Lecture 2b:

Inference in Chains and Trees, Message Passing, Belief Propagation

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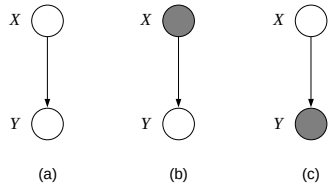
Thursday August 17, 2006
CIAR Summer School, Toronto

Simple Case: Bayes Rule

- For simple models, we can derive the inference formulas by hand using Bayes rule (e.g. responsibility in mixture models).



$$a) \quad p(x,y) = p(x)p(y|x)$$
$$b) \quad p(y|x)$$
$$c) \quad p(x|y) = \frac{p(x)p(y|x)}{\sum_x p(x)p(y|x)}$$

This is called "reversing the arrow".

- In general, the calculation we want to do is:

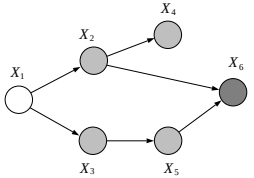
$$p(\mathbf{x}_F|\mathbf{x}_E) = \frac{\sum_{\mathbf{x}_R} p(\mathbf{x}_E, \mathbf{x}_F, \mathbf{x}_R)}{\sum_{\mathbf{x}_F, \mathbf{x}_R} p(\mathbf{x}_E, \mathbf{x}_F, \mathbf{x}_R)}$$

- Q: Can we do these sums efficiently?
  Can we avoid repeating unecessary work each time we do inference?
  A: Yes, if we exploit the factorization of the joint distribution.

Probabilistic Inference

- Partition the random variables in a domain $\mathbf{X}$ into three disjoint subsets, $\mathbf{x}_E$,$\mathbf{x}_F$,$\mathbf{x}_R$. The general *probabilistic inference* problem is to compute the posterior $p(\mathbf{x}_F|\mathbf{x}_E)$ over *query nodes* $\mathbf{x}_F$.
- This involves *conditioning* on *evidence nodes* $\mathbf{x}_E$ and *integrating (summing) out marginal nodes* $\mathbf{x}_R$.
- If the joint distribution is represented as a huge table, this is trivial: just select the appropriate indicies in the columns corresponding to $\mathbf{x}_E$ based on the values, sum over the columns corresponding to $\mathbf{x}_R$, and renormalize the resulting table over $\mathbf{x}_F$.
- If the joint is a known continuous function this can sometimes be done analytically. (e.g. Gaussian: eliminate rows/cols corresponding to $\mathbf{x}_R$; apply conditioning formulas for $p(\mathbf{x}_F|\mathbf{x}_E)$).
- But what if the joint distribution over $\mathbf{X}$ is represented by a directed or undirected graphical model?

Example



The key is to factor and then apply the distributive law.

$$p(\mathbf{x}_1|\bar{\mathbf{x}}_6) = p(\mathbf{x}_1, \bar{\mathbf{x}}_6)/p(\bar{\mathbf{x}}_6)$$
$$= p(\mathbf{x}_1, \bar{\mathbf{x}}_6)/\sum_{\mathbf{x}_1'} p(\mathbf{x}_1', \bar{\mathbf{x}}_6)$$

$$p(\mathbf{x}_1, \bar{\mathbf{x}}_6) = \sum_{\mathbf{x}_2}\sum_{\mathbf{x}_3}\sum_{\mathbf{x}_4}\sum_{\mathbf{x}_5} p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1)p(\mathbf{x}_4|\mathbf{x}_2)p(\mathbf{x}_5|\mathbf{x}_3)p(\bar{\mathbf{x}}_6|\mathbf{x}_2, \mathbf{x}_5)$$
$$= p(\mathbf{x}_1)\sum_{\mathbf{x}_2} p(\mathbf{x}_2|\mathbf{x}_1)\sum_{\mathbf{x}_3} p(\mathbf{x}_3|\mathbf{x}_1)\sum_{\mathbf{x}_4} p(\mathbf{x}_4|\mathbf{x}_2)\sum_{\mathbf{x}_5} p(\mathbf{x}_5|\mathbf{x}_3)p(\bar{\mathbf{x}}_6|\mathbf{x}_2, \mathbf{x}_5)$$
$$= p(\mathbf{x}_1)\sum_{\mathbf{x}_2} p(\mathbf{x}_2|\mathbf{x}_1)\sum_{\mathbf{x}_3} p(\mathbf{x}_3|\mathbf{x}_1)\Phi_5(\mathbf{x}_2, \mathbf{x}_3)\sum_{\mathbf{x}_4} p(\mathbf{x}_4|\mathbf{x}_2)$$
$$= p(\mathbf{x}_1)\sum_{\mathbf{x}_2} p(\mathbf{x}_2|\mathbf{x}_1)\Phi_4(\mathbf{x}_2)\sum_{\mathbf{x}_3} p(\mathbf{x}_3|\mathbf{x}_1)\Phi_5(\mathbf{x}_2, \mathbf{x}_3)$$
$$= p(\mathbf{x}_1)\sum_{\mathbf{x}_2} p(\mathbf{x}_2|\mathbf{x}_1)\Phi_4(\mathbf{x}_2)\Phi_3(\mathbf{x}_1, \mathbf{x}_2)$$
$$= p(\mathbf{x}_1)\Phi_2(\mathbf{x}_1)$$

