Machine Learning

10-701/15-781, Fall 2011

Inference and Learning For Bayesian Networks

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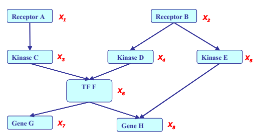
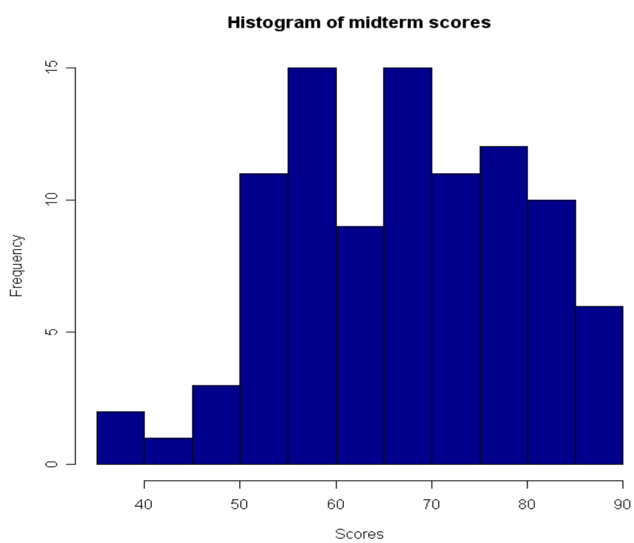


Lecture 14, October 31, 2011

Reading: Chap. 8, C.B book

Midterm



Recap of BN Representation

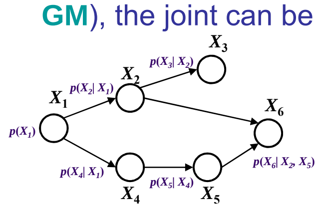
- Joint probability dist. on multiple variables:

$$P(X_1, X_2, X_3, X_4, X_5, X_6)$$
$$= P(X_1)P(X_2 \mid X_1)P(X_3 \mid X_1, X_2)P(X_4 \mid X_1, X_2, X_3)P(X_5 \mid X_1, X_2, X_3, X_4)P(X_6 \mid X_1, X_2, X_3, X_4, X_5)$$

- If X_i's are **independent**: ($P(X_i|\cdot)= P(X_i)$)

$$P(X_1, X_2, X_3, X_4, X_5, X_6)$$
$$= P(X_1)P(X_2)P(X_3)P(X_4)P(X_5)P(X_6) = \prod_i P(X_i)$$

- If X_i's are **conditionally independent** (as described by a **GM**), the joint can be factored to simpler products, e.g.,



$$P(X_1, X_2, X_3, X_4, X_5, X_6)$$
$$= P(X_1)\, P(X_2| X_1)\, P(X_3| X_2)\, P(X_4| X_1)\, P(X_5| X_4)\, P(X_6| X_2, X_5)$$

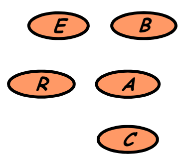
Inference and Learning

- We now have compact representations of probability distributions: **BN**
- A BN *M* describes a unique probability distribution *P*
- Typical tasks:
  - Task 1: How do we answer **queries** about P?
    - We use **inference** as a name for the process of computing answers to such queries
  - Task 2: How do we estimate a **plausible model** *M* from data *D*?
    - i. We use **learning** as a name for the process of obtaining point estimate of *M*.
    - ii. But for *Bayesian*, they seek $p(M \mid D)$, which is actually an **inference** problem.
    - iii. When not all variables are observable, even computing point estimate of *M* need to do **inference** to impute the *missing data*.

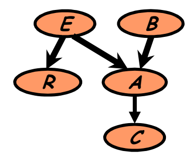
Learning BNs

The goal:

Given set of independent samples (*assignments* of random variables), find the *best* (the most likely?) Bayesian Network (both DAG and CPDs)



(B,E,A,C,R)=(T,F,F,T,F)
(B,E,A,C,R)=(T,F,T,T,F)
....
(B,E,A,C,R)=(F,T,T,T,F)



E	B	P(A | E,B)	
e	b	0.9	0.1
e	$\bar{b}$	0.2	0.8
$\bar{e}$	b	0.9	0.1
$\bar{e}$	$\bar{b}$	0.01	0.99

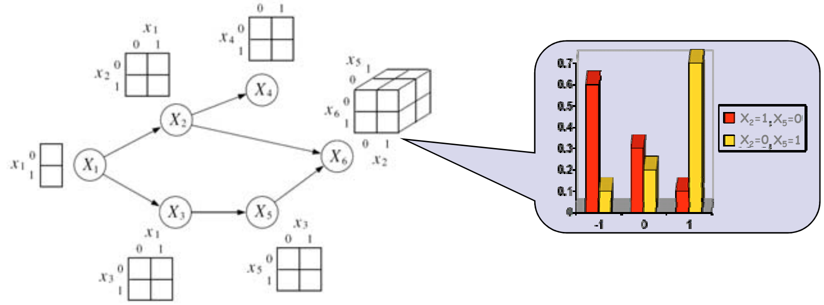
Learning Graphical Models

- Scenarios:
  - completely observed GMs
    - directed
    - undirected
  - partially observed GMs
    - directed
    - undirected (an open research topic)
- Estimation principles:
  - Maximal likelihood estimation (MLE)
  - Bayesian estimation
  - Maximal conditional likelihood
  - Maximal "Margin"
- 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 BN parameters

- 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:

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

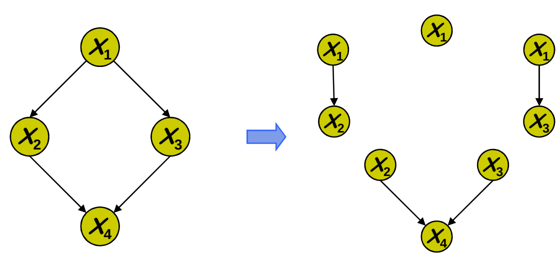


Example: decomposable likelihood of a directed model

- Consider the distribution defined by the directed acyclic GM:

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

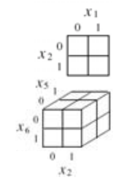
- This is exactly like learning four separate small BNs, each of which consists of a node and its parents.



