PETUUM

Carnegie Mellon University
School of Computer Science

Probabilistic Graphical Models

Learning Partially Observed GM: the Expectation-Maximization algorithm

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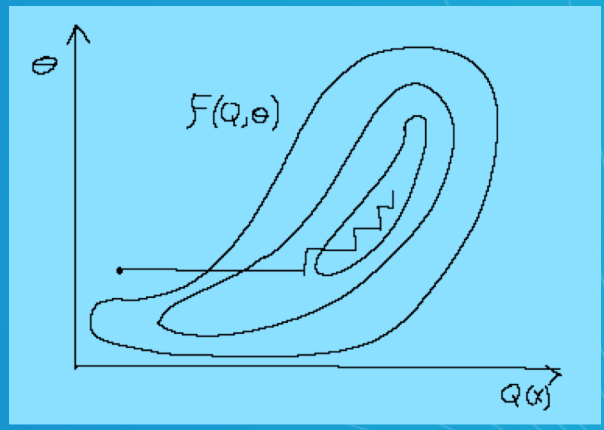
Lecture 6, February 4, 2019



Reading: see class homepage

Before we start, some logistics…

- HW1 was released last week
  - Due date: Wed, Feb 13 (start early!)

- Project:
  - Form teams of 3-4 people (hurry up if you haven't found the team yet)
  - TAs have posted some project suggestions on the course page
  - Project proposals are due Feb 22

- Lecture 5 → self-study (skipping in the interest of time)
  - Some brief highlights will be covered today
  - The scribe team is to write notes based on slides + reading material

Recall: Learning Graphical Models

- Scenarios:
  - Completely observed GMs
    - directed
    - undirected
  - Partially or unobserved GMs
    - directed
    - undirected (an open research topic)

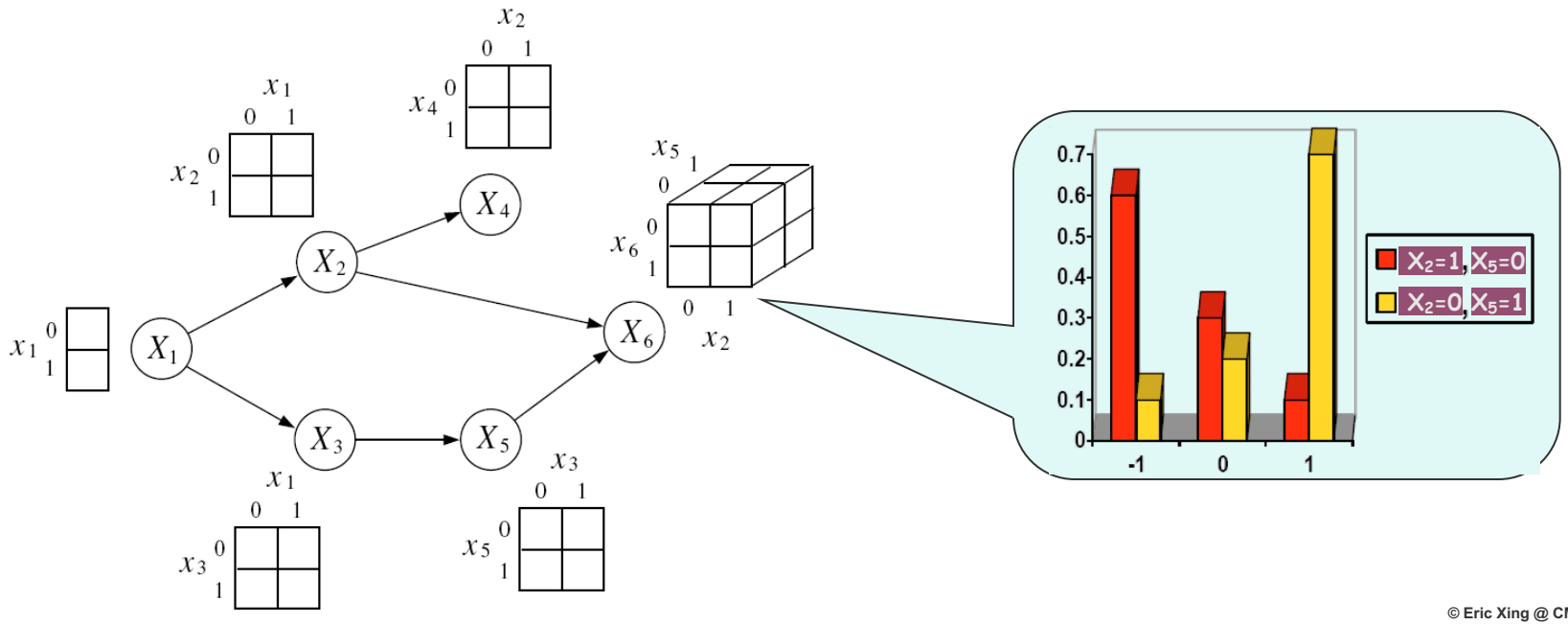
- Estimation principles:
  - Maximal likelihood estimation (MLE)
  - Maximal conditional likelihood
  - Bayesian estimation
  - Maximal "Margin"
  - Maximum entropy

- We use learning as a name for the process of estimating the parameters, and in some cases, the topology of the network, from data.

