School of Computer Science
Carnegie Mellon

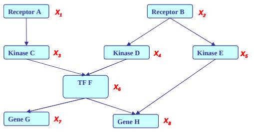
Junction Tree Algorithm

and a case study of the

Hidden Markov Model

Probabilistic Graphical Models (10-708)

Lecture 6, Oct 3, 2007



Eric Xing

Reading: J-Chap 12, 17, KF-Chap. 10

Outline

- So far we have studied exact inference in:
  - Trees
    - message passing on the original graph (which are trees)
  - Poly-trees, Tree-like graphs
    - message passing in factor trees
- Now we will look into exact inference in arbitrary graphs
  - Junction-Tree algorithm
- Inference in Hidden Markov Model

The Junction Tree Algorithm

- Recall: Elimination ≡ message passing on a **clique tree**
- Junction Tree Algorithm:
  - computing messages on a **clique tree**
  - message passing protocol on a **clique tree**
- There are several inference algorithms; some of which operate directly on (special) directed graph
  - Forward-backward algorithm for HMM (we will see it later)
  - Pealing algorithm for trees and phylogenies
- The junction tree algorithm is the most popular and general inference algorithm, it operates on an undirected graph
  - To understand the JT-algorithm, we need to understand how to compile a directed graph into an undirected graph

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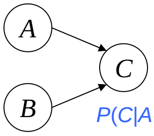
Moral Graph

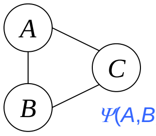
- Note that for both directed GMs and undirected GMs, the joint probability is in a product form:

BN: $P(\mathbf{X}) = \prod_{i=1:d} P(X_i \mid \mathbf{X}_{\pi_i})$ **MRF:** $P(\mathbf{X}) = \frac{1}{Z}\prod_{c \in C} \psi_c(\mathbf{X}_c)$

- So let's convert local conditional probabilities into potentials; then the second expression will be generic, but how does this operation affect the directed graph?
  - We can think of a conditional probability, e.g,. $P(C|A,B)$ as a function of the three variables A, B, and C (we get a real number of each configuration):



$P(C|A,B)$

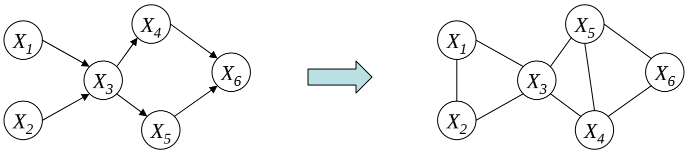


$\Psi(A,B,C) = P(C|A,B)$

  - Problem: But a node and its parent are not generally in the same clique in a BN
  - Solution: Marry the parents to obtain the "moral graph"

Moral Graph (cont.)

- Define the potential on a clique as the product over all conditional probabilities contained within the clique
- Now the product of potentials gives the right answer:



$$\begin{aligned} &P(X_1, X_2, X_3, X_4, X_5, X_6) \\ &= P(X_1)P(X_2)P(X_3 \mid X_1, X_2)P(X_4 \mid X_3)P(X_5 \mid X_3)P(X_6 \mid X_4, X_5) \\ &= \psi(X_1, X_2, X_3)\psi(X_3, X_4, X_5)\psi(X_4, X_5, X_6) \end{aligned}$$

where

$$\psi(X_1, X_2, X_3) = P(X_1)P(X_2)P(X_3 \mid X_1, X_2)$$

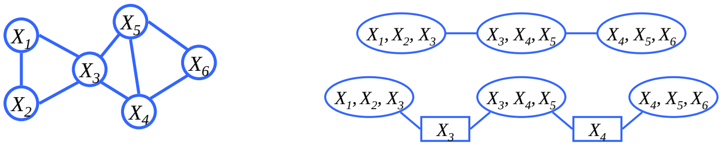
$$\psi(X_3, X_4, X_5) = P(X_4 \mid X_3)P(X_5 \mid X_3)$$

$$\psi(X_4, X_5, X_6) = P(X_6 \mid X_4, X_5)$$

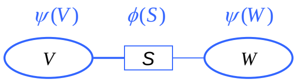
Note that here the interpretation of potential is ambivalent:
it can be either *marginals* or *conditionals*

Clique trees

- A clique tree is an (undirected) tree of cliques



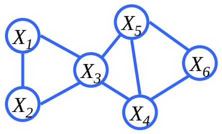
- Consider cases in which two neighboring cliques V and W have an overlap S (e.g., (X_1, X_2, X_3) overlaps with (X_3, X_4, X_5)),

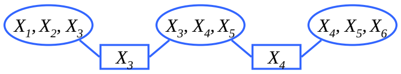


- Now we have an alternative representation of the joint in terms of the potentials:

Clique trees

- A clique tree is an (undirected) tree of cliques





- The alternative representation of the joint in terms of the potentials:

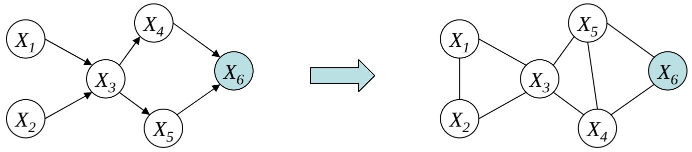
$$\begin{aligned}&P(X_1,X_2,X_3,X_4,X_5,X_6)\\ &=P(X_1)P(X_2)P(X_3\mid X_1,X_2)P(X_4\mid X_3)P(X_5\mid X_3)P(X_6\mid X_4,X_5)\\ &=P(X_1,X_2,X_3)\frac{P(X_3,X_4,X_5)}{P(X_3)}\frac{P(X_4,X_5,X_6)}{P(X_4,X_5)}\\ &=\psi(X_1,X_2,X_3)\frac{\psi(X_3,X_4,X_5)}{\phi(X_3)}\frac{\psi(X_4,X_5,X_6)}{\phi(X_4,X_5)}\end{aligned}$$

Now each potential is isomorphic to the *cluster marginal* of the attendant set of variables

- Generally: $\boxed{P(\mathbf{X})=\frac{\prod_C \psi_C(\mathbf{X}_C)}{\prod_S \phi_S(\mathbf{X}_S)}}$

Why this is useful?

- Propagation of probabilities
  - Now suppose that some evidence has been "absorbed" (i.e., certain values of some nodes have been observed). How do we propagate this effect to the rest of the graph?



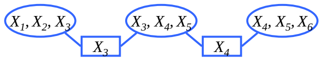
  - What do we mean by propagate?

    Can we adjust all the potentials $\{\psi\}$, $\{\phi\}$ so that they still represent the correct cluster marginals (or unnormalized equivalents) of their respective attendant variables?

  - Utility? $P(X_1 \mid X_6 = x_6) = \sum_{X_2,X_3} \psi(X_1,X_2,X_3)$

$$P(X_3 \mid X_6 = x_6) = \phi(X_3)$$

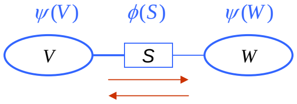
$$P(x_6) = \sum_{X_4,X_5} \psi(X_4,X_5,x_6)$$



Local operations!

Local Consistency

- We have two ways of obtaining $p(S)$



$$P(S) = \sum_{V\setminus S}\psi(V) \qquad P(S) = \sum_{W\setminus S}\psi(W)$$

and they must be the same

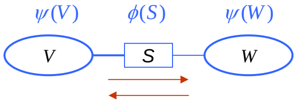
- The following update-rule ensures this:
  - Forward update: $\phi_S^* = \sum_{V\setminus S}\psi_V \quad \psi_W^* = \frac{\phi_S^*}{\phi_S}\psi_W$
  - Backward update $\phi_S^{**} = \sum_{W\setminus S}\psi_W^* \quad \psi_V^{**} = \frac{\phi_S^{**}}{\phi_S^*}\psi_V^*$
- Two important identities can be proven

$$\sum_{V\setminus S}\psi_V^{**} = \sum_{W\setminus S}\psi_W^* = \phi_S^{**} \qquad \frac{\psi_V^*\psi_W^*}{\phi_S^*} = \frac{\psi_V^{**}\psi_W^{**}}{\phi_S^{**}} = \frac{\psi_V\psi_W}{\phi_S}$$

Local Consistency

Invariant Joint

Message Passing Algorithm



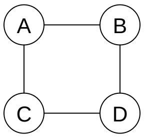
$$\phi_S^* = \sum_{V\setminus S}\psi_V \quad \psi_W^* = \frac{\phi_S^*}{\phi_S}\psi_W$$

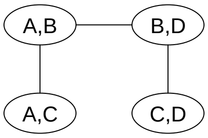
$$\phi_S^{**} = \sum_{W\setminus S}\psi_W^* \quad \psi_V^{**} = \frac{\phi_S^{**}}{\phi_S^*}\psi_V^*$$

- This simple local message-passing algorithm on a clique tree defines the general probability propagation algorithm for directed graphs!
  - Many interesting algorithms are special cases:
    - Forward-backward algorithm for hidden Markov models,
    - Kalman filter updates
    - Pealing algorithms for probabilistic trees
  - The algorithm seems reasonable. Is it correct?

A problem

- Consider the following graph and a corresponding clique tree

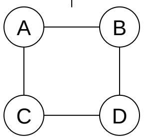




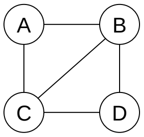
  - Note that C appears in two non-neighboring cliques
- *Question*: with the previous message passage, can we ensure that the probability associated with C in these two (non-neighboring) cliques consistent?
- Answer: No. It is not true that in general local consistency implies global consistency
- What else do we need to get such a guarantee?