E.g.: MLE for BNs with tabular CPDs

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

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

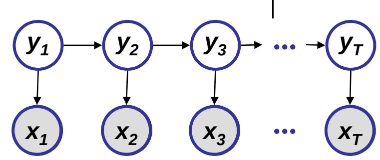


  - Note that in case of multiple parents, $\mathbf{X}_{\pi_i}$ will have a composite state, and the CPD will be a high-dimensional table
  - The sufficient statistics are counts of family configurations

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

- 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: $\theta_{ijk}^{ML} = \dfrac{n_{ijk}}{\sum_{i,j',k} n_{ij'k}}$

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

- Start probabilities

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

- Emission probabilities associated with each state

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

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

Supervised ML estimation

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

$$\ell(\boldsymbol{\theta}; \mathbf{x}, \mathbf{y}) = \log p(\mathbf{x}, \mathbf{y}) = \log \prod_n \left(p(y_{n,1}) \prod_{t=2}^{T} p(y_{n,t} \mid y_{n,t-1}) \prod_{t=1}^{T} p(x_{n,t} \mid x_{n,t}) \right)$$

  - **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:**

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

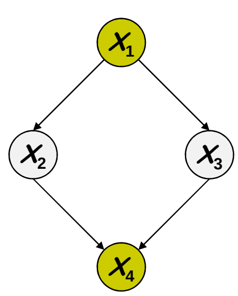
$$b_{ik}^{ML} = \frac{\#(i \to k)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=1}^{T} y_{n,t}^{i} x_{n,t}^{k}}{\sum_n \sum_{t=1}^{T} y_{n,t}^{i}} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

  - **If y is continuous, we can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as $N \times T$ observations of, e.g., a Gaussian, and apply learning rules for Gaussian …**

What if some nodes are not observed?

- Consider the distribution defined by the directed acyclic GM:

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



- Need to compute $p(x_H|x_V)$ → inference

Probabilistic Inference

- Computing statistical queries regarding the network, e.g.:
  - Is node X independent on node Y given nodes Z,W ?
  - What is the probability of X=true if (Y=false and Z=true)?
  - What is the joint distribution of (X,Y) if Z=false?
  - What is the likelihood of some full assignment?
  - What is the most likely assignment of values to all or a subset the nodes of the network?

- General purpose algorithms exist to fully automate such computation
  - Computational cost depends on the topology of the network
  - Exact inference:
    - The junction tree algorithm
  - Approximate inference;
    - Loopy belief propagation, variational inference, Monte Carlo sampling

Inferential Query 1: Likelihood

- Most of the queries one may ask involve **evidence**
  - Evidence $\mathbf{x}_v$ is an assignment of values to a set $\mathbf{X}_v$ of nodes in the GM over varialbe set $\mathbf{X}=\{X_1, X_2, \ldots, X_n\}$
  - Without loss of generality $\mathbf{X}_v=\{X_{k+1}, \ldots , X_n\}$,
  - Write $\mathbf{X}_H=\mathbf{X}\backslash\mathbf{X}_v$ as the set of hidden variables, $\mathbf{X}_H$ can be $\varnothing$ or $\mathbf{X}$

- Simplest query: compute probability of evidence

$$P(\mathbf{x}_v) = \sum_{\mathbf{x}_H} P(\mathbf{X}_H, \mathbf{X}_v) = \sum_{x_1} \cdots \sum_{x_k} P(x_1, \ldots, x_k, \mathbf{x}_v)$$

  - this is often referred to as computing the **likelihood** of $\mathbf{x}_v$

Inferential Query 2: Conditional Probability

- Often we are interested in the **conditional probability distribution** of a variable given the evidence

$$P(\mathbf{X}_H \mid \mathbf{X}_V = \mathbf{x}_V) = \frac{P(\mathbf{X}_H, \mathbf{x}_V)}{P(\mathbf{x}_V)} = \frac{P(\mathbf{X}_H, \mathbf{x}_V)}{\sum_{\mathbf{x}_H} P(\mathbf{X}_H = \mathbf{x}_H, \mathbf{x}_V)}$$

  - this is the ***a posteriori* belief** in $\mathbf{X}_H$, given evidence $\mathbf{x}_v$

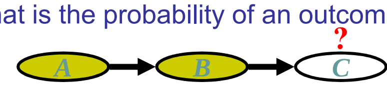
- We usually query a subset $\mathbf{Y}$ of all hidden variables $\mathbf{X}_H=\{\mathbf{Y},\mathbf{Z}\}$ and "don't care" about the remaining, $\mathbf{Z}$:

$$P(\mathbf{Y} \mid \mathbf{x}_V) = \sum_{\mathbf{z}} P(\mathbf{Y}, \mathbf{Z} = \mathbf{z} \mid \mathbf{x}_V)$$

  - the process of summing out the "don't care" variables z is called **marginalization**, and the resulting $P(\mathbf{Y}|\mathbf{x}_v)$ is called a **marginal** prob.

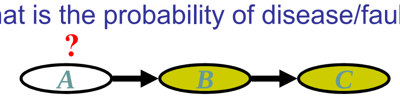
Applications of *a posteriori* Belief

- **Prediction**: what is the probability of an outcome given the starting condition



  - the query node is a descendent of the evidence

- **Diagnosis**: what is the probability of disease/fault given symptoms



  - the query node an ancestor of the evidence

- **Learning** under partial observation
  - fill in the unobserved values under an "EM" setting (more later)

- The directionality of information flow between variables is not restricted by the directionality of the edges in a GM
  - probabilistic inference can combine evidence form all parts of the network

Inferential Query 3: Most Probable Assignment

- In this query we want to find the **most probable joint assignment** (MPA) for ***some*** variables of interest

- Such reasoning is usually performed under some given evidence $\mathbf{x}_v$, and ignoring (the values of) other variables $\mathbf{Z}$:

$$\mathbf{Y}^* \mid \mathbf{x}_V = \arg\max_y P(\mathbf{Y} \mid \mathbf{x}_V) = \arg\max_y \sum_{\mathbf{z}} P(\mathbf{Y}, \mathbf{Z} = \mathbf{z} \mid \mathbf{x}_V)$$

  - this is the **maximum *a posteriori*** configuration of $\mathbf{Y}$.