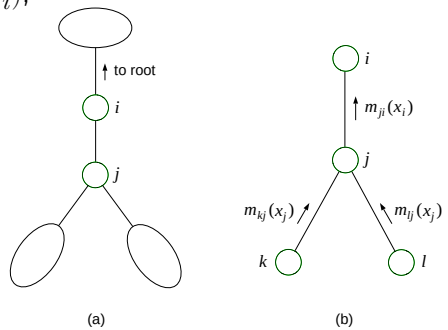
Marginalization without Evidence

- Marginalization of joint distributions represented by graphical models is a special case of probabilistic inference.
- To compute the marginal $p(x_i)$ of a single node, we set it to be the query node and set the evidence set to be empty.
- In directed models, we can ignore all nodes downstream from the query node, and marginalize only the part of the graph before it.
- If the node has no parents, we can read off its marginal directly.
- In directed models, we often know that a certain sum must evaluate to unity, since it is a conditional probability.
- For example, consider the term $\Phi_4(\mathbf{x}_2)$ in our six node example:

$$\Phi_4(\mathbf{x}_2) = \sum_{\mathbf{x}_4} p(\mathbf{x}_4|\mathbf{x}_2) \equiv 1$$

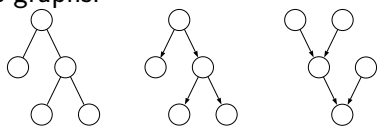
Efficient Summation on Trees: Leaves → Root

- Consider summing out node j which is has node i as its parent:
- Which nodes appear in the factors created by summing over j?
  - nothing in the subtree below j (already summed out)
  - nothing from other subtrees, since the graph is a tree
  - only i, which relates i and j through $p(j|i)$
- Call the factor that is created $m_{ji}(x_i)$, and think of it as a *message* that j passes to i when j is summed.
- This message is created by summing over j the product of all earlier messages $m_{kj}(x_j)$ sent to j as well as $\delta(x_j = x_j^{obs})$ (if j is an evidence node).



Efficient Inference on Tree Structured DAGs

- We want to develop inference algorithms which are correct and efficient when we perform multiple queries (e.g. during learning with latent variables and EM).
- For now, we will focus on tree-structured graphical models, which include all two-node models and all chains as well.
- Exact inference on trees is the basis for the *junction tree algorithm* which solves the general exact inference problem for directed acyclic graphs and for many *approximate* algorithms which can work on intractable or cyclic graphs.



- For starters, let us imagine that the query is a single node (root).

Inference = Efficient Summation = Message Passing

- On a tree, inference can be thought of as passing messages up to the query node at the root from the other nodes at the leaves or interior. Since we ignore subtrees with no evidence, observed (evidence) nodes at always at the leaves.
- The message $m_{ji}(x_i)$ is created when we sum over x_j

$$m_{ji}(x_i) = \sum_{x_j} \left(\psi^E(x_j) p(x_j|x_i) \prod_{k \in c(j)} m_{kj}(x_j) \right)$$

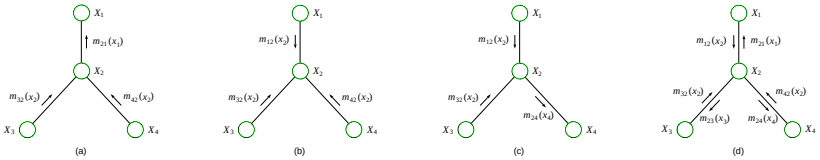
- At the final node x_f, we obtain the answer:

$$p(x_f|\bar{\mathbf{x}}_E) \propto \psi^E(x_f) \prod_{k \in c(f)} m_{kf}(x_f)$$

- If j is an evidence node, $\psi^E(x_j) = \delta(x_j, \bar{x}_j)$, else $\psi^E(x_j) = 1$.
- If j is a leaf node, $c(j)$ is empty, otherwise $c(j)$ are the children of j

Messages are Reused in Multiple Queries

- Consider querying x_1, x_2, x_3 and x_4 in the graph below.
- The messages needed for x_1, x_2, x_4 individually are shown (a-c).
- Also shown in (d) is the set of messages needed to compute all possible marginals over single query nodes.



- Key insight: even though the naive approach (redo the query from scratch) needs to compute N^2 messages to find marginals for all N query nodes, there are only $2N$ possible messages.
- We can compute all possible messages in only double the amount of work it takes to do one query!
- Then we take the product of relevant messages to get marginals.