Triangulation

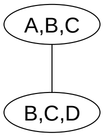
- A triangulated graph is one in which *no cycles* with four or more nodes exist in which there is no *chord*



- We triangulate a graph by adding chords:

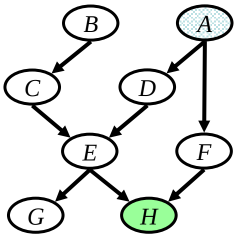


- Now we no longer have our global inconsistency problem.
  - A clique tree for a triangulated graph has the *running intersection property*: If a node appears in two cliques, it appears everywhere on the path between the cliques
  - Thus local consistency implies global consistency



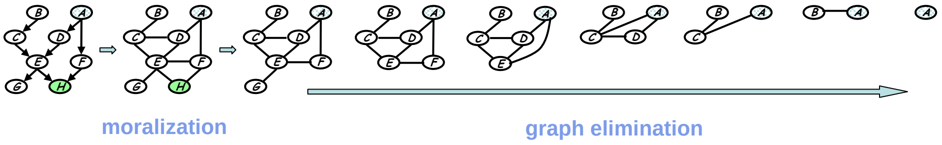
Junction trees

- A clique tree for a triangulated graph is referred to as a *junction tree*
- In junction trees, local consistency implies global consistency. Thus the local message-passing algorithms is (provably) correct
- It is also possible to show that *only* triangulated graphs have the property that their clique trees are junctions. Thus if we want local algorithms, we *must* triangulate
- Are we now all set?
  - How to triangulate?
  - The complexity of building a JT depends on how we triangulate!!
  - Consider this network:
    it turns out that we will need to pay an $O(2^4)$ or $O(2^6)$ cost depending on how we triangulate!



How to triangulate

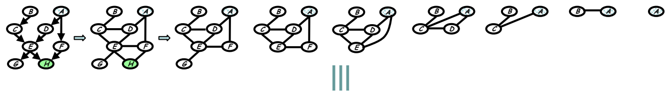
- A graph elimination algorithm

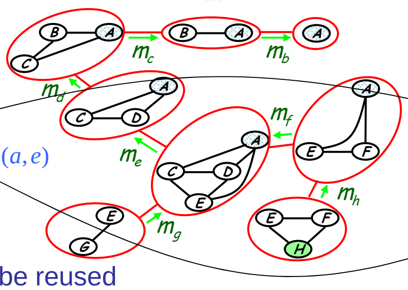


- Intermediate terms correspond to the cliques resulted from elimination
  - "good" elimination orderings lead to **small cliques** and hence reduce complexity (what will happen if we eliminate "e" first in the above graph?)
  - finding the optimum ordering is NP-hard, but for many graph optimum or near-optimum can often be heuristically found

From Elimination to Message Passing

- Our algorithm so far answers only one query (e.g., on one node), do we need to do a complete elimination for every such query?
- Elimination ≡ message passing on a **clique tree**





$$m_e(a,c,d) = \sum_e p(e|c,d) m_g(e) m_f(a,e)$$

Recall this:

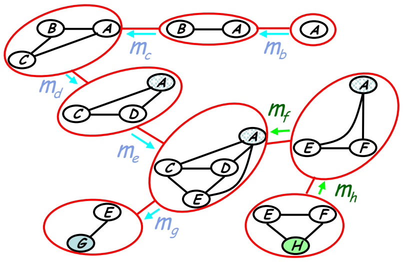
$$\phi_S^* = \sum_{V\setminus S} \psi_V$$

$$\psi_W^* = \frac{\phi_S^*}{\phi_S} \psi_W$$

- Messages can be reused

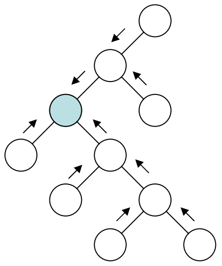
From Elimination to Message Passing

- Our algorithm so far answers only one query (e.g., on one node), do we need to do a complete elimination for every such query?
- Elimination ≡ message passing on a **clique tree**
  - **Another query ...**

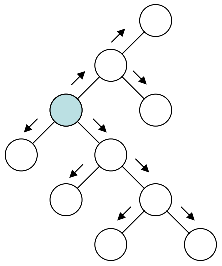


- Messages m_f and m_h are reused, others need to be recomputed

Message-passing algorithms



collect



distribute

- Message update
  - The Hugin update
  - The Shafer-Shenoy update

$$\phi_S^* = \sum_{V\setminus S}\psi_V \qquad \psi_W^* = \frac{\phi_S^*}{\phi_S}\psi_W$$

$$m_{i\to j}(S_{ij}) = \sum_{C_i\setminus S_{ij}} \psi_{C_i} \prod_{k\neq j} m_{k\to i}(S_{ki})$$

A Sketch of the Junction Tree Algorithm

- **The algorithm**

1. Moralize the graph (trivial)
2. Triangulate the graph (good heuristic exist, but actually NP hard)
3. Build a clique tree (e.g., using a maximum spanning tree algorithm
4. Propagation of probabilities --- a local message-passing protocol