Complexity of Inference

Thm:

Computing $P(X_H = x_H \mid x_v)$ in an arbitrary GM is NP-hard

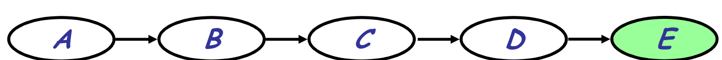
- **Hardness does not mean we cannot solve inference**
  - **It implies that we cannot find a general procedure that works efficiently for arbitrary GMs**
  - **For particular families of GMs, we can have provably efficient procedures**

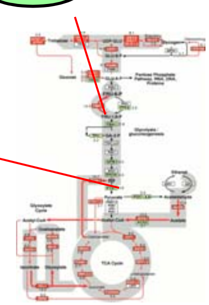
Approaches to inference

- Exact inference algorithms
  - The elimination algorithm
  - Belief propagation
  - The junction tree algorithms (but will not cover in detail here)
- Approximate inference techniques
  - Variational algorithms
  - Stochastic simulation / sampling methods
  - Markov chain Monte Carlo methods

Marginalization and Elimination

- A signal transduction pathway:





What is the likelihood that protein E is active?

- Query: $P(e)$

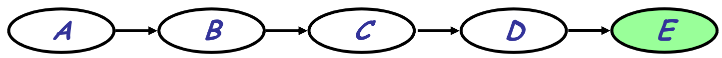
$$P(e) = \underbrace{\sum_d \sum_c \sum_b \sum_a}_{} P(a,b,c,d,e)$$

a naïve summation needs to enumerate over an exponential number of terms

- By chain decomposition, we get

$$= \sum_d \sum_c \sum_b \sum_a P(a)P(b\,|\,a)P(c\,|\,b)P(d\,|\,c)P(e\,|\,d)$$

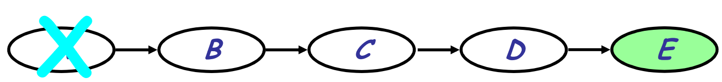
Elimination on Chains



- Rearranging terms ...

$$P(e) = \sum_d \sum_c \sum_b \sum_a P(a)P(b \mid a)P(c \mid b)P(d \mid c)P(e \mid d)$$
$$= \sum_d \sum_c \sum_b P(c \mid b)P(d \mid c)P(e \mid d) \sum_a P(a)P(b \mid a)$$

Elimination on Chains

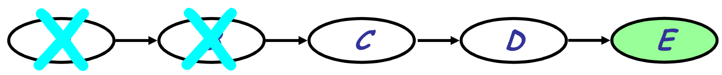


- Now we can perform innermost summation

$$P(e) = \sum_d \sum_c \sum_b P(c \mid b)P(d \mid c)P(e \mid d) \underbrace{\sum_a P(a)P(b \mid a)}$$
$$= \sum_d \sum_c \sum_b P(c \mid b)P(d \mid c)P(e \mid d)\, p(b)$$

- This summation "eliminates" one variable from our summation argument at a "local cost".

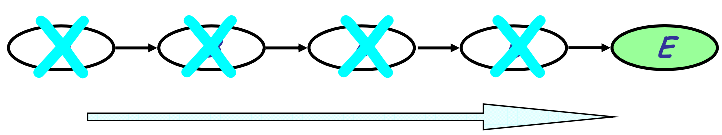
Elimination in Chains



- Rearranging and then summing again, we get

$$
\begin{aligned}
P(e) &= \sum_d \sum_c \sum_b P(c \mid b) P(d \mid c) P(e \mid d) p(b) \\
&= \sum_d \sum_c P(d \mid c) P(e \mid d) \sum_b P(c \mid b) p(b) \\
&= \sum_d \sum_c P(d \mid c) P(e \mid d) p(c)
\end{aligned}
$$

Elimination in Chains

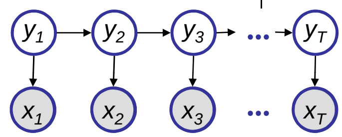


- Eliminate nodes one by one all the way to the end, we get

$$
P(e) = \sum_d P(e \mid d) p(d)
$$

- Complexity:
  - Each step costs $O(|Val(X_i)|*|Val(X_{i+1})|)$ operations: $O(nk^2)$
  - Compare to naïve evaluation that sums over joint values of n-1 variables $O(k^n)$

Hidden Markov Model



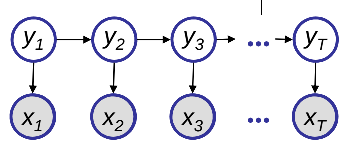
$p(\mathbf{x}, \mathbf{y}) = p(x_1 \ldots\ldots x_T, y_1, \ldots\ldots, y_T)$
$= p(y_1)\, p(x_1 \mid y_1)\, p(y_2 \mid y_1)\, p(x_2 \mid y_2) \ldots p(y_T \mid y_{T-1})\, p(x_T \mid y_T)$

Conditional probability:

$$\begin{aligned} p(y_i|x_1,\ldots,x_T) &= \sum_{y_1}\cdots\sum_{y_{i-1}}\sum_{y_{i+1}}\cdots\sum_{y_T} p(y_i,\ldots,y_T,x_1,\ldots,x_T) \\ &= \sum_{y_1}\cdots\sum_{y_{i-1}}\sum_{y_{i+1}}\cdots\sum_{y_T} p(y_1)p(x_1|y_1)\ldots p(y_T|y_{T-1})p(x_T|y_T) \end{aligned}$$

