Lecture 16:

Structure learning

Wed 10 Nov 2004

Maximizing the score (K&F 14.4.3)

- Consider the family of DAGs G_d with maximum fan-in (number of parents) equal to d.
- Theorem 14.4.3: It is NP-hard to find

$$G^* = \arg \max_{G \in G_d} \text{score}(G, D)$$

  for any $d \geq 2$.
- For $d \leq 1$ (i.e., trees), we can solve the problem in $O(n^2)$ time using max spanning tree.
- In general, we need to use heuristic local search.

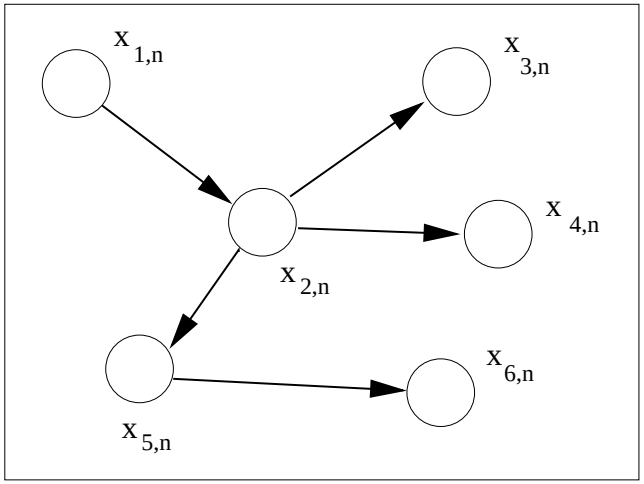
Directed Tree Graphical Models (K&F 14.4.1)

- Directed trees are DAGMs in which each variable x_i has exactly one other variable as its parent x_{π_i} except the "root" x_{root} which has no parents. Thus, the probability of a variable taking on a certain value depends only on the value of its parent:

$$p(\mathbf{x}) = p(x_{\text{root}}) \prod_{i \neq \text{root}} p(x_i | x_{\pi_i})$$

- Trees are the next step up from assuming independence. Instead of considering variables in isolation, consider them in pairs.

NB: each node (except root) has exactly one parent, but nodes may have more than one child.



Undirected Tree Graphical Models

- Undirected trees are connected, acyclic graphs with exactly (D-1) edges if there are D nodes (variables).
- For undirected trees, the cliques are all pairs of connected nodes.

$$p(\mathbf{x}) = \frac{1}{Z} \prod_i \psi_i(x_i, x_{\pi_i})$$

  where we can make $Z = 1$ with the choice $\psi_i = p(x_i|x_{\pi_i})$ except for one clique involving the root: $\psi_j = p(x_r)p(x_j|x_{\pi_j})$
- Trees have no "explaining-away" (converging arrows). Therefore, d-separation and regular separation are equivalent.
- Directed and undirected trees are equivalent and the choice of root is arbitrary (for fully observed models).
- Another characterization of trees: there is exactly one path between any pair of nodes (without doubling back).

Likelihood function

- Notation:

  $\mathbf{y}_i \equiv$ a node x_i and its single parent x_{π_i}.

  $\mathbf{V}_i \equiv$ set of joint configurations of node i and its parent x_{π_i}

  ($\mathbf{y}_{\text{root}} \equiv x_{\text{root}}$ and $\mathbf{V}_{\text{root}} \equiv \mathbf{v}_{\text{root}}$)

- Directed model likelihood:

$$\begin{aligned}
\ell(\theta; \mathcal{D}) &= \sum_n \log p(\mathbf{x}^n) = \sum_n \left[\log p_r(x_r^n) + \sum_{i \neq r} \log p({x_i}^n | {x_{\pi_i}}^n) \right] \\
&= \sum_n \sum_i \sum_{\mathbf{v} \in \mathbf{V}_i} [\mathbf{y}_i^n = \mathbf{v}] \log p_i(\mathbf{v}) \qquad \text{indicator trick} \\
&= \sum_i \sum_{\mathbf{v} \in \mathbf{V}_i} N_i(\mathbf{v}) \log p_i(\mathbf{v})
\end{aligned}$$

  where $N_i(\mathbf{v}) = \sum_n [\mathbf{y}_i^n = \mathbf{v}]$ and $p_i(\mathbf{v}_i) = p(x_i | x_{\pi_i})$.

More on the Likelihood function

- Undirected model likelihood:

$$\begin{aligned}\ell(\theta;\mathcal{D}) &= \sum_n \log \prod_i \psi_i(\mathbf{y}_i^n) \\ &= \sum_n \sum_i \sum_{\mathbf{v}\in\mathbf{V}_i} [\mathbf{y}_i^n = \mathbf{v}] \log \psi_i(\mathbf{v}) \\ &= \sum_i \sum_{\mathbf{v}\in\mathbf{V}_i} N_i(\mathbf{v}) \log \psi_i(\mathbf{v})\end{aligned}$$

  where $N_i(\mathbf{y}) = \sum_n [\mathbf{y}_i^n = \mathbf{y}]$ and $\psi_i(\mathbf{y}_i) = p(x_i|x_{\pi_i})$.
  (Except for one clique involving the root: $\psi_j = p(x_r)p(x_j|x_{\pi_j})$)

- Directed and undirected likelihoods are the same!