- Results in marginal probabilities of all cliques --- solves all queries in a single run
- A **generic** exact inference algorithm for any GM
- **Complexity**: exponential in the size of the maximal clique --- a good elimination order often leads to small maximal clique, and hence a good (i.e., thin) JT

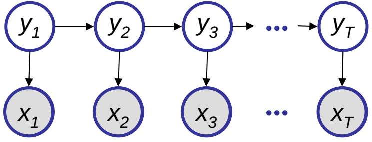
Summary

- Junction tree data-structure for exact inference on general graphs
- Two methods
  - Shafer-Shenoy
  - Belief-update or Lauritzen-Speigelhalter
- Constructing Junction tree from chordal graphs
  - Maximum spanning tree approach

Case study:

- **Hidden Markov Model**

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

- Start probabilities

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

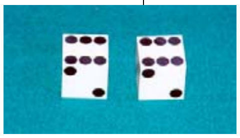
- Emission probabilities associated with each state

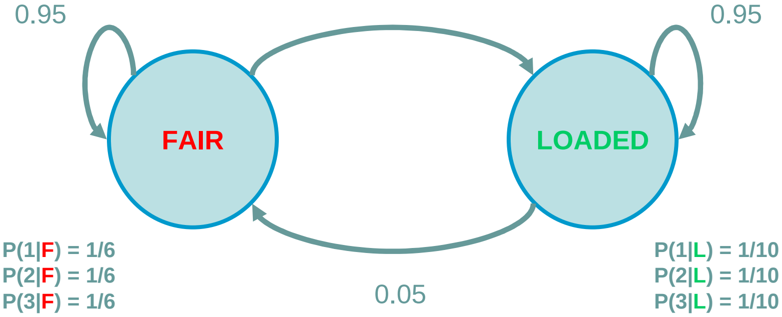
$$p(x_t \mid y_t^i = 1) \sim \text{Multinomial}\left(b_{i,1}, b_{i,2}, \ldots, b_{i,K}\right), \forall i \in \mathbb{I}.$$

or in general: $p(x_t \mid y_t^i = 1) \sim \mathrm{f}\left(\cdot \mid \theta_i\right), \forall i \in \mathbb{I}.$

The Dishonest Casino Model

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

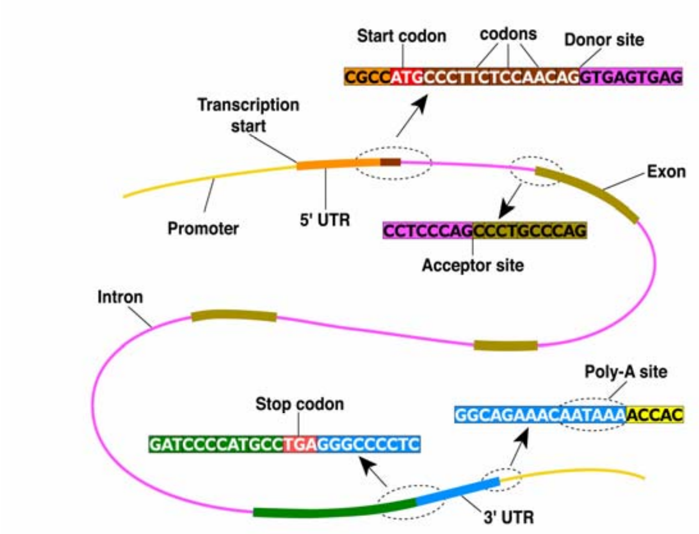




P(1|**F**) = 1/6
P(2|**F**) = 1/6
P(3|**F**) = 1/6
P(4|**F**) = 1/6
P(5|**F**) = 1/6
P(6|**F**) = 1/6

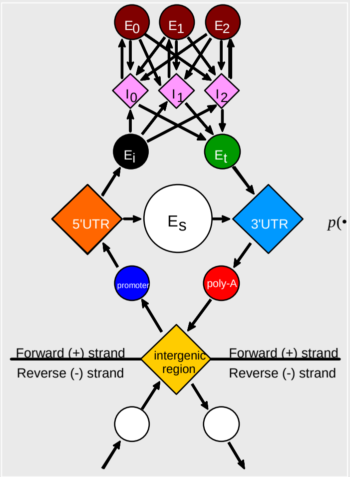
P(1|**L**) = 1/10
P(2|**L**) = 1/10
P(3|**L**) = 1/10
P(4|**L**) = 1/10
P(5|**L**) = 1/10
P(6|**L**) = 1/2

Typical structure of a gene

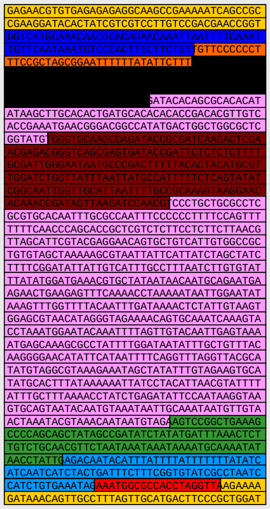


GENSCAN (Burge & Karlin)