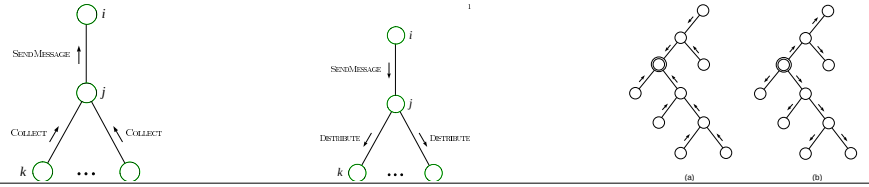
Belief Propagation (Sum-Product) Algorithm

- Choose a root node (arbitrarily or as first query node).
- If j is an evidence node, $\psi^E(x_j) = \delta(x_j, \bar{x}_j)$, else $\psi^E(x_j) = 1$.
- Pass messages from leaves up to root and then back down using:

$$m_{ji}(x_i) = \sum_{x_j} \left(\psi^E(x_j)\psi(x_i, x_j) \prod_{k \in c(j)} m_{kj}(x_j) \right)$$

- Given messages, compute marginals using:

$$p(x_i|\bar{\mathbf{x}}_E) \propto \psi^E(x_i) \prod_{k \in c(i)} m_{ki}(x_i)$$



Computing All Possible Messages

- How can we compute all possible messages efficiently?
- Idea: respect the following Message-Passing-Protocol: *A node can send a message to a neighbour only when it has received messages from all its other neighbours.*
- Protocol is realizable: designate one node (arbitrarily) as the root. Collect messages inward to root then distribute back out to leaves.
- Once we have the messages, we can compute marginals using:

$$p(x_i|\bar{\mathbf{x}}_E) \propto \psi^E(x_i) \prod_{k \in c(i)} m_{ki}(x_i)$$

- Remember that the directed tree on which we pass messages might not be same directed tree we started with.
- We can also consider "synchronous" or "asynchronous" message passing nodes that respect the protocol but don't use the Collect-Distribute schedule above. (Must prove this terminates.)

Computing Joint Pairwise Posteriors

- We can also easily compute the joint pairwise posterior distribution for any pair of connected nodes x_i, x_j.
- To do this, we simply take the product of all messages coming into node i (*except the message from node* j), all the messages coming into node j (*except the message from node* i) and the potentials $\psi_i(x_i), \psi_j(x_j), \psi_{ij}(x_i, x_j)$.
- The posterior is proportional to this product:

$$p(x_i, x_j|\bar{\mathbf{x}}_E) \propto \psi^E(x_i)\psi^E(x_j)\psi(x_i, x_j) \prod_{k \neq j \in c(i)} m_{ki}(x_i) \prod_{\ell \neq i \in c(j)} m_{\ell j}(x_j)$$

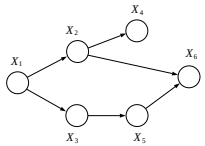
- These joint pairwise posteriors cover all the maximal cliques in the tree, and so those are all we need to do learning.
- Inference of other pairwise or higher order joint posteriors is possible, but more difficult.

Maximizing instead of Summing

- Belief Propagation summed over all possible values of the marginal (non-query, non-evidence) nodes to get a marginal probability.
- What if we wanted to *maximize* over the non-query, non-evidence nodes to find the probabilty of the single best setting consistent with any query and evidence?

$$\max_{\mathbf{x}} p(\mathbf{x}) = \max_{\mathbf{x}_1}\max_{\mathbf{x}_2}\max_{\mathbf{x}_3}\max_{\mathbf{x}_4}\max_{\mathbf{x}_5} p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1)p(\mathbf{x}_3|\mathbf{x}_1)p(\mathbf{x}_4|\mathbf{x}_2)p(\mathbf{x}_5|\mathbf{x}_3)p(\mathbf{x}_6|\mathbf{x}_2,\mathbf{x}_5)$$
$$= \max_{\mathbf{x}_1} p(\mathbf{x}_1)\max_{\mathbf{x}_2} p(\mathbf{x}_2|\mathbf{x}_1)\max_{\mathbf{x}_3} p(\mathbf{x}_3|\mathbf{x}_1)\max_{\mathbf{x}_4} p(\mathbf{x}_4|\mathbf{x}_2)\max_{\mathbf{x}_5} p(\mathbf{x}_5|\mathbf{x}_3)p(\mathbf{x}_6|\mathbf{x}_2,\mathbf{x}_5)$$

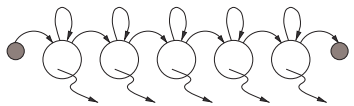
- This is known as the *maximum a-posteriori* or MAP configuration.
- It turns out that (on trees), we can use an algorithm exactly like belief-propagation to solve this problem.



Hidden Markov Models (HMMs)

Add a latent (hidden) variable x_t to a Markov model.