Hidden Markov Model

Conditional probability:



$$\begin{aligned} p(y_i|x_1,\ldots,x_T) &= \sum_{y_1}\cdots\sum_{y_{i-1}}\sum_{y_{i+1}}\cdots\sum_{y_T} p(y_i,\ldots,y_T,x_1,\ldots,x_T) \\ &= \sum_{y_1}\cdots\sum_{y_{i-1}}\sum_{y_{i+1}}\cdots\sum_{y_T} p(y_1)p(x_1|y_1)\ldots p(y_T|y_{T-1})p(x_T|y_T) \end{aligned}$$

Inference on General BN via Variable Elimination

General idea:

- Write query in the form

$$P(X_1, \boldsymbol{e}) = \sum_{x_n} \cdots \sum_{x_3} \sum_{x_2} \prod_i P(x_i \mid pa_i)$$

  - this suggests an "elimination order" of latent variables to be marginalized

- Iteratively
  - Move all irrelevant terms outside of innermost sum
  - Perform innermost sum, getting a new term
  - Insert the new term into the product

- wrap-up

$$P(X_1 \mid \boldsymbol{e}) = \frac{P(X_1, \boldsymbol{e})}{P(\boldsymbol{e})}$$

The Sum-Product Operation

- In general, we can view the task at hand as that of computing the value of an expression of the form:

$$\sum_{\mathbf{z}} \prod_{\phi \in \mathcal{F}} \phi$$

where $\mathcal{F}$ is a set of factors

- We call this task the *sum-product* inference task.

Outcome of elimination

- Let $\mathbf{X}$ be some set of variables,
  let $\mathcal{F}$ be a set of factors such that for each $\phi \in \mathcal{F}$, *Scope*$[\phi] \in \mathbf{X}$,
  let $\mathbf{Y} \subset \mathbf{X}$ be a set of query variables,
  and let $Z = \mathbf{X} - \mathbf{Y}$ be the variable to be eliminated

- The result of eliminating the variable Z is a factor

$$\tau(\mathbf{Y}) = \sum_{\mathbf{z}} \prod_{\phi \in \mathcal{F}} \phi$$

  - This factor does not necessarily correspond to any probability or conditional probability in this network. (example forthcoming)

Dealing with evidence

- Conditioning as a Sum-Product Operation

  - The evidence potential: $$\delta(E_i, \bar{e}_i) = \begin{cases} 1 & \text{if } E_i \equiv \bar{e}_i \\ 0 & \text{if } E_i \neq \bar{e}_i \end{cases}$$

  - Total evidence potential: $$\delta(\mathbf{E}, \bar{\mathbf{e}}) = \prod_{i \in I_{\mathbf{E}}} \delta(E_i, \bar{e}_i)$$

  - Introducing evidence --- restricted factors:

$$\tau(\mathbf{Y}, \bar{\mathbf{e}}) = \sum_{\mathbf{z}, \mathbf{e}} \prod_{\phi \in \mathcal{F}} \phi \times \delta(\mathbf{E}, \bar{\mathbf{e}})$$

The elimination algorithm

Procedure Elimination (

G, // the GM

$\mathbf{E}$, // evidence

Z, // Set of variables to be eliminated

X, // query variable(s)

)

1. Initialize (G)
2. Evidence ($\mathbf{E}$)
3. Sum-Product-Elimination ($\mathcal{F}$, Z, $\prec$)
4. Normalization ($\mathcal{F}$)

The elimination algorithm

Procedure Initialize (G, Z)

1. Let $Z_1, \ldots, Z_k$ be an ordering of Z such that $Z_i \prec Z_j$ iff $i < j$
2. Initialize $\mathcal{F}$ with the full the set of factors

Procedure Evidence ($\mathbf{E}$)

1. **for** each $i \in I_E$,
   $\mathcal{F} = \mathcal{F} \cup \delta(E_i, e_i)$

Procedure Sum-Product-Variable-Elimination ($\mathcal{F}$, Z, $\prec$)

1. **for** i = 1, . . . , k
   $\mathcal{F} \leftarrow$ Sum-Product-Eliminate-Var($\mathcal{F}$, Z_i)
2. $\phi^* \leftarrow \prod_{\phi \in \mathcal{F}} \phi$
3. **return** ϕ^*
4. Normalization (ϕ^*)

The elimination algorithm

Procedure Initialize (G, Z)

1. Let $Z_1, \ldots, Z_k$ be an ordering of Z such that $Z_i \prec Z_j$ iff $i < j$
2. Initialize $\mathcal{F}$ with the full the set of factors

Procedure Evidence $(\mathbf{E})$

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Procedure Sum-Product-Variable-Elimination $(\mathcal{F}, Z, \prec)$

1. **for** $i = 1, \ldots, k$
   $\mathcal{F} \leftarrow$ Sum-Product-Eliminate-Var$(\mathcal{F}, Z_i)$
2. $\phi^* \leftarrow \prod_{\phi \in \mathcal{F}} \phi$
3. **return** ϕ^*
4. Normalization (ϕ^*)

Procedure Normalization (ϕ^*)

1. $P(X|\mathbf{E}) = \phi^*(X) / \sum_x \phi^*(X)$

Procedure Sum-Product-Eliminate-Var (
$\mathcal{F}$, // Set of factors
Z // Variable to be eliminated
)

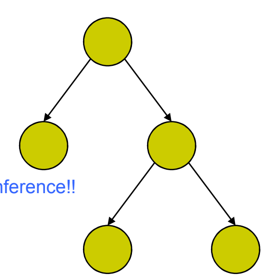
1. $\mathcal{F}' \leftarrow \{\phi \in \mathcal{F} : Z \in Scope[\phi]\}$
2. $\mathcal{F}'' \leftarrow \mathcal{F} - \mathcal{F}'$
3. $\psi \leftarrow \prod_{\phi \in \mathcal{F}'} \phi$
4. $\tau \leftarrow \sum_Z \psi$
5. **return** $\mathcal{F}'' \cup \{\tau\}$