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



$$p(\bullet \mid y) = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix}$$



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CGAAGGATACACTATCGTCGTCCTTGTCCGACGAACCGGT
GGTCATGCAAACAACGCACAGAACAAATTAATTTTCAAAT
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TTCCGCTAGCGGAATTTTTATATTCTTT


GATACACAGCGCACACAT
ATAAGCTTGCACACTGATGCACACACACCGACACGTTGTC
ACCGAAATGAACGGGACGGCCATATGACTGGCTGGCGCTC
GGTATGTGGGTGCAAGCGAGATACCGCGATCAAGACTCGA
ACGAGACGGGTCAGCGAGTGATACCGATTCTCTCTCTTTT
GCGATTGGGAATAATGCCCGACTTTTTACACTACATGCGT
TGGATCTGGTTATTTAATTATGCCATTTTTCTCAGTATAT
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CATCTGTGAAATAGAAATGGCGCCACCTAGGTTAAGAAAA
GATAAACAGTTGCCTTTAGTTGCATGACTTCCCGCTGGAT
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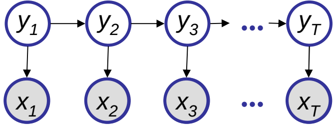
Probability of a parse

- Given a sequence $\mathbf{x} = x_1\ldots\ldots x_T$ and a parse $\mathbf{y} = y_1, \ldots\ldots, y_T$,
- To find how likely is the parse: (given our HMM and the sequence)



$$p(\mathbf{x}, \mathbf{y}) = p(x_1\ldots\ldots x_T, y_1, \ldots\ldots, y_T) \qquad \text{(Joint probability)}$$

$$= p(y_1)\, p(x_1 \mid y_1)\, p(y_2 \mid y_1)\, p(x_2 \mid y_2) \ldots p(y_T \mid y_{T-1})\, p(x_T \mid y_T)$$

$$= p(y_1, \ldots\ldots, y_T)\, p(x_1\ldots\ldots x_T \mid y_1, \ldots\ldots, y_T)$$

Let $\pi_{y_1} \overset{\text{def}}{=} \prod_{i=1}^{M} [\pi_i]^{y_1^i}$, $\quad a_{y_t, y_{t+1}} \overset{\text{def}}{=} \prod_{i,j=1}^{M} [a_{ij}]^{y_t^i y_{t+1}^j}$, $\quad$ and $\; b_{y_t, x_t} \overset{\text{def}}{=} \prod_{i=1}^{M} \prod_{k=1}^{K} [b_{ik}]^{y_t^i x_t^k}$,

$$= \pi_{y_1} a_{y_1, y_2} \cdots a_{y_{T-1}, y_T} \quad b_{y_1, x_1} \cdots b_{y_T, x_T}$$

- Marginal probability: $p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}) = \sum_{y_1} \sum_{y_2} \cdots \sum_{y_N} \pi_{y_1} \prod_{t=2}^{T} a_{y_{t-1}, y_t} \prod_{t=1}^{T} p(x_t \mid y_t)$
- Posterior probability: $p(\mathbf{y} \mid \mathbf{x}) = p(\mathbf{x}, \mathbf{y}) / p(\mathbf{x})$

Applications of HMMs

- **Some early applications of HMMs**
  - finance, but we never saw them
  - speech recognition
  - modelling ion channels
- In the mid-late 1980s HMMs entered genetics and molecular biology, and they are now firmly entrenched.
- **Some current applications of HMMs to biology**
  - mapping chromosomes
  - aligning biological sequences
  - predicting sequence structure
  - inferring evolutionary relationships
  - finding genes in DNA sequence

Three main questions on HMMs

1. Evaluation

GIVEN	an HMM ***M***, and a sequence $\mathbf{x}$,
FIND	Prob ($\mathbf{x}$ | ***M***)
ALGO.	Forward

2. Decoding

GIVEN	an HMM ***M***, and a sequence $\mathbf{x}$,
FIND	the sequence $\mathbf{y}$ of states that maximizes, e.g., P($\mathbf{y}$ | $\mathbf{x}$, ***M***), or the most probable subsequence of states
ALGO.	Viterbi, Forward-backward

3. Learning (next lecture)

GIVEN	an HMM ***M***, with unspecified transition/emission probs., and a sequence $\mathbf{x}$,
FIND	parameters $\theta = (\pi_i, a_{ij}, \eta_{ik})$ that maximize P($\mathbf{x}$ | θ)
ALGO.	Baum-Welch (EM)

The Forward Algorithm

- We want to calculate $P(\mathbf{x})$, the likelihood of $\mathbf{x}$, given the HMM
  - Sum over all possible ways of generating $\mathbf{x}$:

$$p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x},\mathbf{y}) = \sum_{y_1}\sum_{y_2}\cdots\sum_{y_N} \pi_{y_1}\prod_{t=2}^{T} a_{y_{t-1},y_t}\prod_{t=1}^{T} p(x_t \mid y_t)$$