MLE for general BNs

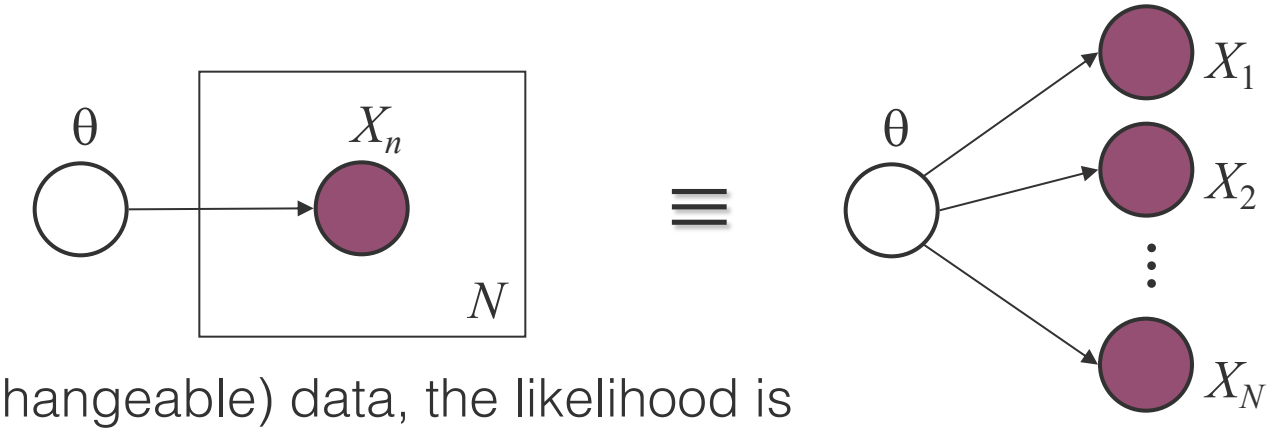
- If we assume the parameters for each CPD are globally independent, and all nodes are fully observed, then the log-likelihood function decomposes into a sum of local terms, one per node:

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



Plates

- A plate is a “macro” that allows subgraphs to be replicated



  - For iid (exchangeable) data, the likelihood is

$$p(D \mid \theta) = \prod_n p(x_n \mid \theta)$$

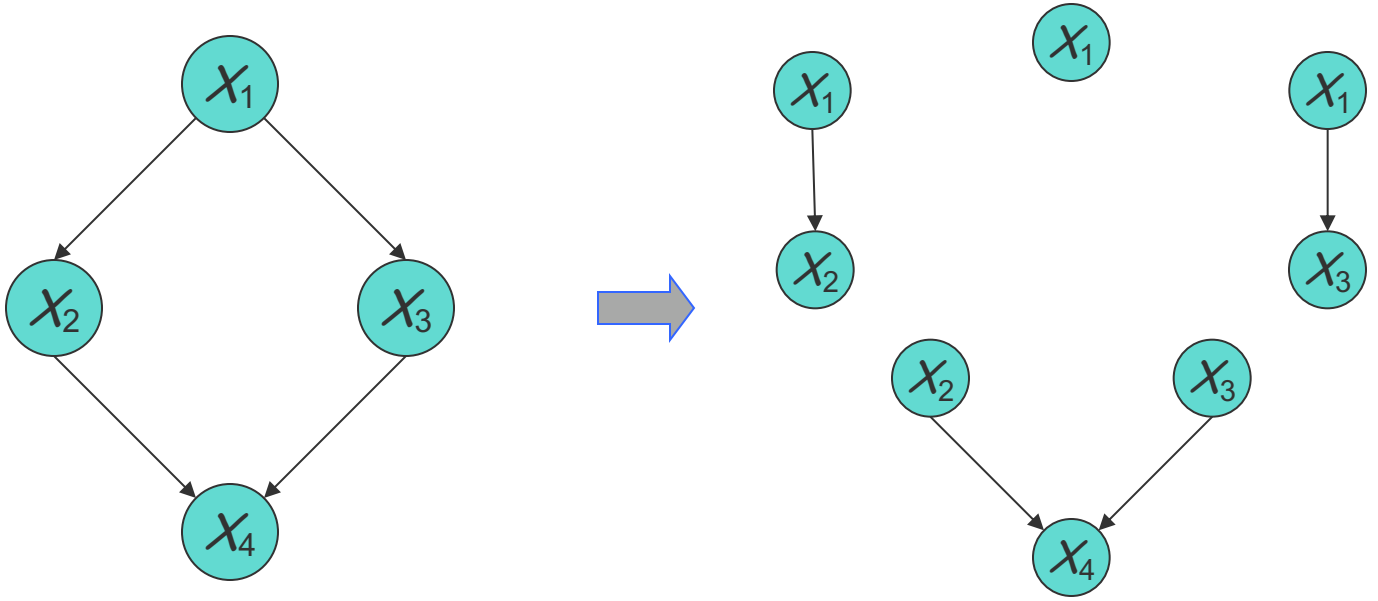
  - We can represent this as a Bayes net with N nodes.
    - The rules of plates are simple: repeat every structure in a box a number of times given by the integer in the corner of the box (e.g. N), updating the plate index variable (e.g. n) as you go.
    - Duplicate every arrow going into the plate and every arrow leaving the plate by connecting the arrows to each copy of the structure.

Decomposable likelihood of a BN

- Consider the distribution defined by the directed acyclic GM:

$$p(x \mid \theta) = p(x_1 \mid \theta_1)\, p(x_2 \mid x_1, \theta_2)\, p(x_3 \mid x_1, \theta_3)\, p(x_4 \mid x_2, x_3, \theta_4)$$

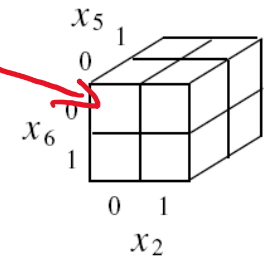
- This is exactly like learning four separate small BNs, each of which consists of a node and its parents.



MLE for BNs with tabular CPDs

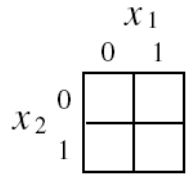
- Assume each CPD is represented as a table (multinomial) where

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



  - Note that in case of multiple parents, $\mathbf{X}_{\pi_i}$ will have a composite state, and the CPD will be a high-dimensional table
  - The sufficient statistics are counts of family configurations

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



- The log-likelihood is

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

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

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

Example: HMM: two scenarios

- 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

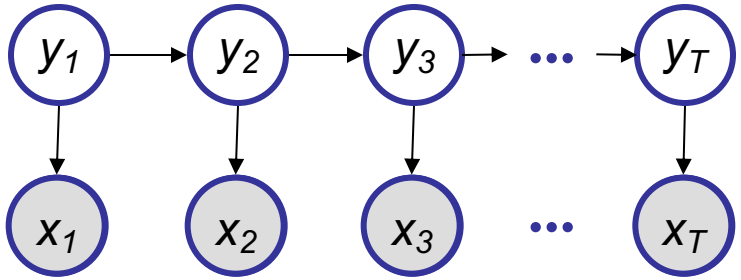
Recall definition of HMM

- Transition probabilities between any two states

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

or

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



- Start probabilities

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

- Emission probabilities associated with each state

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

or in general:

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

Supervised ML estimation

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

    A_{ij} = # times state transition $i \to j$ occurs in $\mathbf{y}$

    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$

  - We can show that the maximum likelihood parameters θ are:

$$a_{ij}^{ML} = \frac{\#(i \to j)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i} y_{n,t}^{j}}{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i}} = \frac{A_{ij}}{\sum_{j'} A_{ij'}}$$

$$b_{ik}^{ML} = \frac{\#(i \to k)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=1}^{T} y_{n,t}^{i} x_{n,t}^{k}}{\sum_n \sum_{t=1}^{T} y_{n,t}^{i}} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

  - What if x is continuous? We can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as NT observations of, e.g., a Gaussian, and apply learning rules for Gaussian …

Supervised ML estimation, cont'd

- Intuition:
  - When we know the underlying states, the best estimate of θ is the average frequency of transitions & emissions that occur in the training data
- Drawback:
  - Given little data, there may be overfitting:
    - $P(x|\theta)$ is maximized, but θ is unreasonable: 0 probabilities – VERY BAD
- Example:
  - Given 10 casino rolls, we observe

    x = 2, 1, 5, 6, 1, 2, 3, 6, 2, 3

    y = F, F, F, F, F, F, F, F, F, F
  - Then: $a_{FF} = 1$; $a_{FL} = 0$

    $b_{F1} = b_{F3} = .2$;

    $b_{F2} = .3$; $b_{F4} = 0$; $b_{F5} = b_{F6} = .1$

Pseudocounts

- Solution for small training sets:
  - Add pseudocounts
    A_{ij} = # times state transition $i \to j$ occurs in $\mathbf{y}$ + R_{ij}
    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$ + S_{ik}
  - R_{ij}, S_{ij} are pseudocounts representing our prior belief
  - Total pseudocounts: $R_i = \Sigma_j R_{ij}$, $S_i = \Sigma_k S_{ik}$,
    - --- "strength" of prior belief,
    - --- total number of imaginary instances in the prior
- Larger total pseudocounts ⇒ strong prior belief
- Small total pseudocounts: just to avoid 0 probabilities ⇒ smoothing
- This is equivalent to Bayesian est. under a uniform prior with "parameter strength" equals to the pseudocounts

Summary: Learning fully observed GMs

- For fully observed BN, the log-likelihood function decomposes into a sum of local terms, one per node; thus learning is also factored
- See lecture 5 for the following:
  - Structural learning
    - Chow-Liu algorithm
    - Neighborhood selection
  - Learning single-node GM – density estimation: exponential family dist.
    - Typical discrete distribution
    - Typical continuous distribution
    - Conjugate priors
  - Learning two-node BN: GLIM
    - Conditional Density Est.
    - Classification
  - Learning BN with more nodes
    - Local operations

Partially observed GMs

- Speech recognition

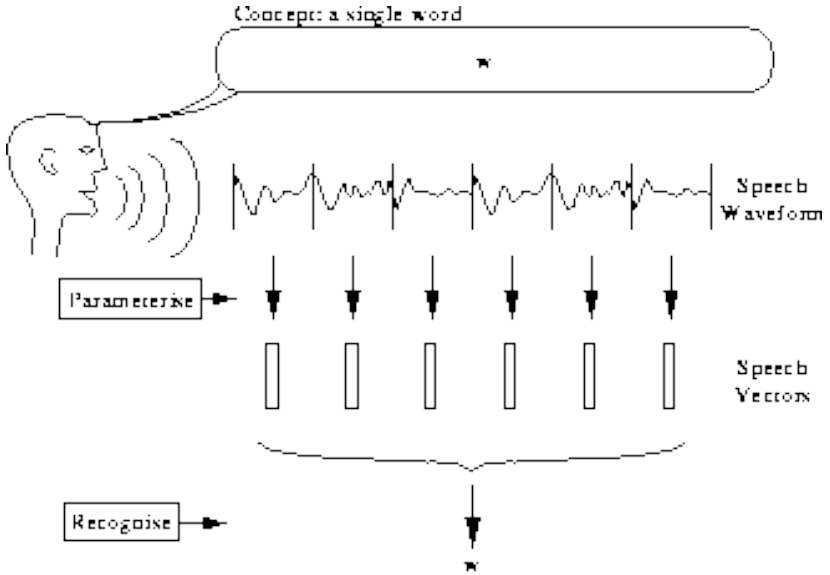
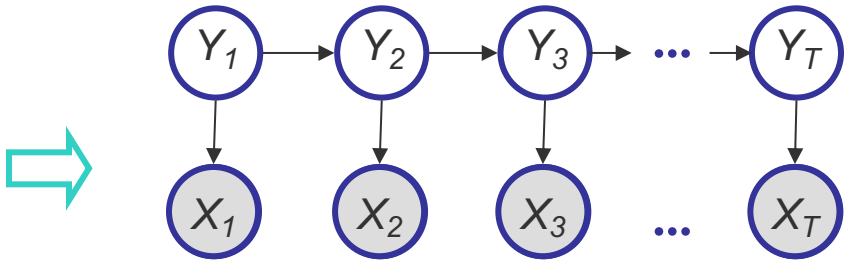
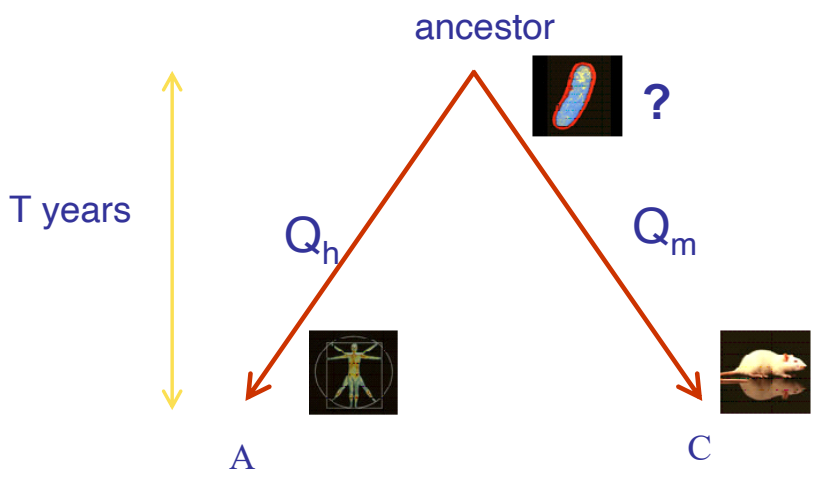