From elimination to message passing

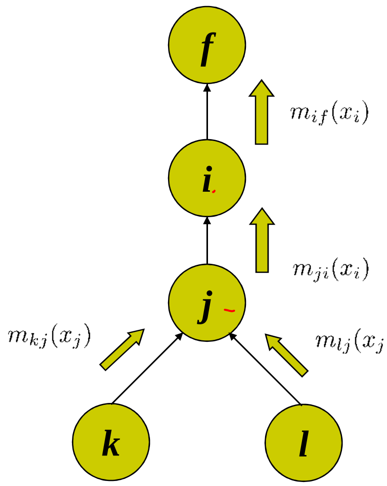
- Recall ELIMINATION algorithm:

  - Choose an ordering $\mathcal{Z}$ in which query node f is the final node
  - Place all potentials on an active list
  - Eliminate node i by removing all potentials containing i, take sum/product over x_i.
  - Place the resultant factor back on the list

- For a TREE graph:
  - Choose query node f as the root of the tree
  - View tree as a directed tree with edges pointing towards from f
  - Elimination ordering based on depth-first traversal
  - Elimination of each node can be considered as message-passing (or Belief Propagation) directly along tree branches, rather than on some transformed graphs
  - → thus, we can use the tree itself as a data-structure to do general inference!!



Message passing for trees



$$m_{ji}(x_i) = \sum_{x_j}\left(\psi(x_j)\psi(x_i,x_j)\prod_{k\in N(j)\backslash i} m_{kj}(x_j)\right)$$

Let $m_{ij}(x_i)$ denote the factor resulting from eliminating variables from bellow up to i, which is a function of x_i:

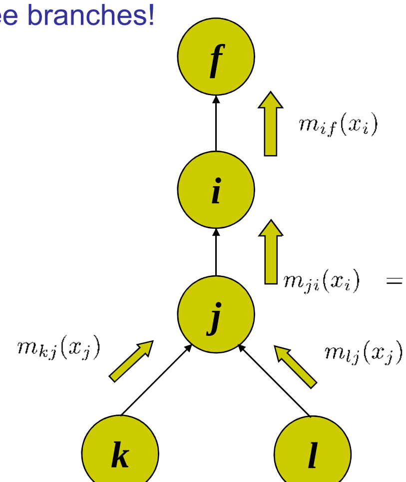
$$m_{ji}(x_i) = \sum_{x_j}\left(\psi(x_j)\psi(x_i,x_j)\prod_{k\in N(j)\backslash i} m_{kj}(x_j)\right)$$

This is reminiscent of a ***message*** sent from j to i.

$$p(x_f) \propto \psi(x_f) \prod_{e\in N(f)} m_{ef}(x_f)$$

$m_{ij}(x_i)$ represents a "belief" of x_i from x_j!

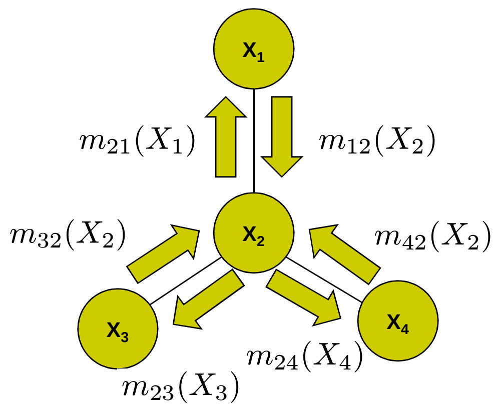
- Elimination on trees is equivalent to message passing along tree branches!



$$m_{ji}(x_i) = \sum_{x_j}\left(\psi(x_j)\psi(x_i,x_j)\prod_{k\in N(j)\backslash i} m_{kj}(x_j)\right)$$

The message passing protocol:

- A two-pass algorithm:



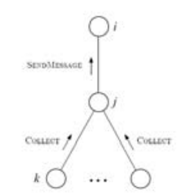
Belief Propagation (SP-algorithm): Sequential implementation

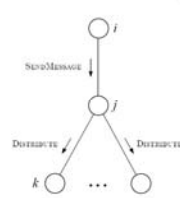
```
SUM-PRODUCT(T, E)
    EVIDENCE(E)
    f = CHOOSEROOT(V)
    for e ∈ N(f)
        COLLECT(f, e)
    for e ∈ N(f)
        DISTRIBUTE(f, e)
    for i ∈ V
        COMPUTEMARGINAL(i)

EVIDENCE(E)
    for i ∈ E
        ψ^E(x_i) = ψ(x_i)δ(x_i, x̄_i)
    for i ∉ E
        ψ^E(x_i) = ψ(x_i)

COLLECT(i, j)
    for k ∈ N(j)\i
        COLLECT(j, k)
    SENDMESSAGE(j, i)

DISTRIBUTE(i, j)
    SENDMESSAGE(i, j)
    for k ∈ N(j)\i
        DISTRIBUTE(j, k)

SENDMESSAGE(j, i)
```

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

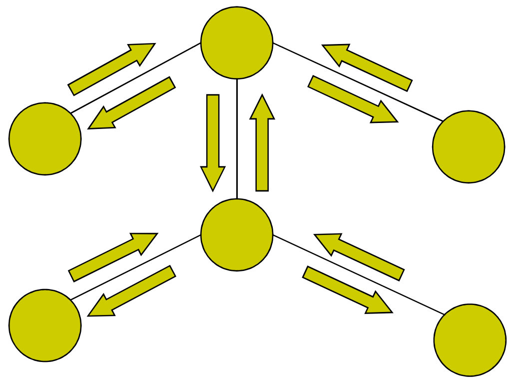
```
COMPUTEMARGINAL(i)
```

$$p(x_i) \propto \psi^E(x_i) \prod_{j \in \mathcal{N}(i)} m_{ji}(x_i)$$





Belief Propagation (SP-algorithm): Parallel synchronous implementation



- For a node of degree d, whenever messages have arrived on any subset of d-1 node, compute the message for the remaining edge and send!
  - A pair of messages have been computed for each edge, one for each direction
  - All incoming messages are eventually computed for each node

Correctness of BP on tree

- Collollary: the synchronous implementation is "non-blocking"
- Thm: The Message Passage Guarantees obtaining all marginals in the tree

$$m_{ji}(x_i) = \sum_{x_j}\left(\psi(x_j)\psi(x_i,x_j)\prod_{k\in N(j)\setminus i} m_{kj}(x_j)\right)$$

- What about non-tree?

