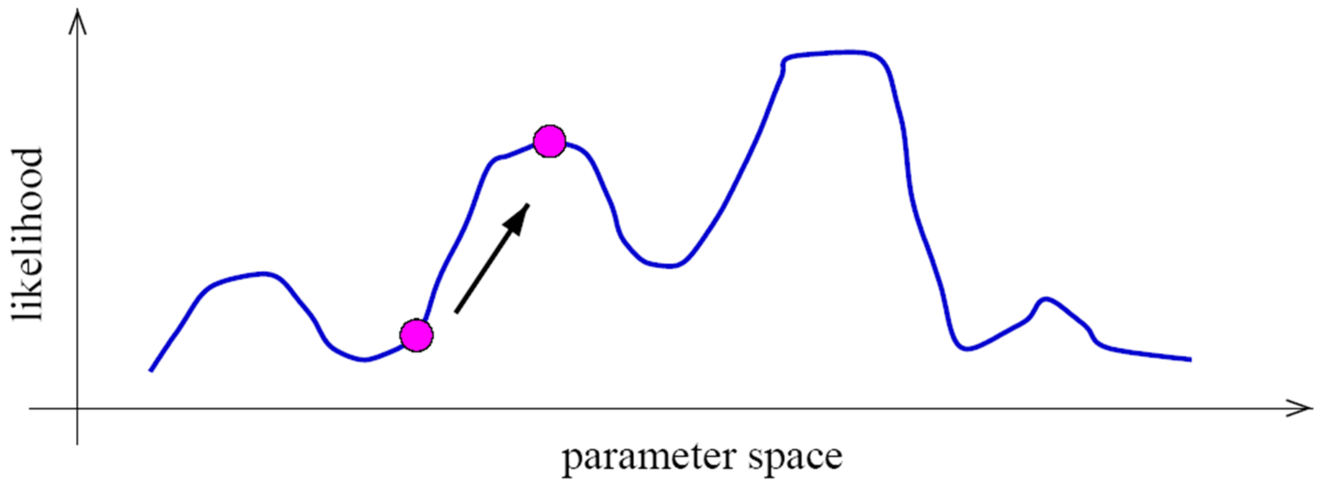
the parameters $\gamma_i, \lambda_i, \eta_{ij} \in \mathbb{R}$ are unconstrained.

  - Use chain rule to compute $\frac{\partial \ell}{\partial \pi}, \frac{\partial \ell}{\partial \mathbf{A}}$.

$$\frac{\partial \ell}{\partial \xi} = \frac{\partial \ell}{\partial \Sigma}\frac{\partial \Sigma}{\partial A}\frac{\partial A}{\partial \lambda}$$

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.



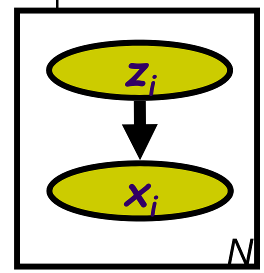
Identifiability

π_1

π_2 π_3

$$\begin{bmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix} = \begin{bmatrix} 0.1 \\ 0.3 \\ 0.6 \end{bmatrix} \qquad \begin{bmatrix} \\ \\ \\ \end{bmatrix} = \begin{bmatrix} 0.6 \\ 0.1 \\ 0.3 \end{bmatrix}$$

Toward the EM algorithm



- Recall MLE for completely observed data

- Data log-likelihood

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

- MLE

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

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

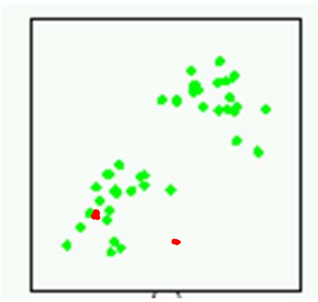
$$\hat{\sigma}_{k,MLE} = \arg\max_{\sigma} \ell(\boldsymbol{\theta}; D)$$

- 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?