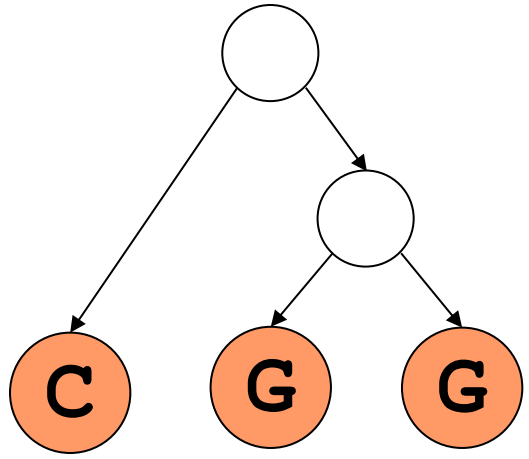
Fig. 1.2 Isolated Word Problem



Partially observed GM

- Biological Evolution

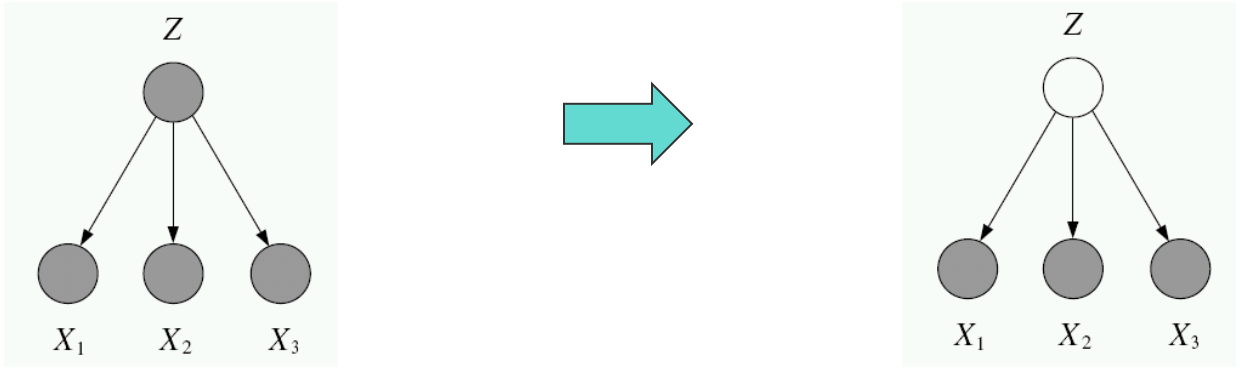




Inference is a subroutine for Learning

- Directed, but partially observed GM: imputing miss variables

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



- Undirected, but fully observed GM: compute clique marginals

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

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

Probabilistic Inference

- We now have compact representations of probability distributions: Graphical Models
- A GM $\mathcal{M}$ describes a unique probability distribution P
- Typical tasks:
  - Task 1: How do we answer queries about P_M, *e.g.*, $P_M(X|Y)$?
    - We use inference as a name for the process of computing answers to such queries
  - Task 2: How do we estimate a plausible model $\mathcal{M}$ from data $\mathcal{D}$?
    i. We use learning as a name for the process of obtaining point estimate of $\mathcal{M}$
    ii. But for *Bayesian*, they seek $p(\mathcal{M}|\mathcal{D})$, which is actually an inference problem
    iii. Inference can be a subroutine of many more types of learning problems

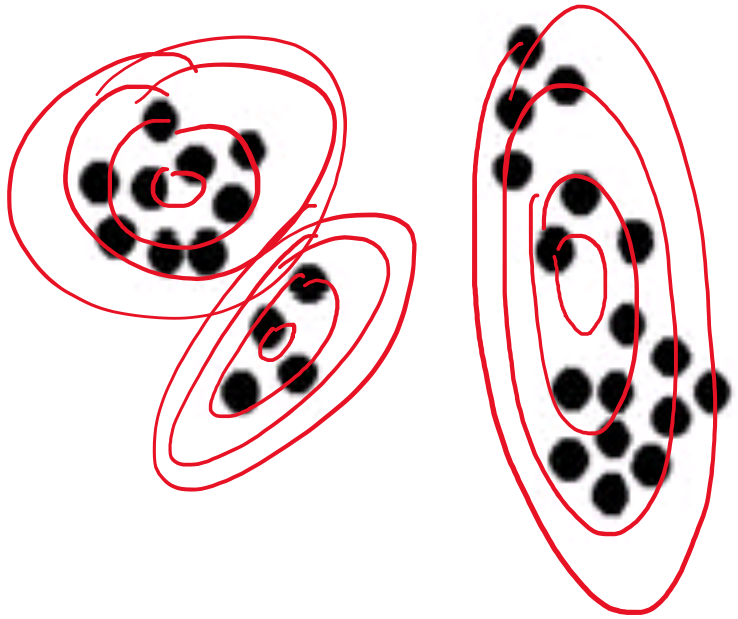
To learn partially observable GMs => iterate between Task 1 & 2