- HMM $\equiv$ " probabilistic function of a Markov chain":
  1. 1st-order Markov chain generates hidden state sequence (path):
  $$\mathrm{P}(x_{t+1} = j|x_t = i) = S_{ij} \qquad \mathrm{P}(x_1 = j) = \pi_j$$
  2. A set of output probability distributions $A_j(\cdot)$ (one per state) converts state path into sequence of observable symbols/vectors
  $$\mathrm{P}(\mathbf{y}_t = y|x_t = j) = A_j(y)$$

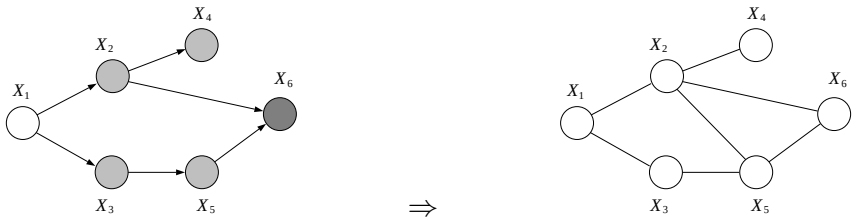


(state transition diagram)

- Even though hidden state seq. is 1st-order Markov, the output process is not Markov of *any* order [ex. 1111121111311121111131...]

Moralization in Non-Tree DAGs

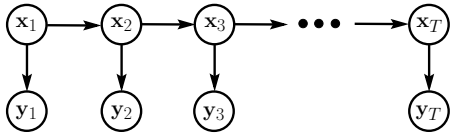
- For directed graphs, the parents may not be explicitly connected, but they are involved in the same potential function $p(x_i|\mathbf{x}_{\pi_i})$.
- Thus to correctly account for all the dependencies, we first must connect all the parents of every node and the drop the directions on the links.
- This step is known as "Moralization" and it is essential: since conditioning couples parents in directed models ("explaining away") we need a mechanism for respecting this when we do inference.



Applications of HMMs

- Speech recognition.
- Language modeling.
- Information retrieval.
- Motion video analysis/tracking.
- Protein sequence and genetic sequence alignment and analysis.
- Financial time series prediction.
- ...

HMM Graphical Model



- Hidden states $\{x_t\}$, outputs $\{\mathbf{y}_t\}$
  Joint probability factorizes:

$$\begin{aligned}\mathsf{P}(\{\mathbf{x}\},\{\mathbf{y}\}) &= \prod_{t=1}^{T} \mathsf{P}(x_t|\mathbf{x}_{t-1})\mathsf{P}(\mathbf{y}_t|x_t) \\ &= \pi_{\mathbf{x}_1} \prod_{t=1}^{T-1} S_{x_t,x_{t+1}} \prod_{t=1}^{T} A_{x_t}(\mathbf{y}_t)\end{aligned}$$

- NB: Data are *not* i.i.d.
  There is no easy way to use plates to show this model. (Why?)

Example: HMM Likelihood Calculation

- To evaluate the probability $\mathsf{P}(\{\mathbf{y}\})$, we want:

$$\mathsf{P}(\{\mathbf{y}\}) = \sum_{\{\mathbf{x}\}} \mathsf{P}(\{\mathbf{x}\},\{\mathbf{y}\})$$

$$\mathsf{P}(\text{observed sequence}) = \sum_{\text{all paths}} \mathsf{P}(\text{ observed outputs , state path })$$

- Looks hard! (#paths = #states^T). But joint probability factorizes:

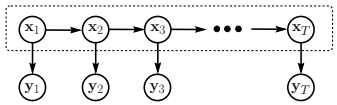
$$\mathsf{P}(\{\mathbf{y}\}) = \sum_{\mathbf{x}_1}\sum_{\mathbf{x}_2}\cdots\sum_{\mathbf{x}_T}\prod_{t=1}^{T} \mathsf{P}(x_t|\mathbf{x}_{t-1})\mathsf{P}(\mathbf{y}_t|x_t)$$

$$= \sum_{\mathbf{x}_1} \mathsf{P}(\mathbf{x}_1)\mathsf{P}(\mathbf{y}_1|\mathbf{x}_1) \sum_{\mathbf{x}_2} \mathsf{P}(\mathbf{x}_2|\mathbf{x}_1)\mathsf{P}(\mathbf{y}_2|\mathbf{x}_2)\cdots\sum_{\mathbf{x}_T} \mathsf{P}(\mathbf{x}_T|\mathbf{x}_{T-1})\mathsf{P}(\mathbf{y}_T|\mathbf{x}_T)$$

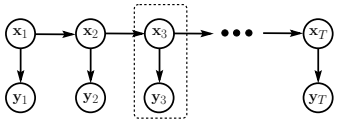
- By moving the summations inside, we can save a lot of work.

Links to Other Models

- You can think of an HMM as:
  A Markov chain with stochastic measurements.



  or
  A mixture model with states coupled across time.



- The future is independent of the past given the present.
  However, conditioning on all the observations couples hidden states.