  - To avoid summing over an exponential number of paths $\mathbf{y}$, define

$$\alpha(y_t^k = 1) = \alpha_t^k \overset{\text{def}}{=} P(x_1,\ldots,x_t, y_t^k = 1)$$

(the forward probability)

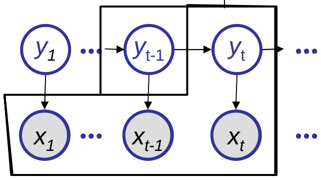
  - The recursion:

$$\alpha_t^k = p(x_t \mid y_t^k = 1)\sum_i \alpha_{t-1}^i a_{i,k}$$

$$P(\mathbf{x}) = \sum_k \alpha_T^k$$

The Forward Algorithm – derivation

- Compute the forward probability:



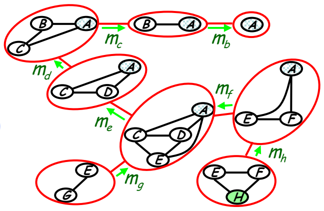
$$\alpha_t^k = P(x_1,\ldots,x_{t-1},x_t,y_t^k=1)$$
$$=\sum_{y_{t-1}} P(x_1,\ldots,x_{t-1},x_t,y_{t-1},y_t^k=1)$$
$$=\sum_{y_{t-1}} P(x_1,\ldots,x_{t-1},y_{t-1})P(y_t^k=1\mid y_{t-1},x_1,\ldots,x_{t-1})P(x_t\mid y_t^k=1,x_1,\ldots,x_{t-1},y_{t-1})$$
$$=\sum_{y_{t-1}} P(x_1,\ldots,x_{t-1},y_{t-1})P(y_t^k=1\mid y_{t-1})P(x_t\mid y_t^k=1)$$
$$=P(x_t\mid y_t^k=1)\sum_i P(x_1,\ldots,x_{t-1},y_{t-1}^i=1)P(y_t^k=1\mid y_{t-1}^i=1)$$
$$=P(x_t\mid y_t^k=1)\sum_i \alpha_{t-1}^i a_{i,k}$$

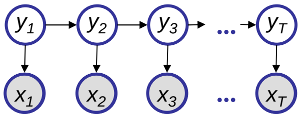
Chain rule: $P(A,B,C)=P(A)P(B\mid C)P(C\mid A,B)$

Recall the Elimination and Message Passing Algorithm

- Elimination $\equiv$ message passing on a **clique tree**

$$m_e(a,c,d) = \sum_e p(e\mid c,d)m_g(e)m_f(a,e)$$





$$\alpha_t^k = p(x_t\mid y_t^k=1)\sum_i \alpha_{t-1}^i a_{i,k}$$

$$P(\mathbf{x}) = \sum_k \alpha_T^k$$

The Forward Algorithm

- We can compute α_t^k for all k, t, using dynamic programming!

Initialization:

$$\alpha_1^k = P(x_1 \mid y_1^k = 1)\pi_k$$

$$\begin{aligned}\alpha_1^k &= P(x_1, y_1^k = 1) \\ &= P(x_1 \mid y_1^k = 1)P(y_1^k = 1) \\ &= P(x_1 \mid y_1^k = 1)\pi_k\end{aligned}$$

Iteration:

$$\alpha_t^k = P(x_t \mid y_t^k = 1)\sum_i \alpha_{t-1}^i a_{i,k}$$

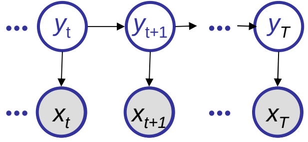
Termination:

$$P(\mathbf{x}) = \sum_k \alpha_T^k$$

The Backward Algorithm

- We want to compute $P(y_t^k = 1 \mid \mathbf{x})$,

  the posterior probability distribution on the t th position, given $\mathbf{x}$



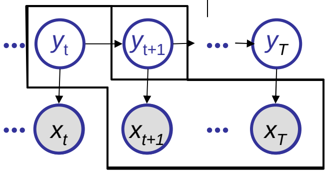
  - We start by computing

$$\begin{aligned}P(y_t^k = 1, \mathbf{x}) &= P(x_1, \dots, x_t, y_t^k = 1, x_{t+1}, \dots, x_T) \\ &= P(x_1, \dots, x_t, y_t^k = 1)P(x_{t+1}, \dots, x_T \mid x_1, \dots, x_t, y_t^k = 1) \\ &= \underbrace{P(x_1 \dots x_t, y_t^k = 1)}_{\text{Forward, } \alpha_t^k}\underbrace{P(x_{t+1} \dots x_T \mid y_t^k = 1)}_{\text{Backward, } \beta_t^k = P(x_{t+1}, \dots, x_T \mid y_t^k = 1)}\end{aligned}$$