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

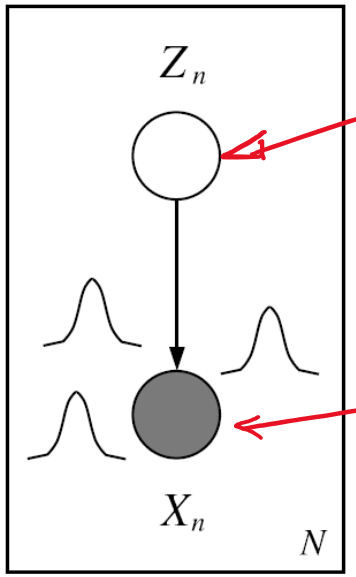
Mixture Models



Represent a complex density through a mixture of simpler densities

Mixture Models, cont'd

- A density model $p(x)$ may be multi-modal.
- But we may be able to model it as a mixture of uni-modal distributions (e.g., Gaussians).
- Example: each mode of the distribution may correspond to a different sub-population (e.g., male and female).



discrete latent variables index modes

model intra-mode distrib's

Unobserved Variables

- A variable can be unobserved (latent) because:
  1. **imaginary quantity:** meant to provide some simplified and abstractive view of the data generation process
     - e.g., speech recognition models, mixture models, …
  2. **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 …
  3. **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

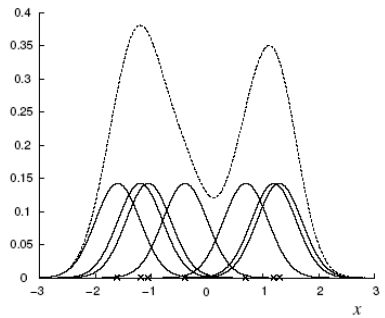
- Continuous latent variables (factors) can be used for dimensionality reduction (e.g., factor analysis, etc.)

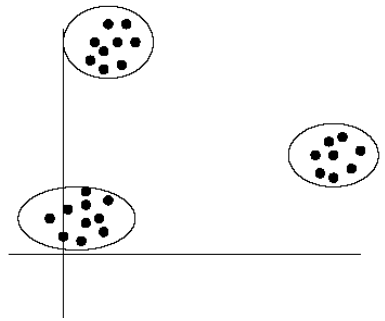
Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

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

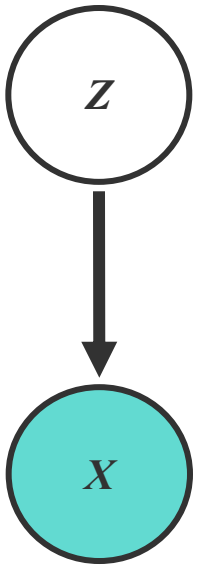
mixture proportion mixture component





- 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

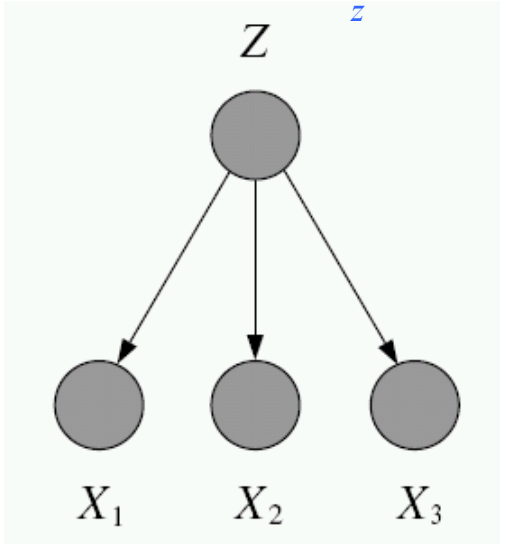
Why is Learning Harder?

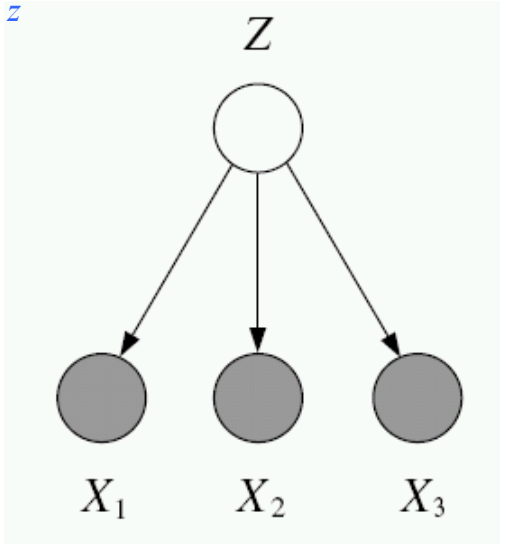
- In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models)

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

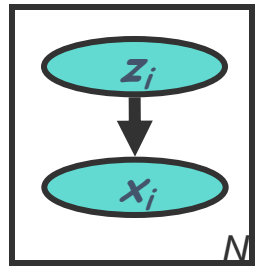
- With latent variables, all the parameters become coupled together via marginalization

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





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?

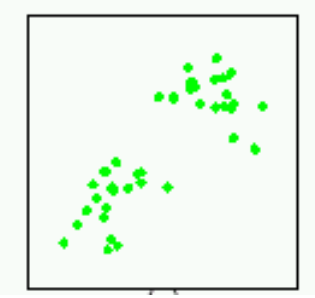
Question

- " … We solve problem X using Expectation-Maximization …"
  - What does it mean?

- E-step
  - What do we take expectation with?
  - What do we take expectation over?

- M-step
  - What do we maximize?
  - What do we maximize with respect to?