The forward (α) recursion

- We want to compute:

$$L = \mathsf{P}(\{\mathbf{y}\}) = \sum_{\{\mathbf{x}\}} \mathsf{P}(\{\mathbf{x}\},\{\mathbf{y}\})$$

- There is a clever "forward recursion" to compute the sum efficiently.

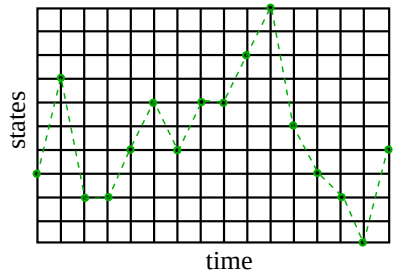
$$\begin{aligned}\alpha_j(t) &= \mathsf{P}(\ \mathbf{y}_1^t\ ,\ x_t = j\ ) \\ \alpha_j(1) &= \pi_j A_j(\mathbf{y}_1) \\ \alpha_k(t+1) &= \{\sum_j \alpha_j(t) S_{jk}\} A_k(\mathbf{y}_{t+1})\end{aligned}$$

- Notation: $\mathbf{x}_a^b \equiv \{\mathbf{x}_a,\ldots,\mathbf{x}_b\}$; $\mathbf{y}_a^b \equiv \{\mathbf{y}_a,\ldots,\mathbf{y}_b\}$
- This enables us to easily (cheaply) compute the desired likelihood L since we know we must end in some possible state:

$$L = \sum_k \alpha_k(T)$$

HMM Inference: Bugs on a Grid

- Naive algorithm:
  1. start bug in each state at t=1 holding value 0
  2. move each bug forward in time: make copies & increment the value of each copy by transition prob. + output emission prob.
  3. go to 2 until all bugs have reached time T
  4. sum up values on all bugs



HMMs: Inference of Hidden States

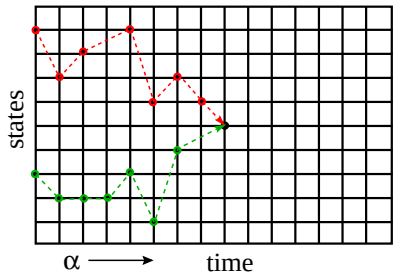
- What if we we want to estimate the hidden states given observations? To start with, let us estimate a single hidden state:

$$p(x_t|\{\mathbf{y}\}) = \gamma(x_t) = \frac{p(\{\mathbf{y}\}|x_t)p(x_t)}{p(\{\mathbf{y}\})}$$
$$= \frac{p(\mathbf{y}_1^t|x_t)p(\mathbf{y}_{t+1}^T|x_t)p(x_t)}{p(\mathbf{y}_1^T)}$$
$$= \frac{p(\mathbf{y}_1^t, x_t)p(\mathbf{y}_{t+1}^T|x_t)}{p(\mathbf{y}_1^T)}$$
$$p(x_t|\{\mathbf{y}\}) = \gamma(x_t) = \frac{\alpha(x_t)\beta(x_t)}{p(\mathbf{y}_1^T)}$$

where
$$\alpha_j(t) = p(\, \mathbf{y}_1^t \,,\, x_t = j \,)$$
$$\beta_j(t) = p(\mathbf{y}_{t+1}^T \mid x_t = j \,)$$
$$\gamma_i(t) = p(x_t = i \mid \mathbf{y}_1^T)$$

Bugs on a Grid - Trick

- Clever recursion:
  adds a step between 2 and 3 above which says: at each node, replace all the bugs with a single bug carrying the sum of their values



- This trick is called *dynamic programming*, and can be used whenever we have a summation, search, or maximization problem that can be set up as a grid in this way. The axes of the grid don't have to be "time" and "states".

Forward-Backward Algorithm

- We compute these quantites efficiently using another recursion. Use total prob. of all paths going through state i at time t to compute the *conditional* prob. of being in state i at time t:

$$\gamma_i(t) = p(x_t = i \mid \mathbf{y}_1^T)$$
$$= \alpha_i(t)\beta_i(t)/L$$

  where we defined:

$$\beta_j(t) = p(\mathbf{y}_{t+1}^T \mid x_t = j \,)$$

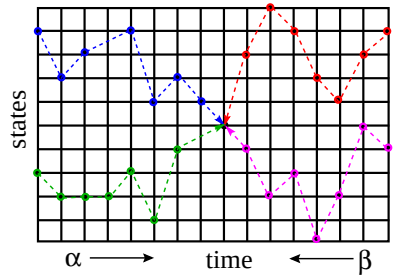
- There is also a simple recursion for $\beta_j(t)$:

$$\beta_j(t) = \sum_i S_{ji}\beta_i(t+1)A_i(\mathbf{y}_{t+1})$$
$$\beta_j(T) = 1$$

- $\alpha_i(t)$ gives total *inflow* of prob. to node (t, i)
  $\beta_i(t)$ gives total *outflow* of prob.