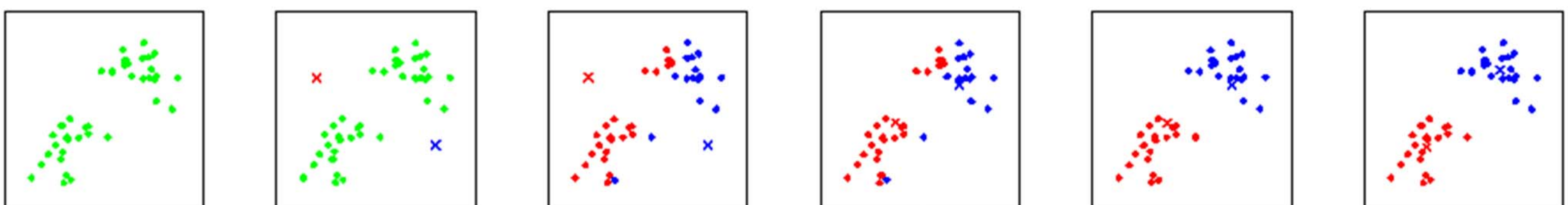
Recall: K-means



$\Sigma = (\ddots)$

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

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

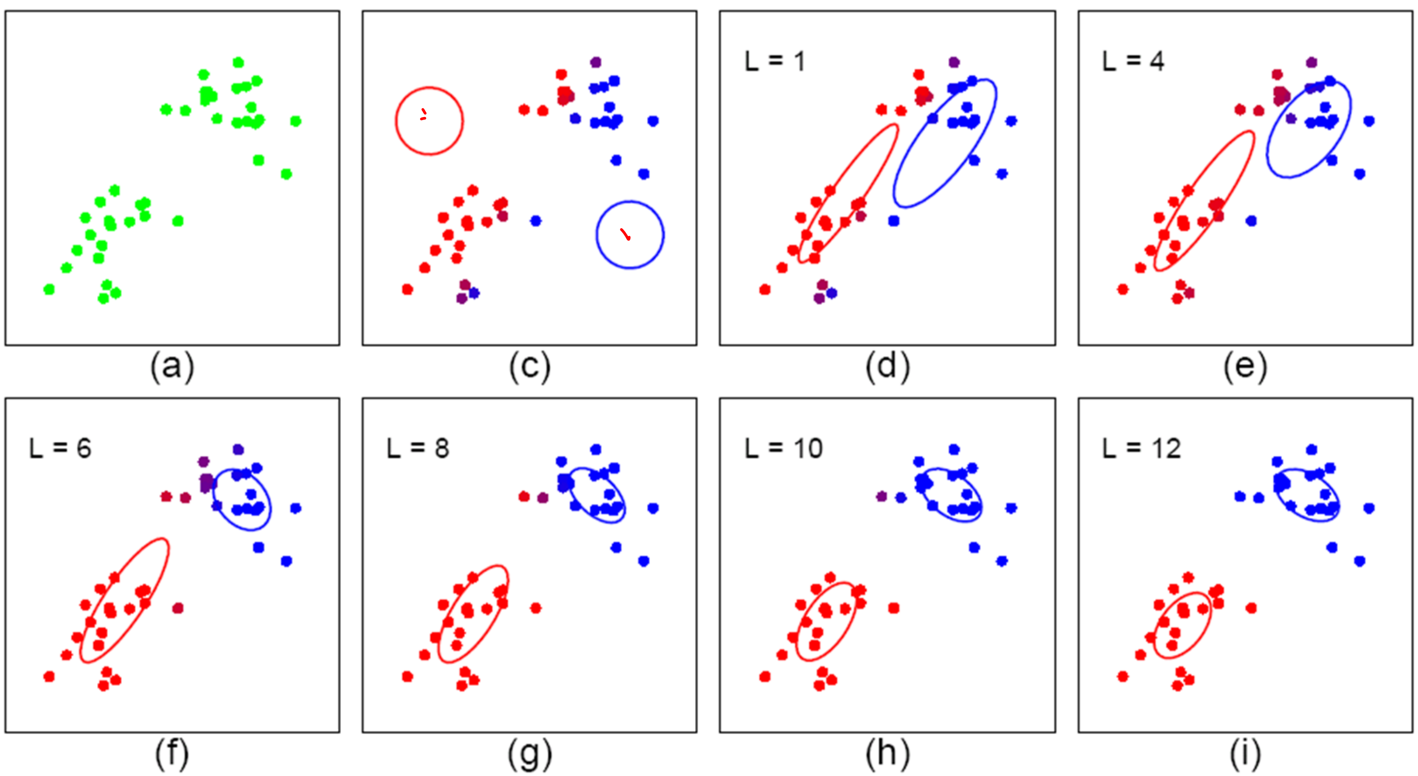


(a) (b) (c) (d) (e) (f)