Inference on general GM

- Now, what if the GM is not a tree-like graph?
- Can we still directly run message
  message-passing protocol along its edges?
- For non-trees, we do not have the guarantee that message-passing will be consistent!
- Then what?
  - Construct a graph data-structure from P that has a tree structure, and run message-passing on it!

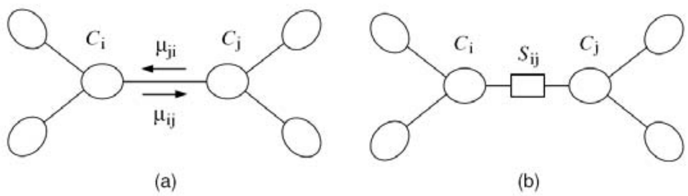
→ Junction tree algorithm

A Sketch of the Junction Tree Algorithm

- **The algorithm**
  - Construction of junction trees --- a special **clique tree**
  - Propagation of probabilities --- a 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
- Many well-known algorithms are special cases of JT
  - Forward-backward, Kalman filter, Peeling, Sum-Product ...

The Shafer Shenoy Algorithm

- Shafer-Shenoy algorithm



  - Message from clique i to clique j :

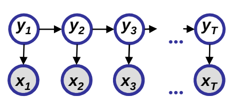
$$\mu_{i \to j} = \sum_{C_i \setminus S_{ij}} \psi_{C_i} \prod_{k \neq j} \mu_{k \to i}(S_{ki})$$

  - Clique marginal

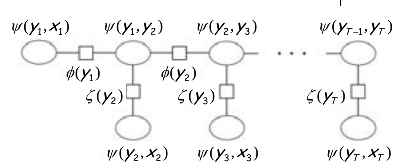
$$p(C_i) \propto \psi_{C_i} \prod_{k} \mu_{k \to i}(S_{ki})$$

The Junction tree algorithm for HMM

- A junction tree for the HMM

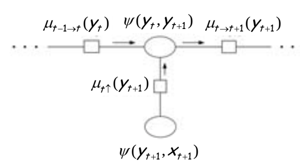


$\Rightarrow$



- Rightward pass

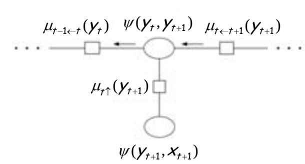
$$\mu_{t \to t+1}(y_{t+1}) = \sum_{y_t} \psi(y_t, y_{t+1}) \mu_{t-1 \to t}(y_t) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{y_t} p(y_{t+1} \mid y_t) \mu_{t-1 \to t}(y_t) p(x_{t+1} \mid y_{t+1})$$
$$= p(x_{t+1} \mid y_{t+1}) \sum_{y_t} a_{y_t, y_{t+1}} \mu_{t-1 \to t}(y_t)$$



  - 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*!

Summary

- The simple Eliminate algorithm captures the key algorithmic Operation underlying probabilistic inference:
  --- That of taking a sum over product of potential functions

- The computational complexity of the Eliminate algorithm can be reduced to purely graph-theoretic considerations.

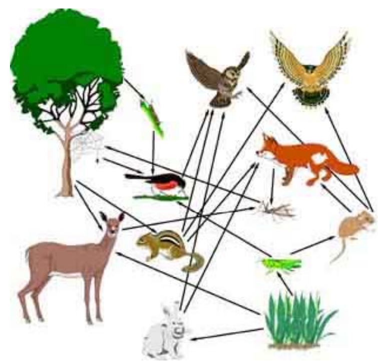
- This graph interpretation will also provide hints about how to design improved inference algorithms

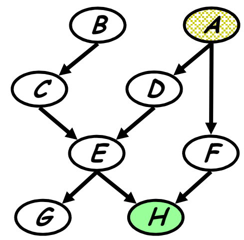
- What can we say about the overall computational complexity of the algorithm? In particular, how can we control the "size" of the summands that appear in the sequence of summation operation.

Extra reading:

From Elimination to JT on a general Bayesian network

A food web





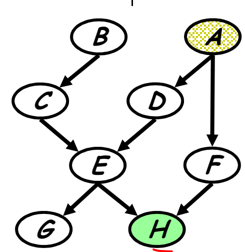
What is the probability that hawks are leaving given that the grass condition is poor?

Example: Variable Elimination

- Query: *P(A |h)*
  - Need to eliminate: *B,C,D,E,F,G,H*
- Initial factors:

$$P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)P(g\,|\,e)P(h\,|\,e,f)$$

- Choose an elimination order: *H,G,F,E,D,C,B*

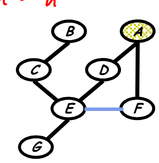


- Step 1:
  - **Conditioning** (fix the evidence node (i.e., *h*) on its observed value (i.e., $\tilde{h}$)):

$h \to \tilde{h}$

$$m_h(e,f) = p(h = \tilde{h}\,|\,e,f)$$

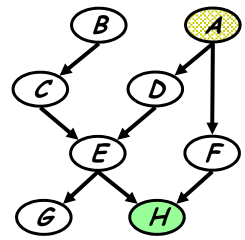
  - This step is isomorphic to a marginalization step:



$$m_h(e,f) = \sum_h p(h\,|\,e,f)\,\delta(h = \tilde{h})$$

Example: Variable Elimination

- Query: $P(B\,|\,h)$
  - Need to eliminate: B,C,D,E,F,G
- Initial factors:

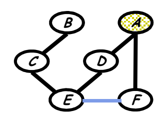


$$P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)P(g\,|\,e)P(h\,|\,e,f)$$
$$\Rightarrow P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)P(g\,|\,e)m_h(e,f)$$