Forward-Backward Algorithm

- $\alpha_i(t)$ gives total *inflow* of prob. to node (t, i)
  $\beta_i(t)$ gives total *outflow* of prob.



- Bugs again: we just let the bugs run forward from time 0 to t and backward from time T to t.
- In fact, we can just do one forward pass to compute all the $\alpha_i(t)$ and one backward pass to compute all the $\beta_i(t)$ and then compute any $\gamma_i(t)$ we want. Total cost is $O(K^2T)$.

Parameter Estimation using EM (Baum-Welch)

- S_{ij} are transition probs; state j has output distribution $A_j(\mathbf{y})$

$$\mathsf{P}(x_{t+1} = j | x_t = i) = S_{ij} \qquad \mathsf{P}(x_1 = j) = \pi_j$$
$$\mathsf{P}(\mathbf{y}_t = y | x_t = j) = A_j(y)$$

- Complete log likelihood:

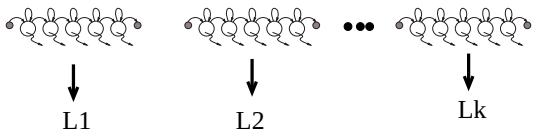
$$\log p(x, y) = \log\{\pi_{\mathbf{x}_1} \prod_{t=1}^{T-1} S_{x_t, x_{t+1}} \prod_{t=1}^{T} A_{x_t}(\mathbf{y}_t)\}$$
$$= \log\{\prod_i \pi_i^{[\mathbf{x}_1^i]} \prod_{t=1}^{T-1} \prod_{ij} S_{ij}^{[x_t^i, x_{t+1}^j]} \prod_{t=1}^{T} \prod_k A_k(\mathbf{y}_t)^{[\mathbf{x}_t^k]}\}$$
$$= \sum_i [\mathbf{x}_1^i] \log \pi_i + \sum_{t=1}^{T-1} \sum_{ij} [x_t^i, x_{t+1}^j] \log S_{ij} + \sum_{t=1}^{T} \sum_k [x_t^k] \log A_k(\mathbf{y}_t)$$

  where the indicator $[x_t^i] = 1$ if $x_t = i$ and 0 otherwise

- For EM, we need to compute the *expected complete log likelihood*.

Using HMMs for Recognition

- Use many HMMs for recognition by:
  1. training one HMM for each class (requires *labelled* training data)
  2. evaluating probability of an unknown sequence under each HMM
  3. classifying unknown sequence: HMM with highest likelihood



- This requires the solution of two problems:
  1. Given model, evaluate prob. of a sequence.
     (We can do this exactly & efficiently.)
  2. Give some training sequences, estimate model parameters.
     (We can find the local maximum of parameter space nearest our starting point using Baum-Welch (EM).)

State expectations required from the E-Step

- The expected complete log likelihood requires
  $\gamma_i(t) =< [x_t^i] >$ *and* $x_{iij}(t) =< [x_t^i, x_{t+1}^j] >$
- So in the E-step we need to compute both
  $\gamma_i(t) = p(x_t = i | \{\mathbf{y}\})$ and $x_{iij}(t) = p(x_t = i, x_{t+1} = j | \{\mathbf{y}\})$.
- We already know how to compute $\gamma_i(t)$ using α and β recursions. We can compute $x_{iij}(t)$ the same way (recall BP):

$$x_{iij}(t) = p(x_{it}, x_{jt+} | \{\mathbf{y}\}) = p(x_{it} | \{\mathbf{y}\}) p(x_{jt+} | x_{it}, \{\mathbf{y}\})$$
$$= p(x_{it}, y_1^t | y_{t+1}^T) p(x_{jt+} | x_{it}, y_{t+1}^T) / p(y_1^t | y_{t+1}^T)$$
$$= \frac{p(x_{it}, y_1^t) p(y_{t+1}^T | x_{it}, y_1^t)}{p(y_1^t | y_{t+1}^T) p(y_{t+1}^T)} \frac{p(y_{t+1}^T | x_{jt+}, x_{it}) p(x_{jt+} | x_{it})}{p(y_{t+1}^T | x_i = t)}$$
$$= \frac{p(x_{it}, y_1^t) p(y_{t+1}^T | x_{it})}{p(y_1^T)} \frac{p(y_{t+1} | x_{jt+}) p(y_{t+2}^T | x_{jt+}) p(x_{jt+} | x_{it})}{p(y_{t+1}^T | x_i = t)}$$
$$= \alpha_i(t) A_j(y_{t+1}) S_{ij} \beta_j(t+1) / L$$

M-step: New Parameters are just Ratios of Frequency Counts

- Initial state distribution: expected #times in state i at time 1:

$$\hat{\pi}_i = \gamma_i(1)$$

- Expected #transitions from state i to j which begin at time t:

$$x_{iij}(t) = \alpha_i(t) S_{ij} A_j(\mathbf{y}_{t+1}) \beta_j(t+1)/L$$

so the estimated transition probabilities are:

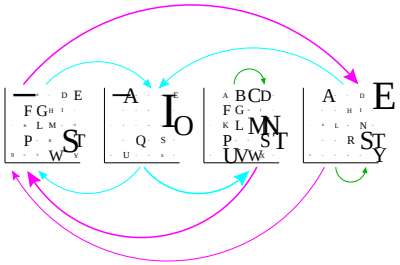
$$\hat{S}_{ij} = \sum_{t=1}^{T-1} x_{iij}(t) \Big/ \sum_{t=1}^{T-1} \gamma_i(t)$$

- The output distributions are the expected number of times we observe a particular symbol in a particular state:

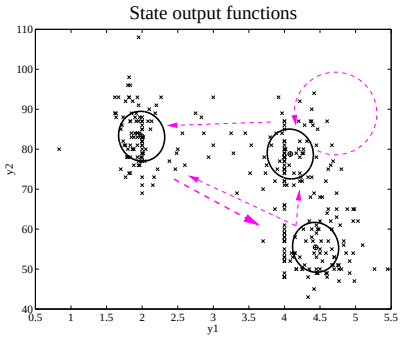
$$\hat{A}_j(y_0) = \sum_{t|\mathbf{y}_t = y_0} \gamma_j(t) \Big/ \sum_{t=1}^{T} \gamma_j(t)$$

HMM Examples

English character sequences



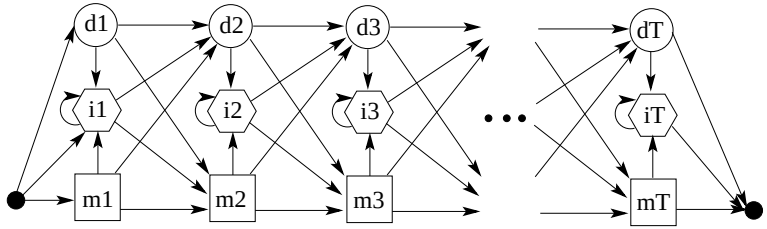
Geyser data (continuous)



Viterbi Decoding

- The numbers $\gamma_j(t)$ above gave the probability distribution over all states at any time.
- By choosing the state $\gamma_*(t)$ with the largest probability at each time, we can make a "best" state path. This is the path with the *maximum expected number of correct states*.
- But it *is not* the single path with the highest likelihood of generating the data. In fact it may be a path of prob. zero!
- To find the single best path, we do *Viterbi decoding* which is just Bellman's dynamic programming algorithm applied to this problem.
- The recursions look the same, except with $\max$ instead of $\sum$.
- Bugs once more: same trick except at each step kill all bugs but the one with the highest value at the node.

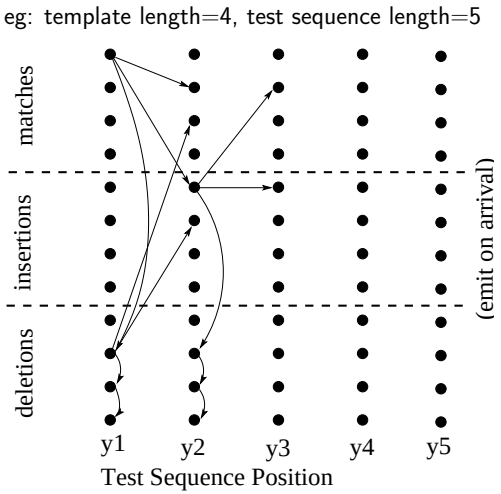
Profile (String-Edit) HMMs



- A "profile HMM" or "string-edit" HMM is used for probabilistically matching an observed input string to a stored template pattern with possible insertions and deletions.
- Three kinds of states: match, insert, delete.
  m_n – use position n in the template to match an observed symbol
  i_n – insert extra symbol(s) observations after template position n
  d_n – delete (skip) template position n

DP for Profile HMMs

- How do we fill in the costs for a DP grid using a string-edit HMM?
- Almost the same as normal except:
  - Now the grid is 3 times its normal height.
  - It is possible to move down without moving right if you move into a deletion state.



Forward-Backward for Profile HMMs

- The equations for the delete states in profile HMMs need to be modified slightly, since they don't emit any symbols.
- For delete states k, the forward equations become:

$$\alpha_k(t) = \sum_j \alpha_j(t) S_{jk}$$

  which should be evaluated after the insert and match state updates.
- For all states, the backward equations become:

$$\beta_k(t) = \sum_{i \in \text{match,ins}} S_{ki} \beta_i(t+1) A_i(\mathbf{y}_{t+1}) + \sum_{j \in \text{del}} S_{kj} \beta_j(t)$$

  which should be evaluated first for delete states k; then for the rest.
- The gamma equations remain the same:

$$\gamma_i(t) = p(x_t = i \mid \mathbf{y}_1^T) = \alpha_i(t)\beta_i(t)/L$$

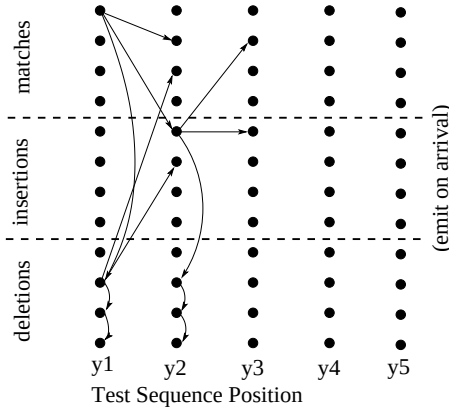
- Notice that each summation above contains only three terms, regardless of the total number of states!