Expectation-Maximization

$P(Z|X) = \begin{cases} 0.1 \\ 0.2 \\ 0.7 \end{cases}$

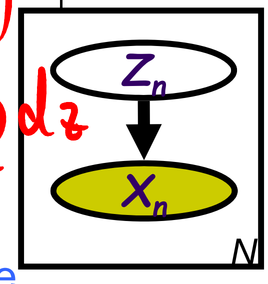
- Start:
  - "Guess" the centroid μ_k and coveriance Σ_k of each of the K clusters
- Loop



Example: Gaussian mixture model

$\langle p(z,x) \rangle_{p(z)}$

$\int p(z,x) \frac{f(z)}{q(z)} dz$



- 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

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

$\langle p(z,x) \rangle_q$

$q(z) = p(z|x)$

  - The likelihood of a sample:

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

- The expected complete log likelihood

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

E-step

$\{ \mu_k^{t-1} \Sigma_k^{t-1} \pi_k^{t-1} \}$

$p(z, x; \{\pi, \mu, \Sigma\})$

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

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

  – 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).

$t+1$

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

- Here we are essentially doing **inference**

M-step

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

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

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

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

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

Fact:

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

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

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

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

$\langle \ell(\theta, x, z) \rangle$

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

$\langle \ell_c \rangle \le \ell(x)$

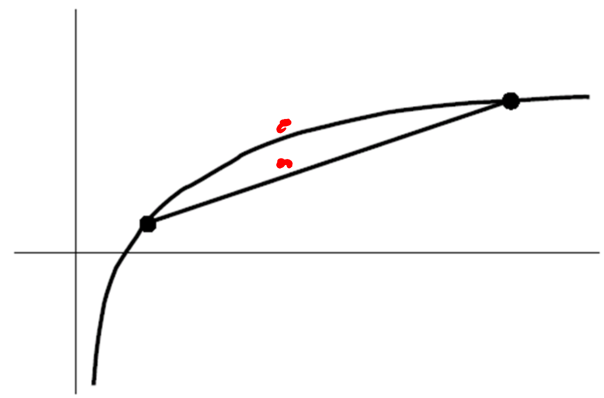
- For ***any*** distribution $q(z)$, define *expected complete log likelihood*:

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

  - 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

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



Lower Bounds and Free Energy

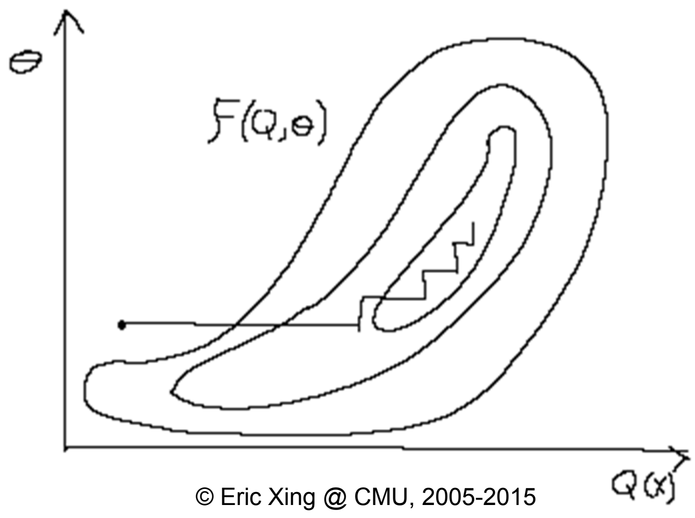
- For fixed data x, define a functional called the free energy:

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

$\ell(x, \theta)$

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

M↑



→ G

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

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

$F_{(q)} < \ell(\theta - x)$

$q = p(z(x)$

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

E-step ≡ plug in posterior expectation of latent variables

$\langle z_i \rangle \langle z_j \rangle$

$\langle z_i z \rangle$

$p(z_i, z \mid x)$

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

$F(\theta) = \ell(x)$

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

$q \rightarrow p(z|x)$

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

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

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

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

- Note that the free energy breaks into two terms:

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

  - 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:

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

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

Example: HMM

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

    GIVEN: a genomic region $x = x_1 \dots x_{1,000,000}$ 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:**

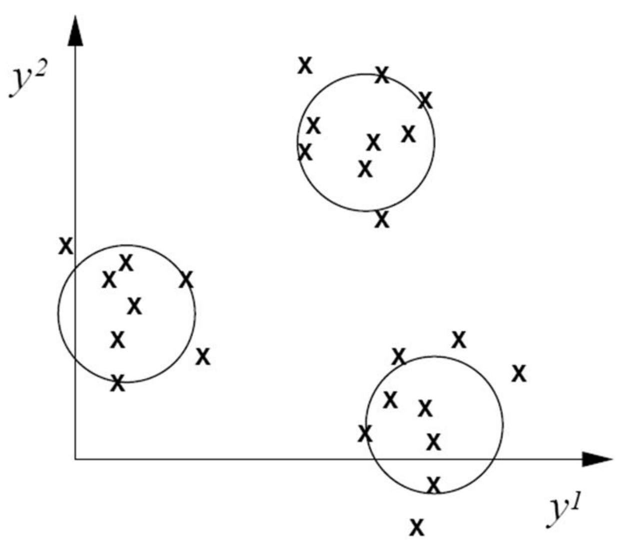
    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition

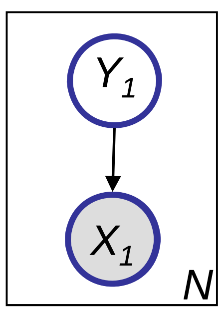
    GIVEN: 10,000 rolls of the casino player, but we don't see when he changes dice

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

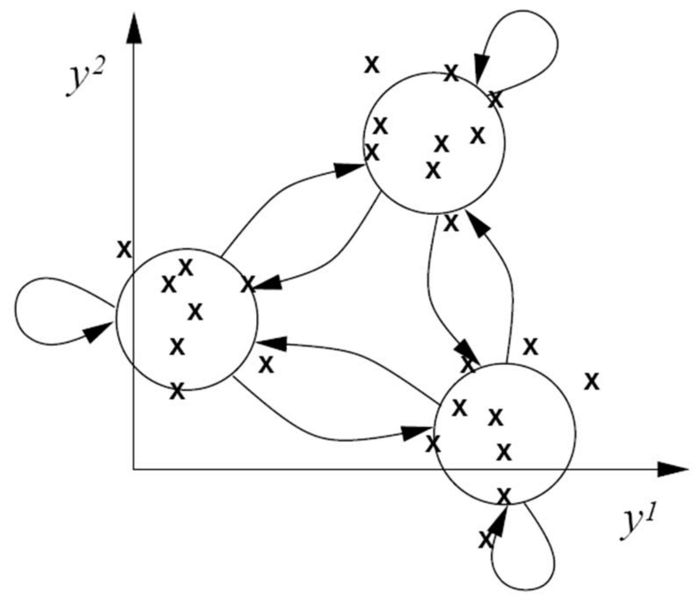
Hidden Markov Model:
from static to dynamic mixture models

Static mixture





Dynamic mixture



The underlying source:

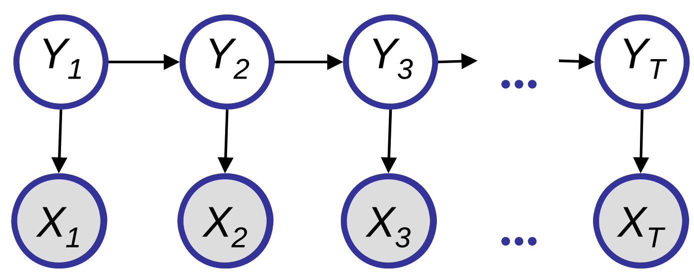
Speech signal,

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

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

- EM
  - The **E** step

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

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

  - 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? $A_{ij} = \sum_{n,t} \langle y_{n,t-1}^i y_{n,t}^j \rangle$, $B_{ik} = \sum_{n,t} \langle y_{n,t}^i \rangle x_{n,t}^k$,
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*