- Step 2: Eliminate G
  - compute

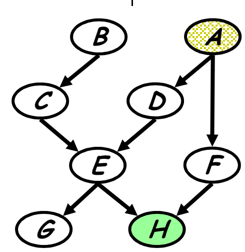
$$m_g(e)=\sum_g p(g\,|\,e)=1$$

$$\Rightarrow P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)m_g(e)m_h(e,f)$$
$$= P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)m_h(e,f)$$



Example: Variable Elimination

- Query: $P(B\,|\,h)$
  - Need to eliminate: B,C,D,E,F
- Initial factors:

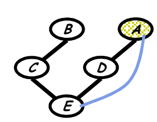


$$P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)P(g\,|\,e)P(h\,|\,e,f)$$
$$\Rightarrow P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)P(g\,|\,e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)P(f\,|\,a)m_h(e,f)$$

- Step 3: Eliminate F
  - compute

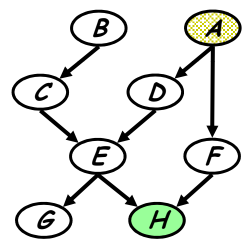
$$m_f(e,a)=\sum_f p(f\,|\,a)m_h(e,f)$$

$$\Rightarrow P(a)P(b)P(c\,|\,b)P(d\,|\,a)P(e\,|\,c,d)m_f(a,e)$$



Example: Variable Elimination

- Query: $P(B\,|\,h)$
  - Need to eliminate: B,C,D,E
- Initial factors:

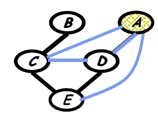


$$P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)\underline{P(e|c,d)m_f(a,e)}$$

- Step 4: Eliminate E
  - compute

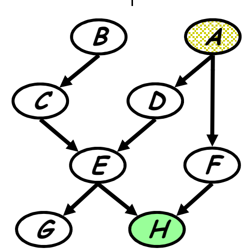
$$m_e(a,c,d)=\sum_e p(e|c,d)m_f(a,e)$$

$$\Rightarrow P(a)P(b)P(c|b)P(d|a)\underline{m_e(a,c,d)}$$



Example: Variable Elimination

- Query: $P(B\,|\,h)$
  - Need to eliminate: B,C,D
- Initial factors:

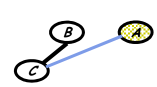


$$P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)m_f(a,e)$$
$$\Rightarrow P(a)P(b)P(c|b)\underline{P(d|a)m_e(a,c,d)}$$

- Step 5: Eliminate D
  - compute

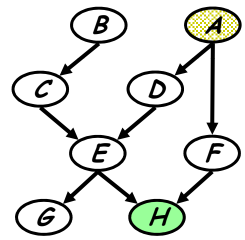
$$m_d(a,c)=\sum_d p(d|a)m_e(a,c,d)$$

$$\Rightarrow P(a)P(b)P(c|d)\underline{m_d(a,c)}$$



Example: Variable Elimination

- Query: $P(B \mid h)$
  - Need to eliminate: B, C



- Initial factors:

$$P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)P(g \mid e)P(h \mid e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)P(g \mid e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)m_f(a,e)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)m_e(a,c,d)$$
$$\Rightarrow P(a)P(b)\underline{P(c \mid d)m_d(a,c)}$$

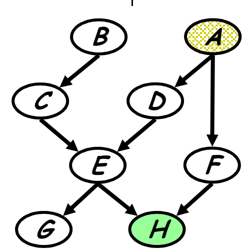
- Step 6: Eliminate C

  - compute $$m_c(a,b) = \sum_c p(c \mid b) m_d(a,c)$$

$$\Rightarrow P(a)P(b)\underline{P(c \mid d)m_d(a,c)}$$

Example: Variable Elimination

- Query: $P(B \mid h)$
  - Need to eliminate: B



- Initial factors:

$$P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)P(g \mid e)P(h \mid e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)P(g \mid e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)P(f \mid a)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c,d)m_f(a,e)$$
$$\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)m_e(a,c,d)$$
$$\Rightarrow P(a)P(b)P(c \mid d)m_d(a,c)$$
$$\Rightarrow P(a)\underline{P(b)m_c(a,b)}$$

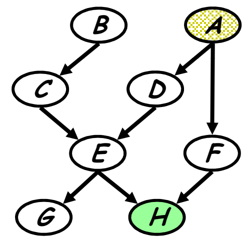
- Step 7: Eliminate B

  - compute $$m_b(a) = \sum_b p(b) m_c(a,b)$$

$$\Rightarrow P(a)\underline{m_b(a)}$$

Example: Variable Elimination

- Query: *P(B | h)*
  - Need to eliminate: *B*



- Initial factors:

$$P(a)P(b)P(c|d)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)$$
$$\Rightarrow P(a)P(b)P(c|d)P(d|a)P(e|c,d)P(f|a)P(g|e)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|d)P(d|a)P(e|c,d)P(f|a)m_h(e,f)$$
$$\Rightarrow P(a)P(b)P(c|d)P(d|a)P(e|c,d)m_f(a,e)$$
$$\Rightarrow P(a)P(b)P(c|d)P(d|a)m_e(a,c,d)$$
$$\Rightarrow P(a)P(b)P(c|d)m_d(a,c)$$
$$\Rightarrow P(a)P(b)m_c(a,b)$$
$$\Rightarrow P(a)m_b(a)$$