String-Edit HMM Grid Costs

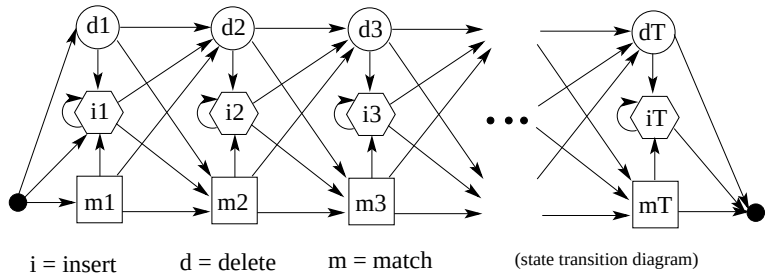
$C_{x \to x'} = -\log T_{x,x'} - \log A_{x'}(\mathbf{y}_t)$ if x' is match or insert

$C_{x \to x'} = -\log T_{x,x'}$ if x' is a delete state

State $x \in \{m_n, i_n, d_n\}$ has nonzero transition probabilities only to states $x' \in \{m_{n+1}, i_n, d_{n+1}\}$.



Profile HMMs have Linear Costs



- number of states = 3(length_template)
- Only insert and match states can generate output symbols.
- Once you visit or skip a match state you can never return to it.
- At most 3 destination states from any state, so S_{ij} very sparse.
- Storage/Time cost *linear* in #states, not quadratic.
- State variables and observations no longer in sync. (e.g. y1:m1 ; d2 ; y2:i2 ; y3:i2 ; y4:m3 ; ...)

Initializing Forward-Backward for Profile HMMs

- The initialization equations for Profile HMMs also need to be fixed up, to reflect the fact that the model can only begin in states m_1, i_1, d_1 and can only finish in states m_N, i_N, d_N.
- In particular, $\pi_j = 0$ if j is not one of m_1, i_1, d_1.
- When initializing $\alpha_k(1)$, delete states k have zeros, and all other states have the product of the transition probabilities through only delete states up to them, plus the final emission probability.
- When initializing $\beta_k(T)$, similar adjustments must be made.
- To enforce the condition that the model finishes in states m_N, i_N, d_N, we create a special END state, accessible only from m_N, i_N, d_N, and append a special "END" symbol in the final position of each sequence. We then define $A(END, k)$ to be zero unless k is the END state, in which case $A(END, k)$ is one. [$A(z, END)$ is also zero for any z other than the END symbol.]

M-step for Profile HMMs

- The emission probabilities $A_j()$ for match and insert states and the initial state distribution π (for m_1, i_1, d_1) are updated exactly as in the regular M-step.
- The expected #transitions from state i to j which begin at time t are different when j is a delete state:

$$x_{iij}(t) = \alpha_i(t) S_{ij} \beta_j(t) / L$$

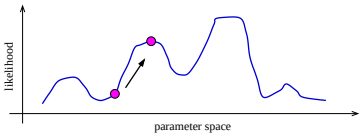
- Given this change, the updates to the transition parameters is the same as in the normal M-step.

Summary: Probabilistic Graphical Models

- Graphical models provide a *compact factorizations* of large joint probability distributions by exploiting *conditional independencies*.
- Efficient algorithms exist for learning the parameters of a graphical model and for inferring distributions over certain variables in the model given observations of other variables.
- The simplest graphical models have only a single node and represent parametric distributions as in traditional statistics.
- The next most complex models have two nodes and represent classification, regression, clustering and latent factor models.
- Even more complex models have chain and tree structures.
- For fully observed models, maximum likelihood learning decouples across the network and each node can learn its parameters given only observations of itself and its parents.

Summary: EM and Belief Propagation

- In networks with hidden or latent variables, learning is much harder and requires inferring the distribution over the unobserved variables given the observed variables.
- Given the results of such inference, the EM algorithm can be used to update the parameters in a way that never decreases the likelihood of the training data.



- Inference in two-node models is just a simple application of Bayes' rule. This is used at test time in supervised models and at training time in unsupervised models.
- In more complex models such as chains and trees, efficient inference can be performed with the belief propagation (BP) algorithm which is the natural extension of dynamic programming to statistical models.