  - The recursion: $\beta_t^k = \sum_i a_{k,i}\, p(x_{t+1} \mid y_{t+1}^i = 1)\beta_{t+1}^i$

The Backward Algorithm – derivation

- Define the backward probability:



$$\beta_t^k = P(x_{t+1},\dots,x_T \mid y_t^k = 1)$$
$$= \sum_{y_{t+1}} P(x_{t+1},\dots,x_T, y_{t+1} \mid y_t^k = 1)$$
$$= \sum_i P(y_{t+1}^i = 1 \mid y_t^k = 1) p(x_{t+1} \mid y_{t+1}^i = 1, y_t^k = 1) P(x_{t+2},\dots,x_T \mid x_{t+1}, y_{t+1}^i = 1, y_t^k = 1)$$
$$= \sum_i P(y_{t+1}^i = 1 \mid y_t^k = 1) p(x_{t+1} \mid y_{t+1}^i = 1) P(x_{t+2},\dots,x_T \mid y_{t+1}^i = 1)$$
$$= \sum_i a_{k,i} p(x_{t+1} \mid y_{t+1}^i = 1) \beta_{t+1}^i$$

$$\text{Chain rule}: \; P(A,B,C \mid \alpha) = P(A,\alpha)P(B \mid C,\alpha)P(C \mid A,B,\alpha)$$

The Backward Algorithm

- We can compute β_t^k for all k, t, using dynamic programming!

Initialization:

$$\beta_T^k = 1, \ \forall k$$

Iteration:

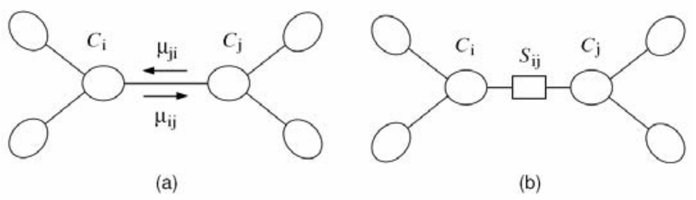
$$\beta_t^k = \sum_i a_{k,i} P(x_{t+1} \mid y_{t+1}^i = 1) \beta_{t+1}^i$$

Termination:

$$P(\mathbf{x}) = \sum_k \alpha_1^k \beta_1^k$$

Shafer Shenoy for HMMs

- Recap: Shafer-Shenoy algorithm



  - Message from clique *i* to clique *j* :

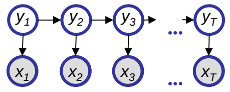
$$\mu_{i\to j}=\sum_{C_i\setminus S_{ij}}\psi_{C_i}\prod_{k\neq j}\mu_{k\to i}(S_{ki})$$

  - Clique marginal

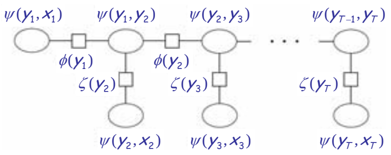
$$p(C_i)\propto\psi_{C_i}\prod_{k}\mu_{k\to i}(S_{ki})$$

Message Passing for HMMs (cont.)

- A junction tree for the HMM

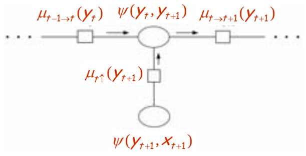


$\Rightarrow$



- Rightward pass

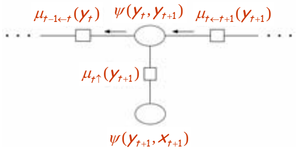
$$\mu_{t\to t+1}(y_{t+1})=\sum_{y_t}\psi(y_t,y_{t+1})\mu_{t-1\to t}(y_t)\mu_{t\uparrow}(y_{t+1})$$
$$=\sum_{y_t}p(y_{t+1}\mid y_t)\mu_{t-1\to t}(y_t)p(x_{t+1}\mid y_{t+1})$$
$$=p(x_{t+1}\mid y_{t+1})\sum_{y_t}a_{y_t,y_{t+1}}\mu_{t-1\to t}(y_t)$$



  - This is exactly the *forward algorithm*!

- Leftward pass …

$$\mu_{t-1\leftarrow t}(y_t)=\sum_{y_{t+1}}\psi(y_t,y_{t+1})\mu_{t\leftarrow t+1}(y_{t+1})\mu_{t\uparrow}(y_{t+1})$$
$$=\sum_{y_{t+1}}p(y_{t+1}\mid y_t)\mu_{t\leftarrow t+1}(y_{t+1})p(x_{t+1}\mid y_{t+1})$$



  - This is exactly the *backward algorithm*!