- Trees are in the exponential family with $\mathbf{y}_i$ as sufficient statistics.

Maximum Likelihood Parameters Given Structure

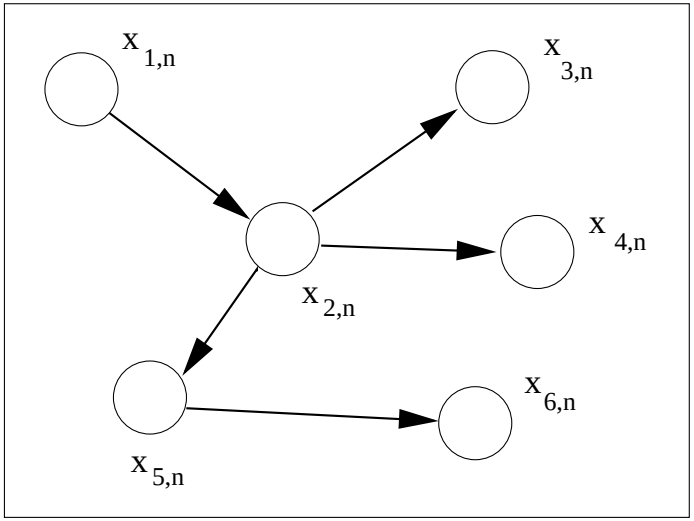
- Trees are just a special case of fully observed graphical models.
- For discrete data x_i with values v_i, each node stores a conditional probability table (CPT) over its values given its parent's value. The ML parameter estimates are just the empirical histograms of each node's values given its parent:

$$p^*(x_i = v_i | x_{\pi_i} = v_j) = \frac{N(x_i = v_i, x_{\pi_i} = v_j)}{\sum_{\mathbf{v}_i} N(x_i = v_i, x_{\pi_i} = v_j)} = \frac{N_i(\mathbf{y}_i)}{N_{\pi_i}(v_j)}$$

  except for the root which uses marginal counts $N_r(v_r)/N$.
- For continuous data, the most common model is a two-dimensional Gaussian at each node. The ML parameters are just to set the mean of $p_i(\mathbf{y}_i)$ to be the sample mean of $[x_i; x_{\pi_i}]$ and the covariance matrix to the sample covariance.
- In practice we should use some kind of smoothing/regularization.

Structure Learning

- What about the tree structure (links)?
  How do we know which nodes to make parents of which?



- Bold idea: how can we also *learn* the optimal structure?
  In principle, we could search all combinatorial structures, for each compute the ML parameters, and take the best one.
- But is there a better way? Yes. It turns out that structure learning in tree models can be converted to a good old computer science problem: maximum weight spanning tree.

Optimal Structure

- Let us rewrite the likelihood function:

$$\ell(\theta;\mathcal{D}) = \sum_{\mathbf{x}\in\mathbf{V}_{\text{all}}} N(\mathbf{x}) \log p(\mathbf{x})$$

$$= \sum_{\mathbf{x}} N(\mathbf{x}) \left(\log p(\mathbf{x}_r) + \sum_{i\neq r} \log p(x_i|x_{\pi_i}) \right)$$

- ML parameters, are equal to the observed frequency counts $q(\cdot)$:

$$\frac{\ell^*}{N} = \sum_{\mathbf{x}\in\mathbf{V}_{\text{all}}} q(\mathbf{x}) \left(\log q(\mathbf{x}_r) + \sum_{i\neq r} \log q(x_i|x_{\pi_i}) \right)$$

$$= \sum_{\mathbf{x}} q(\mathbf{x}) \left(\log q(\mathbf{x}_r) + \sum_{i\neq r} \log \frac{q(x_i, x_{\pi_i})}{q(x_{\pi_i})} \right)$$

$$= \sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i\neq r} \log \frac{q(x_i, x_{\pi_i})}{q(x_i)q(x_{\pi_i})} + \sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i} \log q(\mathbf{x}_i)$$

- NB: second term does not depend on structure.