Recall: K-means

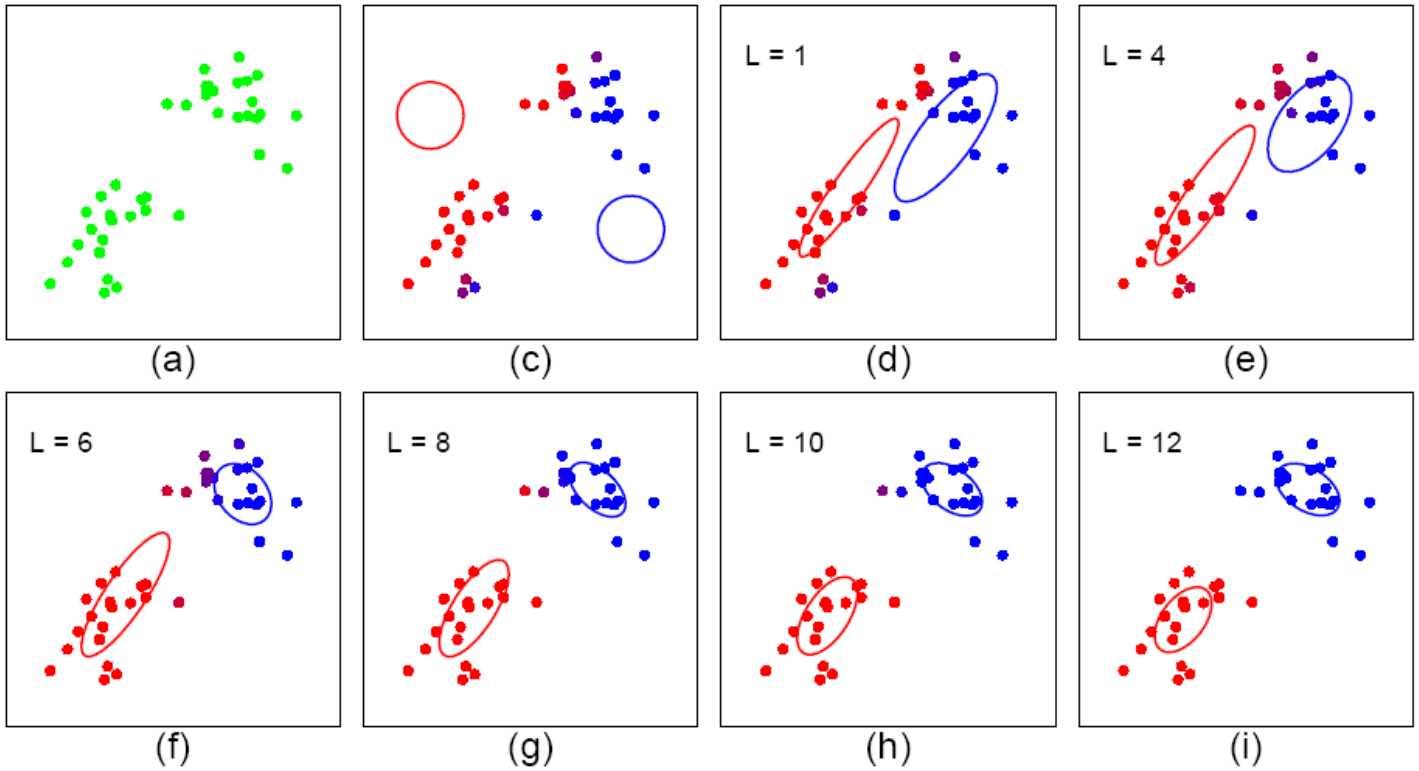


$$z_n^{(t)} = \arg\max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

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

Expectation-Maximization

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



Example: Gaussian mixture model

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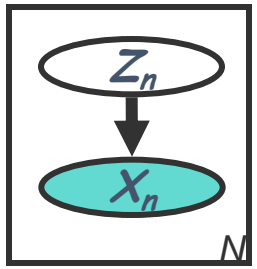
  - Z is a latent class indicator vector

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



  - 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:

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

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

we want to est. parameters

- The expected <u>complete</u> 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

- 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).

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

$p(z_n^k = 1, x, \mu^{(t)}, \Sigma^{(t)})$

$p(x, \mu^{(t)}, \Sigma^{(t)})$

} Bayes rule

(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 :

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

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

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

- 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

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

- 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:

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

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 (or marginal) 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*:

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

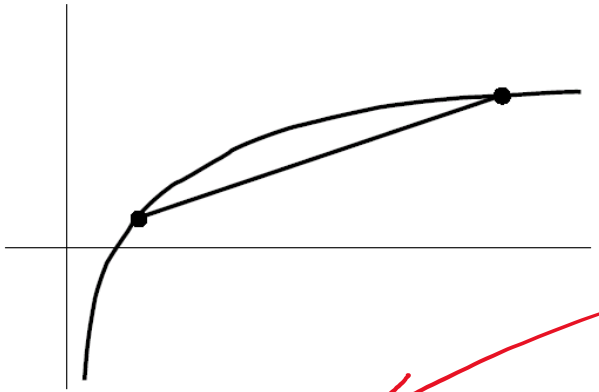
  - A deterministic function of θ
  - Linear in $\ell_c()$ →inherit its factorizability
  - Does maximizing this surrogate yield a maximizer of the likelihood?

- Jensen's inequality

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

when is it tight?

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



lower bound!

Lower Bounds and Free Energy

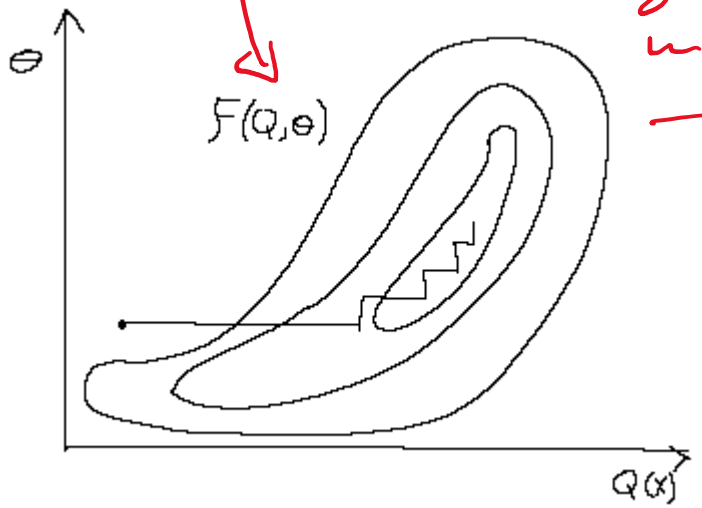
- For fixed data **x**, define a functional called the free energy:

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

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

(generalization of EM: the MM-algorithm)

Even if the marginal likelihood is computable, coordinate ascent has better convergence rate than gradient method!