$\theta_i := \mathrm{MLE}(ESS_i)$

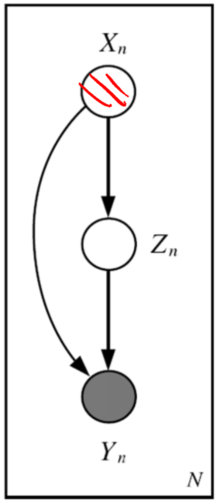
Summary: EM Algorithm

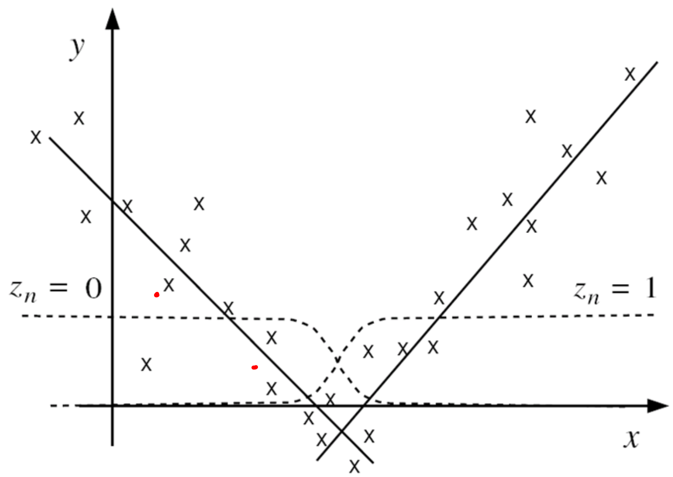
- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:
  1. Estimate some “missing” or “unobserved” data from observed data and current parameters.
  2. Using this “complete” data, find the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

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

  - Each expert can be a linear regression model:

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

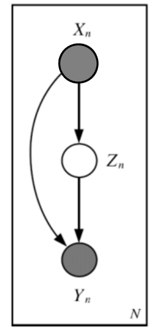
  - The posterior expert responsibilities are

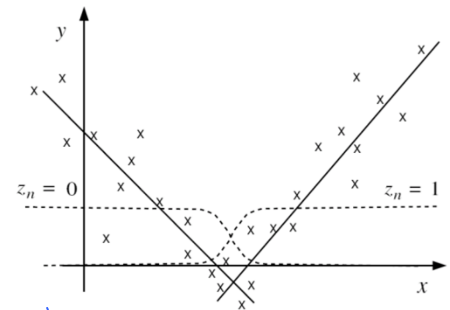
$$P(z^k = 1|x, y, \theta) = \frac{p(z^k = 1|x) p_k(y|x, \theta_k, \sigma_k^2)}{\sum_j p(z^j = 1|x) p_j(y|x, \theta_j, \sigma_j^2)}$$

EM for conditional mixture model

- Model:

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





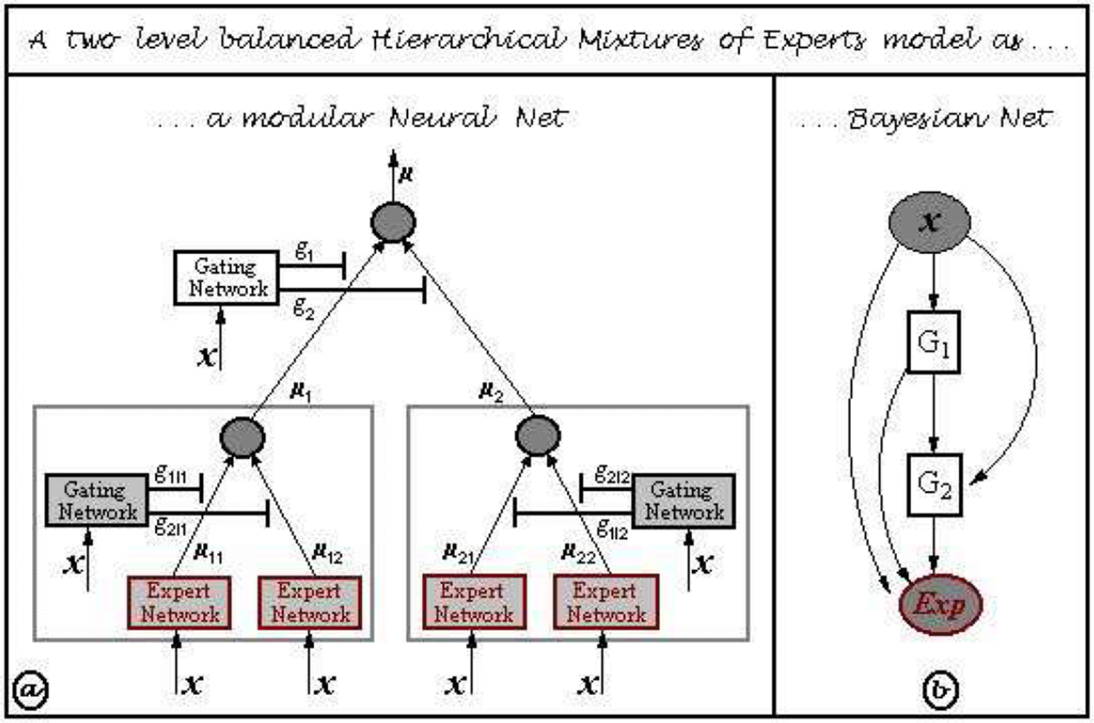
- The objective function

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

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

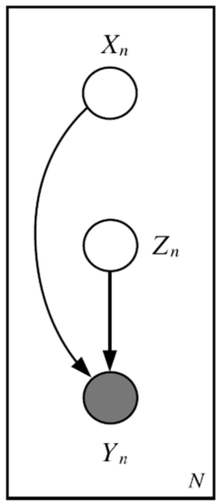
- EM:
  - E-step: $$\tau_n^{k(t)} = P(z_n^k = 1 | x_n, y_n, \theta) = \frac{p(z_n^k = 1|x_n) p_k(y_n|x_n, \theta_k, \sigma_k^2)}{\sum_j p(z_n^j = 1|x_n) p_j(y_n|x_n, \theta_j, \sigma_j^2)}$$
  - M-step:
    - using the normal equation for standard LR $\theta = (X^T X)^{-1} X^T Y$, but with the data re-weighted 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?)

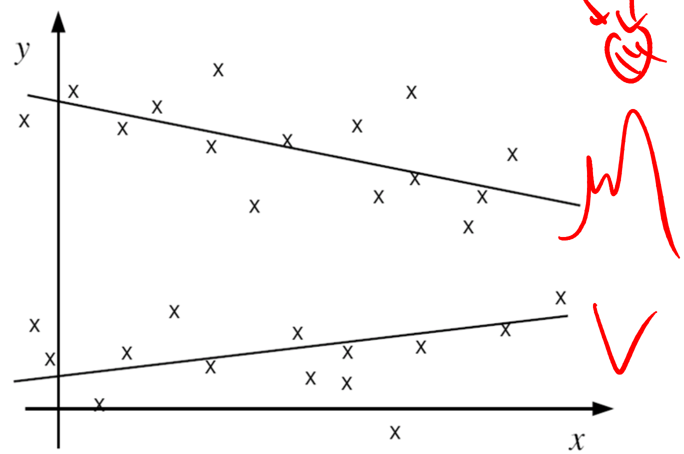
Hierarchical mixture of experts

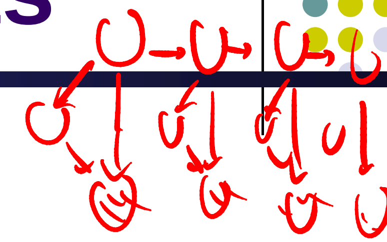


- This is like a soft version of a depth-2 classification/regression tree.
- $P(Y \mid X, G_1, G_2)$ can be modeled as a GLIM, with parameters dependent on the values of G_1 and G_2 (which specify a "conditional path" to a given leaf in the tree).

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.

$\mu = \frac{\sum x_n}{\sum n}$

- 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

- Some recent development: convex relaxation, direct non-convex optimization …(see references)