Edge Weights

- Each term in sum $i \neq r$ corresponds to an edge from i to its parent.

$$\begin{aligned}
\frac{\ell^*}{N} &= \sum_{\mathbf{x}} q(\mathbf{x}) \sum_{i \neq r} \log \frac{q(x_i, x_{\pi_i})}{q(x_i) q(x_{\pi_i})} + C \\
&= \sum_{i \neq r} \sum_{x_i, x_{\pi_i}} q(x_i, x_{\pi_i}) \log \frac{q(x_i, x_{\pi_i})}{q(x_i) q(x_{\pi_i})} + C \\
&= \sum_{i \neq r} \sum_{\mathbf{y}_i} q(\mathbf{y}_i) \log \frac{q(\mathbf{y}_i)}{q(x_i) q(x_{\pi_i})} + C \\
&= \sum_{i \neq r} W(i; \pi_i) + C
\end{aligned}$$

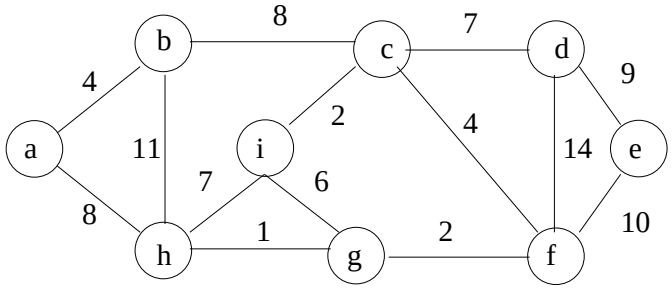
  where the edge weights W are defined by *mutual information*:

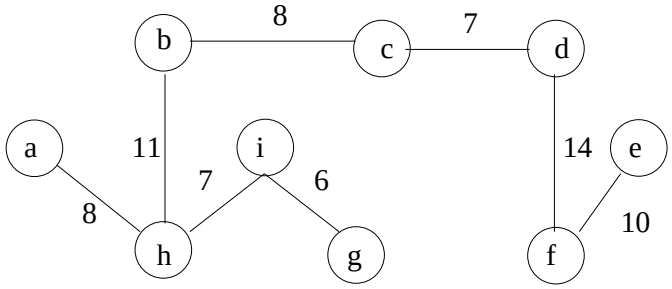
$$W(i; j) = \sum_{x_i, x_j} q(x_i, x_j) \log \frac{q(x_i, x_j)}{q(x_i) q(x_j)}$$

- So overall likelihood is sum of weights on edges that we use. We need the maximum weight spanning tree.

Kruskal's algorithm (Greedy Search)

- To find the maximum weight spanning tree A on a graph with nodes U and weighted edges E:
  1. $A \leftarrow \text{empty}$
  2. Sort edges E by nonincreasing weight: $e_1, e_2, \ldots, e_K$.
  3. for $k = 1$ to K $\{A \mathrel{+}= e_k$ unless doing so creates a cycle$\}$





Maximum Likelihood Trees

We can now completely solve the tree learning problem:

1. Compute the marginal counts $q(x_i)$ for each node and pairwise counts $q(x_i, x_j)$ for all pairs of nodes.
2. Set the weights to the mutual informations:

$$W(i;j) = \sum_{x_i, x_j} q(x_i, x_j) \log \frac{q(x_i, x_j)}{q(x_i) q(x_j)}$$

3. Find the maximum weight spanning tree A=MWST(W).
4. Using the undirected tree A chosen by MWST, pick a root arbitrarily and orient the edges away from the root.
   Set the conditional functions to the observed frequencies:

$$p(x_i | x_{\pi_i}) = \frac{q(x_i, x_{\pi_i})}{\sum_{x_i} q(x_i, x_{\pi_i})} = \frac{q(x_i, x_{\pi_i})}{q(x_{\pi_i})}$$

Notes

- *Any* directed tree consistent with the undirected tree found by the algorithm above will assign the same likelihood to any dataset.
- Amazingly, as far as likelihood goes, the root is arbitrary.
  We can just pick one node and orient the edges away from it.
  Or we can work with undirected models.
- For continuous nodes (e.g. Gaussian), the situation is similar, except that computing the mutual information requires an integral.
- Mutual information is the *Kullback-Leibler* divergence (cross-entropy) between a distribution and the product of its marginals. Measures how far from independent the joint distribution is.

$$W(i;j) = \mathrm{I}[x_i; x_j] = \mathrm{KL}[q(x_i, xj) \| q(x_i) q(x_j)]$$

Beyond trees

- Mixtures of trees - add hidden variables
- General graphs - local search

Bayesian model averaging (K&F 14.5)

- So far, we have just tried to find the mode of $P(G|D)$, i.e., the best scoring network.
- But the mode may be untypical of the distribution: most of the mass may be elsewhere.
- Suppose we are trying to determine if there is an edge $X \rightarrow Y$ in the "true" model.
- We can compute features like this using

$$P(f|D) = \sum_G f(G) P(G|D)$$

  where $P(G|D) \propto P(D|G)P(G) \propto \prod_i \exp \mathsf{FamScore}(D(X_i, \Pi_i))$.
- The main problem is that there are $2^{\Theta(n^2)}$ DAGs on n nodes.
- Even if we restrict indegree to $\leq d$, there are still $2^{\Theta(dn \log n)}$ DAGs.