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

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

Bayes rule

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

$$= \log p(x \mid \theta^t) = \ell(\theta^t; x)$$

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

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

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

- Note that the free energy breaks into two terms:

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

  - 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:

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

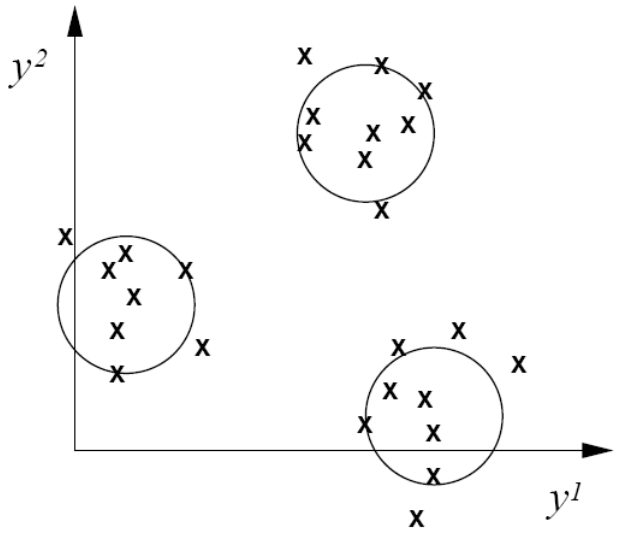
  - Under optimal q^{t+1}, this is equivalent to solving a standard MLE of fully observed model $p(x,z|\theta)$, with the sufficient statistics involving z replaced by their expectations w.r.t. $p(z|x,\theta)$.

Example: HMM

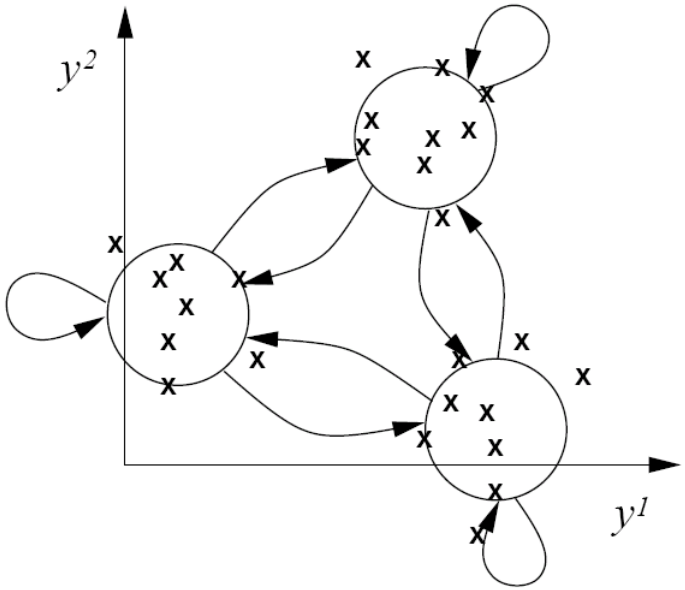
- Supervised learning: estimation when the "right answer" is known
  - Examples:
    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands
    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 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

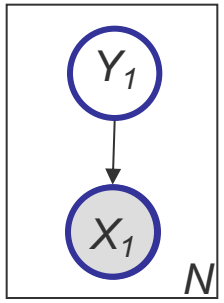
Hidden Markov Model: from static to dynamic mixture models

Static mixture



Dynamic mixture



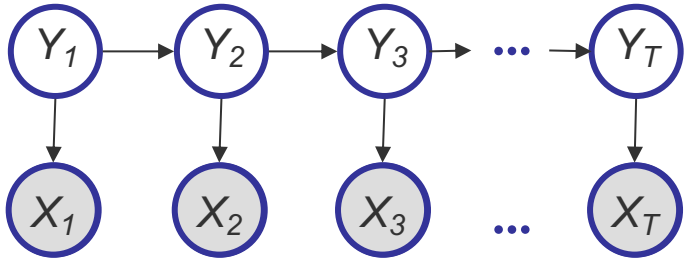


The underlying source:

Speech signal, dice, …

The sequence:

Phonemes, sequence of rolls, …



Supervised ML estimation

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

    A_{ij} = # times state transition $i \to j$ occurs in $\mathbf{y}$

    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$

  - We can show that the maximum likelihood parameters θ are:

$$a_{ij}^{ML} = \frac{\#(i \to j)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i} y_{n,t}^{j}}{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i}} = \frac{A_{ij}}{\sum_{j'} A_{ij'}}$$

$$b_{ik}^{ML} = \frac{\#(i \to k)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=1}^{T} y_{n,t}^{i} x_{n,t}^{k}}{\sum_n \sum_{t=1}^{T} y_{n,t}^{i}} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

  - What if x is continuous? We can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as $N \cdot T$ observations of, e.g., a Gaussian, and apply learning rules for Gaussian …

The Baum Welch algorithm (or EM for HMM)

- 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)

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

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

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

Summary: EM Algorithm

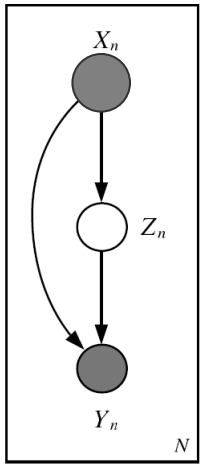
- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:
  1. Estimate some "missing" or "unobserved" data from observed data and current parameters.
  2. Using this "complete" data, find the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

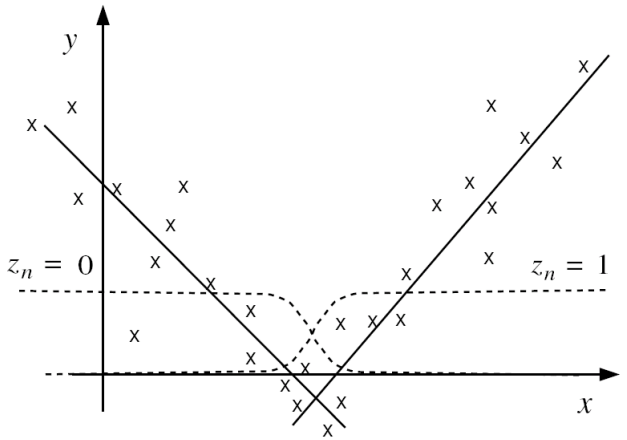
- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:

  - 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:

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

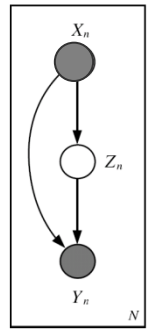
  - The posterior expert responsibilities are

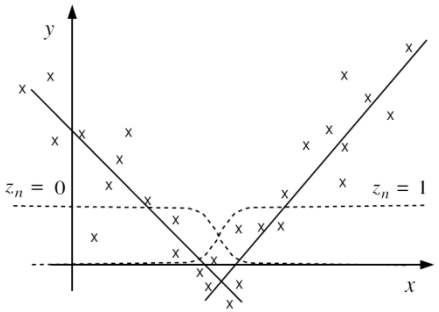
$$P(z^k = 1|x, y, \theta) = \frac{p(z^k = 1|x) p_k(y|x, \theta_k, \sigma_k^2)}{\sum_j p(z^j = 1|x) p_j(y|x, \theta_j, \sigma_j^2)}$$

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

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

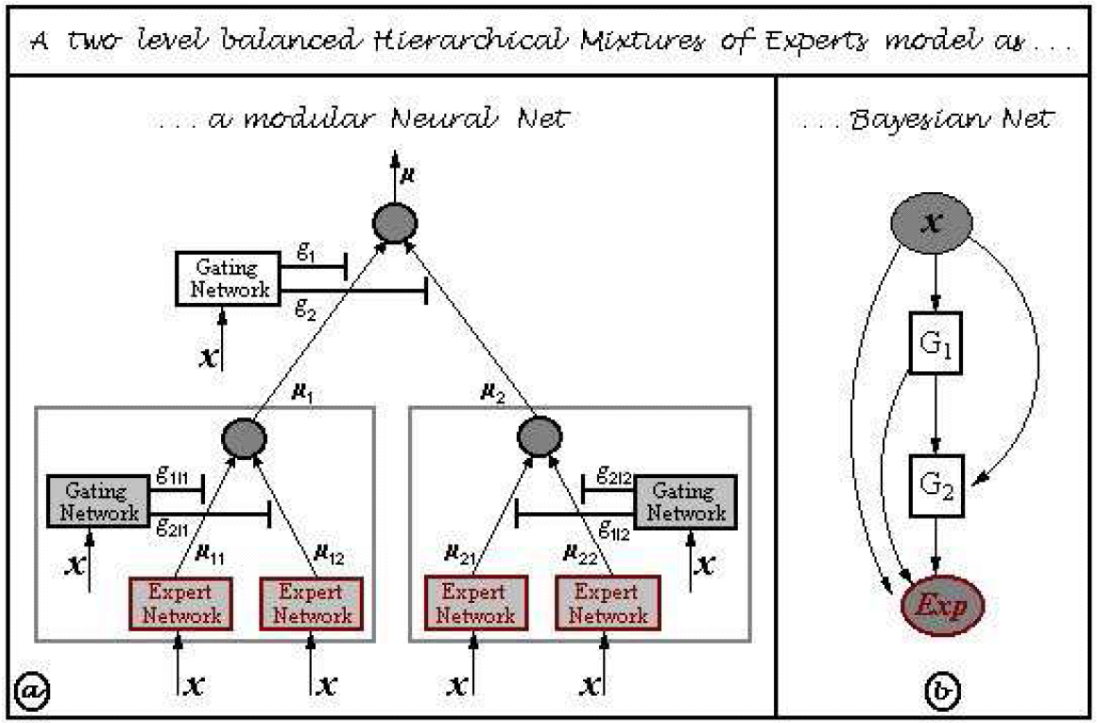
$$= \sum_n \sum_k \left\langle z_n^k \right\rangle \log\left(\text{softmax}(\xi_k^T x_n)\right) - \frac{1}{2} \sum_n \sum_k \left\langle z_n^k \right\rangle \left(\frac{(y_n - \theta_k^T x_n)}{\sigma_k^2} + \log \sigma_k^2 + C \right)$$

- EM:
  - E-step:

$$\tau_n^{k(t)} = P(z_n^k = 1 | x_n, y_n, \boldsymbol{\theta}) = \frac{p(z_n^k = 1|x_n)\, p_k(y_n|x_n, \theta_k, \sigma_k^2)}{\sum_j p(z_n^j = 1|x_n)\, p_j(y_n|x_n, \theta_j, \sigma_j^2)}$$

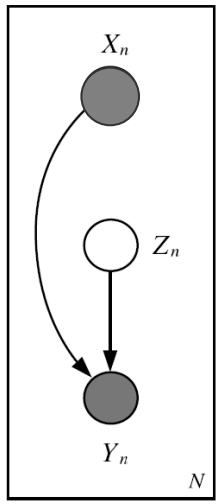
  - M-step:
    - using the normal equation for standard LR $\theta = (X^T X)^{-1} X^T y$, but with the data re-weighted by τ (homework)
    - IRLS and/or weighted IRLS algorithm to update $\{\xi_k, \theta_k, \sigma_k\}$ based on data pair (x_n, y_n), with weights (homework)

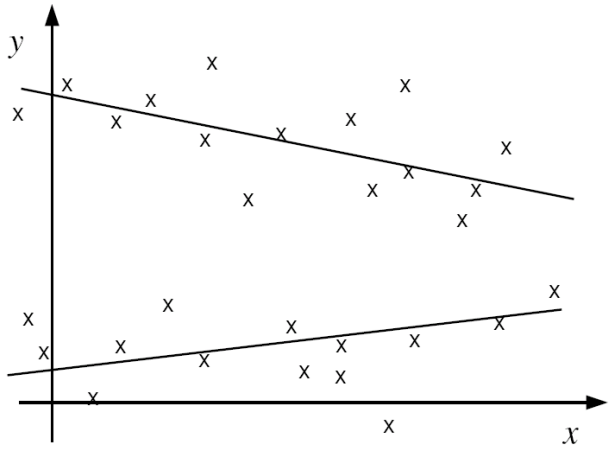
Hierarchical mixture of experts



- 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 the likelihood

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