Posterior decoding

- We can now calculate

$$P(y_t^k = 1 | \mathbf{x}) = \frac{P(y_t^k = 1, \mathbf{x})}{P(\mathbf{x})} = \frac{\alpha_t^k \beta_t^k}{P(\mathbf{x})}$$

- Then, we can ask
  - What is the most likely state at position *t* of sequence $\mathbf{x}$:

$$k_t^* = \arg\max_k P(y_t^k = 1 | \mathbf{x})$$

  - Note that this is an MPA of a single hidden state, what if we want to a MPA of a whole hidden state sequence?
  - Posterior Decoding: $\left\{ y_t^{k_t^*} = 1 : t = 1 \cdots T \right\}$
  - This is different from MPA of a whole sequence of hidden states
  - This can be understood as *bit error rate* vs. *word error rate*

Example:
MPA of *X* ?
MPA of *(X, Y)* ?

x	*y*	*P(x,y)*
0	*0*	*0.35*
0	*1*	*0.05*
1	*0*	*0.3*
1	*1*	*0.3*

Viterbi decoding

- GIVEN $\mathbf{x} = x_1, \ldots, x_T$, we want to find $\mathbf{y} = y_1, \ldots, y_T$, such that $P(\mathbf{y}|\mathbf{x})$ is maximized:

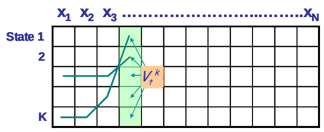
$$\mathbf{y}^* = \text{argmax}_{\mathbf{y}} P(\mathbf{y}|\mathbf{x}) = \text{argmax}_{\pi} P(\mathbf{y},\mathbf{x})$$

  - Let

$$V_t^k = \max_{\{y_1,\ldots y_{t-1}\}} P(x_1,\ldots,x_{t-1},y_1,\ldots,y_{t-1},x_t,y_t^k = 1)$$

= Probability of most likely **sequence of states** ending at state $y_t = k$

  - The recursion:



$$V_t^k = p(x_t | y_t^k = 1) \max_i a_{i,k} V_{t-1}^i$$

  - Underflows are a significant problem

$$p(x_1,\ldots,x_t,y_1,\ldots,y_t) = \pi_{y_1} a_{y_1,y_2} \cdots a_{y_{t-1},y_t} b_{y_1,x_1} \cdots b_{y_t,x_t}$$

    - These numbers become extremely small – underflow
    - Solution: Take the logs of all values: $V_t^k = \log p(x_t | y_t^k = 1) + \max_i \left(\log(a_{i,k}) + V_{t-1}^i\right)$

The Viterbi Algorithm – derivation

- Define the viterbi probability:

$$
\begin{aligned}
V_{t+1}^{k} &= \max_{\{y_1,\dots y_t\}} P(x_1,\dots,x_t,y_1,\dots,y_t,x_{t+1,}y_{t+1}^{k}=1)\\
&= \max_{\{y_1,\dots y_t\}} P(x_{t+1,}y_{t+1}^{k}=1 \mid x_1,\dots,x_t,y_1,\dots,y_t)P(x_1,\dots,x_t,y_1,\dots,y_t)\\
&= \max_{\{y_1,\dots y_t\}} P(x_{t+1,}y_{t+1}^{k}=1 \mid y_t)P(x_1,\dots,x_{t-1},y_1,\dots,y_{t-1},x_t,y_t)\\
&= \max_i P(x_{t+1,}y_{t+1}^{k}=1 \mid y_t^i=1)\max_{\{y_1,\dots y_{t-1}\}} P(x_1,\dots,x_{t-1},y_1,\dots,y_{t-1},x_t,y_t^i=1)\\
&= \max_i P(x_{t+1,} \mid y_{t+1}^{k}=1)a_{i,k}V_t^i\\
&= P(x_{t+1,} \mid y_{t+1}^{k}=1)\max_i a_{i,k}V_t^i
\end{aligned}
$$

The Viterbi Algorithm

- Input: $\mathbf{x} = x_1, \dots, x_T,$

Initialization:

$$V_1^k = P(x_1 \mid y_1^k = 1)\pi_k$$

Iteration:

$$V_t^k = P(x_{t,} \mid y_t^k = 1)\max_i a_{i,k}V_{t-1}^i$$

$$\mathrm{Ptr}(k,t) = \arg\max_i a_{i,k}V_{t-1}^i$$

Termination:

$$P(\mathbf{x},\mathbf{y}^*) = \max_k V_T^k$$

TraceBack:

$$y_T^* = \arg\max_k V_T^k$$

$$y_{t-1}^* = \mathrm{Ptr}(y_t^*, t)$$

Computational Complexity and implementation details

- What is the running time, and space required, for Forward, and Backward?

$$\alpha_t^k = p(x_t \mid y_t^k = 1) \sum_i \alpha_{t-1}^i a_{i,k}$$

$$\beta_t^k = \sum_i a_{k,i}\, p(x_{t+1} \mid y_{t+1}^i = 1) \beta_{t+1}^i$$

$$V_t^k = p(x_t \mid y_t^k = 1) \max_i a_{i,k} V_{t-1}^i$$

Time: $O(K^2N)$; Space: $O(KN)$.

- Useful implementation technique to avoid underflows
  - Viterbi: sum of logs
  - Forward/Backward: rescaling at each position by multiplying by a constant