MCMC FOR FEATURE PROBABILITY

- Suppose we can find a set G' of high-scoring networks. Then

$$P(f|D) \approx \frac{\sum_{G \in G'} P(G|D) f(G)}{\sum_{G \in G'} P(G|D)}$$

- If we can uniformly sample graphs from $P(G|D)$, we can approximate this using

$$P(f|D) \approx \frac{1}{T} f(G_t)$$

  where G_k is the k'th sample.

- Markov chain Monte Carlo (MCMC) provides a way of sampling from complex distributions such as this.

MCMC

- We define a Markov chain on graph structures (in this case) with transition probability given by the Metropolis-Hastings rule

$$P(G'|G) = \min\left(1, \frac{P(G'|D)Q(G'|G)}{P(G|D)Q(G|Q')}\right)$$

  where $Q(G'|G)$ is the *proposal probability* and the ratio is the *acceptance probability*.

- The proposal Q has to be such that the Markov chain is ergodic, i.e., we can get to any state from any other state.

- We start the chain off in some inital state and then perform a random walk according to the above dynamics.

- Theory shows the stationary distribution of such a Markov chain is $P(G|D)$.

MCMC convergence

- The *mixing time* is how long it takes the chain to converge from a random starting point.
- Once the chain has converged (after the *burnin*), we can draw (correlated) samples from $P(G|D)$.
- We can diagnose convergence by running the chain from multiple starting points and comparing the results. (Diagnosing convergence is an open problem.)

MCMC for DAG structure

- Suppose the proposal Q picks randomly from the following operators (where legal): add an edge, delete an edge, reverse an edge.
- The MH acceptance probability requires computing the Bayes factor $P(G'|D)/P(G|D)$, which is efficient for decomposable scores.
- However, small changes to the graph can result in large changes to the score, resulting in a jagged landscape.
- So the chain does not mix rapidly (it gets stuck in local optima).

Rao-Blackwellised MCMC

- An alternative idea is to do MCMC sampling in the space of node orderings $\prec$, which "only" has size $n!$.
- Given an ordering, we can sum over all graphs efficiently (see below). Hence

$$P(f|D) \approx \frac{1}{T} P(f|D, \prec_t)$$

- This combination of sampling and exact integration/ marginalization is called Rao-Blackwellised sampling.
- This is named after the Rao-Blackwell theorem, which says (roughly) that variance is reduced if you sample in a smaller space:

$$\mathsf{Var}E\left[E[f(G)|\prec]\right] \leq \mathsf{Var}E[f(G)]$$

MCMC over orderings

- We use Metropolis-Hastings as before.
- One proposal is to flip 2 variables in the order, leaving the rest unchanged:

$$(X_{i_1}, \ldots, \mathbf{X_{i_j}}, \ldots, \mathbf{X_{i_k}}, \ldots, X_{i_n}) \rightarrow (X_{i_1}, \ldots, \mathbf{X_{i_k}}, \ldots, \mathbf{X_{i_j}}, \ldots, X_{i_n})$$

- Using score decomposability, only family scores for nodes inside the bold range need to be recomputed.
- This is much more expensive than MCMC in DAG space, but each move is much more powerful, and the space is much smaller.

Marginal likelihood given known node ordering

- If we know the ordering (eg. temporal), we have

$$P(D|\prec) = \sum_{G \in G_{d,\prec}} P(G|\prec) P(D|G)$$

- Given $\prec$, we can pick the parents for each node independently. Let $U_{i,\prec} = \{U : U \prec X_i, |U| \leq d\}$. Assuming $P(G|\prec)$ is uniform for legal graphs,

$$\begin{aligned} P(D|\prec) &= \sum_{G \in G_{d,\prec}} \prod_i \exp \mathsf{FamScore}(D(X_i, \pi_i)) \\ &= \prod_i \sum_{U_i \in U_{i,\prec}} \exp \mathsf{FamScore}(D(X_i, \pi_i)) \end{aligned}$$

- We marginalize out parameters θ and graph structures G.
- This is what we need to evaluate the MH acceptance probability.

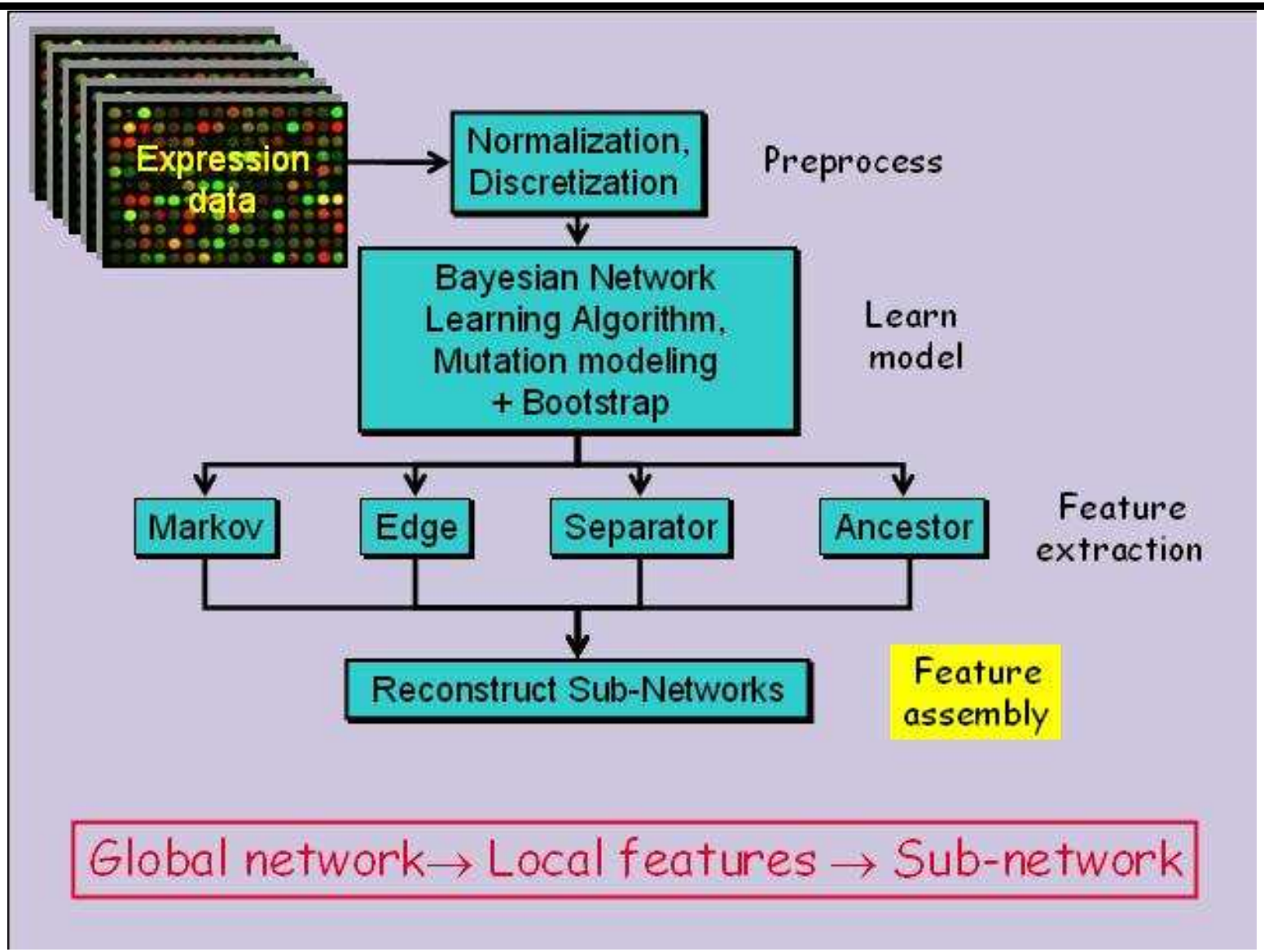
Prob. feature given known node ordering

- Given a sampled ordering, we can compute the probability of a parent set

$$P(\pi_i^G = U | D, \prec) = \frac{\exp \mathsf{FamScore}(D(X_i, U))}{\sum_{U' \in U_{i,\prec}} \exp \mathsf{FamScore}(D(X_i, U'))}$$

- From this, we can sample parents and hence graphs compatible with $\prec$.
- From this, we can compute probability of features such as "There is a directed path from X_i to X_j".
- Useful for determining features of biological networks from small sets of data.

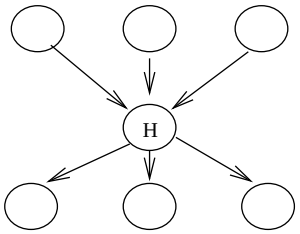
Learning gene regulatory pathways



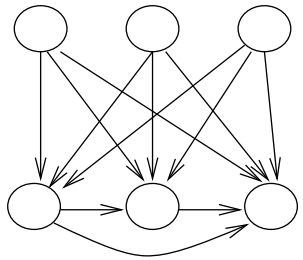
(Slide from Nir Friedman)

Hidden variables (K&F 15.7)

- So far, we have assumed all variables have been observed.
- In this case, we can compute the Bayesian score (evidence) exactly.
- But hidden variables can simplify a model a lot
  eg. mixture models, HMMs.



17 parameters

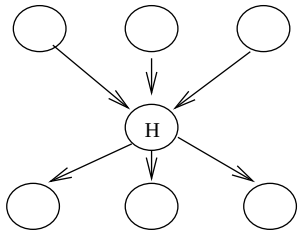


59 parameters

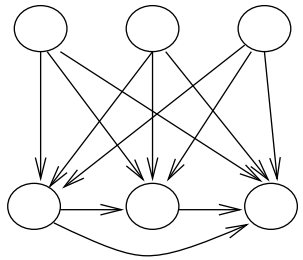
- Can still run local search to pick best model.
- But hidden variables raise various problems:
  - Efficiently computing the score from partially observed data.
  - Detecting the presence of latent (confounding) factors.
  - Inferring the dimensionality/ cardinality of latent factors.

Detecting presence of hidden variables

- One idea is to look for dense semi-cliques.



17 parameters



59 parameters

- Then insert a hidden variable "in the middle", and let the search algorithm figure out the detailed "wiring".
- Unfortunately, many scoring criteria (e.g., BIC) produce very sparse graphs, which makes such semi-cliques rare.
- Constraint-based methods sometimes can be used to detect confounding.
- In general, this is an open problem.

Structural EM algorithm (K&F 15.6)

- Assume the number of hidden variables is given. Let y be the observed nodes, s be hidden, and $z = (x, y)$ be all nodes.
- We can compute the BIC score for each candidate structure G' by applying EM to each one:

$$\text{score}_{BIC}(G'|y) = \log P(y|G', \hat{\theta}) - \frac{d(G)}{2} \log N$$

- But this is very expensive.
- Idea of structural EM: use current model (G, θ) to compute the expected sufficient statistics (ESS) needed to evaluate each neighbor G', i.e., compute the expected BIC score.
- This requires computing ESS for nodes and potentially new parents; such sets may not reside inside a clique of the jtree for G.
- Application: phylogenetic trees.

Approximating the evidence in latent variable models

- When there are hidden variables, the parameter posterior has an exponential number of modes.
- Hence computing the marginal likelihood is intractable.
- There are various possible approximations:
  - Laplace
  - BIC
  - Cheeseman-Stutz (CS) lower bound
  - Variational Bayes EM lower bound
  - Sampling

Expectation-Maximization (EM) Algorithm

- EM is an optimization strategy for objective functions that can be interpreted as likelihoods in the presence of missing data.
- It is much simpler than gradient methods:
  - No need to choose step size.
  - Enforces constraints automatically.
  - Calls inference and fully observed learning as subroutines.
- EM is an Iterative algorithm with two linked steps:
  - E-step: fill-in hidden values using inference, $p(\mathbf{z}|\mathbf{x}, \theta^t)$.
  - M-step: update parameters θ^{t+1} using standard MLE/MAP method applied to completed data
- We will prove that this procedure monotonically improves ℓ (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.

Complete & Incomplete Log Likelihoods

- Observed variables $\mathbf{x}$, latent variables $\mathbf{z}$, parameters θ:

$$\ell_c(\theta; \mathbf{x}, \mathbf{z}) = \log p(\mathbf{x}, \mathbf{z}|\theta)$$

  is the *complete log likelihood*.

- Usually optimizing $\ell_c(\theta)$ given both $\mathbf{z}$ and $\mathbf{x}$ is straightforward. (e.g. class conditional Gaussian fitting, linear regression)

- With $\mathbf{z}$ unobserved, we need the log of a marginal probability:

$$\ell(\theta; \mathbf{x}) = \log p(\mathbf{x}|\theta) = \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta)$$

  which is the *incomplete log likelihood*.

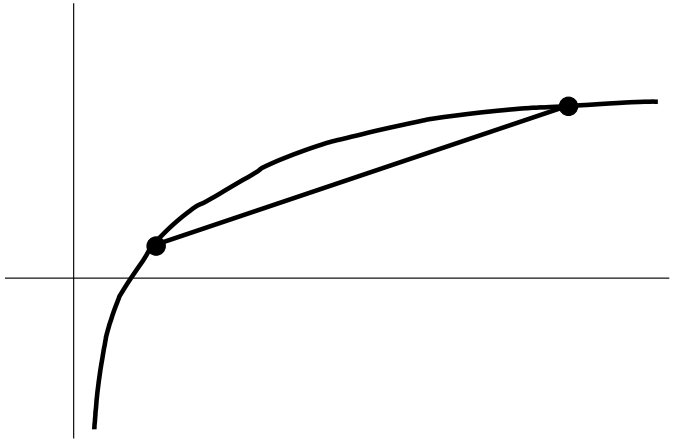
Expected Complete Log Likelihood

- For *any* distribution $q(\mathbf{z})$ define *expected complete log likelihood*:

$$\ell_q(\theta; \mathbf{x}) = \langle \ell_c(\theta; \mathbf{x}, \mathbf{z}) \rangle_q \equiv \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$$

- Amazing fact: $\ell(\theta) \geq \ell_q(\theta) + \mathcal{H}(q)$ because of concavity of $\log$:

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



- Where the inequality is called *Jensen's inequality*.
  (It is only true for distributions: $\sum q(\mathbf{z}) = 1;\ q(\mathbf{z}) > 0$.)

Lower Bounds and Free Energy

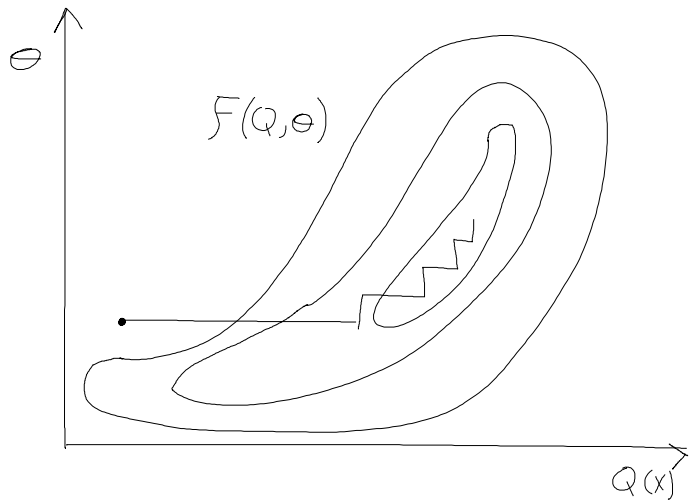
- For fixed data $\mathbf{x}$, define a functional called the *free energy*:

$$F(q,\theta) \equiv \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{x},\mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \leq \ell(\theta)$$

- The EM algorithm is coordinate-ascent on F:

$$\textbf{E-step:} \quad q^{t+1} = \operatorname{argmax}_q \; F(q,\theta^t)$$

$$\textbf{M-step:} \quad \theta^{t+1} = \operatorname{argmax}_\theta \; F(q^{t+1},\theta^t)$$



M-step: maximization of expected ℓ_c

- Note that the free energy breaks into two terms:

$$\begin{aligned} F(q,\theta) &= \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{x},\mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \\ &= \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x},\mathbf{z}|\theta) - \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log q(\mathbf{z}|\mathbf{x}) \\ &= \ell_q(\theta;\mathbf{x}) + \mathcal{H}(q) \end{aligned}$$

  (this is where its name comes from)

- 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:

$$\theta^{t+1} = \operatorname{argmax}_\theta \ell_q(\theta;\mathbf{x}) = \operatorname{argmax}_\theta \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x},\mathbf{z}|\theta)$$

E-step: inferring latent posterior

- Claim: the optimim setting of q in the E-step is:

$$q^{t+1} = p(\mathbf{z}|\mathbf{x}, \theta^t)$$

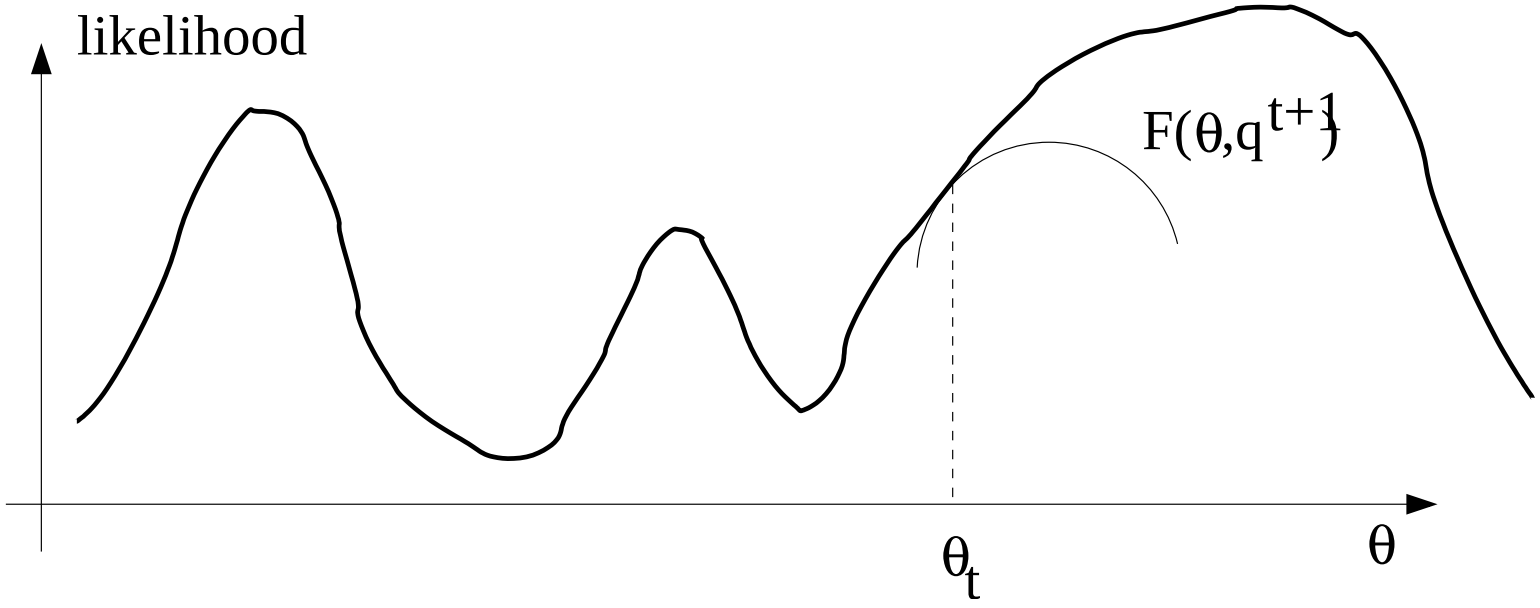
- This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform classification).
- Proof (easy): this setting saturates the bound $\ell(\theta; \mathbf{x}) \geq F(q, \theta)$

$$\begin{aligned} F(p(\mathbf{z}|\mathbf{x}, \theta^t), \theta^t) &= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \log \frac{p(\mathbf{z}|\mathbf{x}, \theta^t) p(\mathbf{x}|\theta^t)}{p(\mathbf{z}|\mathbf{x}, \theta^t)} \\ &= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \log p(\mathbf{x}|\theta^t) \\ &= \log p(\mathbf{x}|\theta^t) \textstyle\sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \\ &= \ell(\theta; \mathbf{x}) \cdot 1 \end{aligned}$$

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

EM Constructs Sequential Convex Lower Bounds

- Consider the likelihood function and the function $F(q^{t+1}, \cdot)$.



Recap: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds ML 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 our best guess (posterior) and updating the paramters based on this guess:
  E-step: $q^{t+1} = p(\mathbf{z}|\mathbf{x}, \theta^t)$
  M-step: $\theta^{t+1} = \text{argmax}_\theta \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

Variational Bayes EM (VBEM) algorithm

- Latent variables are now x *and parameters* θ, observations are y.
- Goal: Maximize lower bound on marginal likelihood $P(y)$.
- Key assumption: assume a factorized posterior $q(x, \theta) \approx q_x(x) q_\theta(\theta)$:

$$\log p(y) \geq \int q_x(x) q_\theta(\theta) \log \frac{p(y, x, \theta)}{q_x(x) q_\theta(\theta)} \; dx d\theta \stackrel{\text{def}}{=} F(q_x(x), q_\theta(\theta), y)$$

- Replaces stochastic dependence between x and θ with deterministic constraints on moments.
- VB E step:

$$q_x^{t+1}(x) \propto \exp\left[\int \log p(x, y|\theta) q_\theta^t(\theta) d\theta\right]$$

- VB M step:

$$q_\theta^{t+1}(\theta) \propto p(\theta) \exp\left[\int \log p(x, y|\theta) q_x^{t+1}(x) dx\right]$$

Conjugate exponential models

- Assumption 1: the complete-data log-likelihood is that of an exponential family:

$$p(x, y|\theta) = f(x, y)g(\theta)\exp(\phi(\theta)^T u(x, u))$$

- Assumption 2: the parameter prior is conjugate to the likelihood:

$$p(\theta|\eta, \nu) = h(\eta, \nu)g(\theta)^\eta \exp(\phi(\theta)^T \nu)$$

- Thm: at every step of VBEM, the parameter posterior is

$$q(\theta|\eta + n, \nu + \sum_{i=1}^{n} \overline{u}(y_i)), \text{ where } \overline{u}(y_i) = E_{q_{x_i}} u(x_i, y_i)$$

and the latent variable posterior is $q_x(x) = \prod_i q_{x_i}(x_i)$ where

$$q_{x_i}(x_i) = p(x_i|y, \overline{\phi}) \propto f(x_i, y_i)\exp\left[\overline{\phi}^T u(x_i, y_i)\right] \text{ where } \overline{\phi} = E_{q_\theta}\phi(\theta)$$

VBEM in practice

- E-step: Do inference as usual, but use parameters $\tilde{\theta}$ s.t. $\phi(\tilde{\theta}) = \overline{\phi}$ (expected natural parameters)
- M-step: update hyper-parameters using expected sufficient statistics.
- The normalizing constant of inference is a lower bound on $p(y)$.
- Examples: HMMs, factor analysis (PCA), linear dynamical systems
- Variational message passing (VMP) is a way of implementing VBEM for any conjugate-exponential model, but makes the additional mean-field approximation that $q(x) = \prod_k q(x_k)$.

VBEM for model selection