- Step 8: Wrap-up $p(a,\tilde{h}) = p(a)m_b(a)\,, \quad p(\tilde{h}) = \sum_a p(a)m_b(a)$

$$\Rightarrow P(a|\tilde{h}) = \frac{p(a)m_b(a)}{\sum p(a)m_b(a)}$$

Complexity of variable elimination

- Suppose in one elimination step we compute

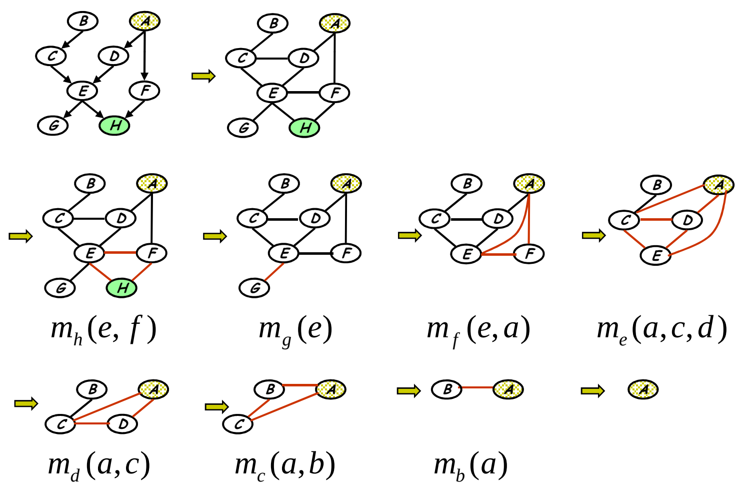
$$m_x(y_1,\ldots,y_k) = \sum_x m'_x(x,y_1,\ldots,y_k)$$
$$m'_x(x,y_1,\ldots,y_k) = \prod_{i=1}^{k} m_i(x,\mathbf{y}_{c_i})$$

This requires

- $k \bullet |\mathrm{Val}(X)| \bullet \prod_i |\mathrm{Val}(\mathbf{Y}_{C_i})|$ multiplications
  - For each value of *x*, y_1, …, y_k, we do *k* multiplications
- $|\mathrm{Val}(X)| \bullet \prod_i |\mathrm{Val}(\mathbf{Y}_{C_i})|$ additions
  - For each value of y_1, …, y_k, we do *|Val(X)|* additions

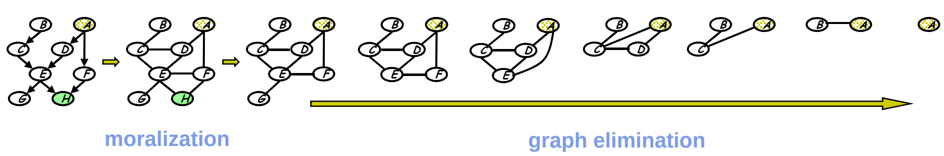
Complexity is **exponential** in number of variables in the intermediate factor

Elimination Cliques



Understanding Variable Elimination

- A graph elimination algorithm

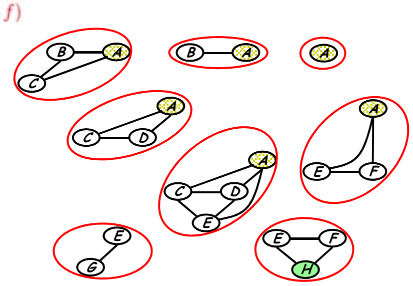


- Intermediate terms correspond to the cliques resulted from elimination
  - "good" elimination orderings lead to **small cliques** and hence reduce complexity
    (what will happen if we eliminate "e" first in the above graph?)
  - finding the optimum ordering is NP-hard, but for many graph optimum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

Elimination Clique

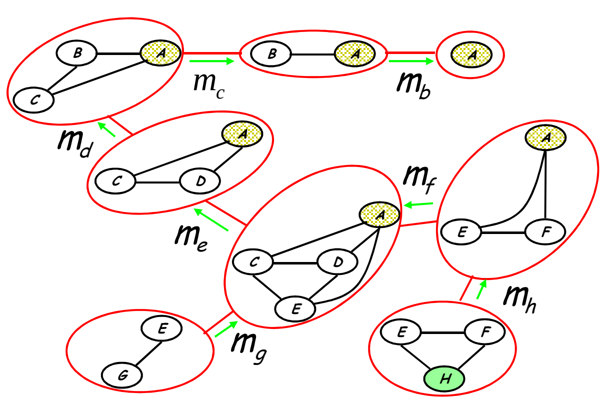
- Recall that Induced dependency during marginalization is captured in elimination cliques
  - Summation <-> elimination
  - Intermediate term <-> elimination clique

$$
\begin{aligned}
& P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)\phi_h(e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)\phi_g(e)\phi_h(e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)\phi_f(a,e) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)\phi_e(a,c,d) \\
\Rightarrow\ & P(a)P(b)P(c|b)\phi_d(a,c) \\
\Rightarrow\ & P(a)P(b)\phi_c(a,b) \\
\Rightarrow\ & P(a)\phi_b(a) \\
\Rightarrow\ & \phi(a)
\end{aligned}
$$



  - Can this lead to an generic inference algorithm?

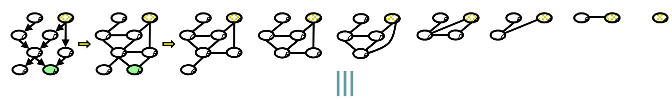
A Clique Tree

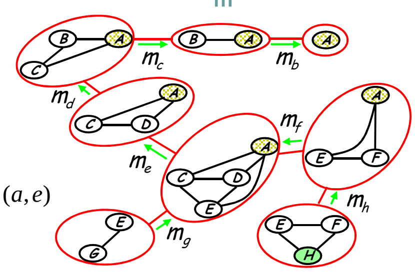


$$
m_e(a,c,d) = \sum_e p(e\,|\,c,d)\,m_g(e)\,m_f(a,e)
$$

From Elimination to Message Passing

- Elimination ≡ message passing on a **clique tree**



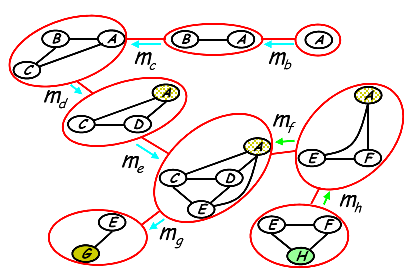


$$m_e(a,c,d) = \sum_e p(e \mid c,d) m_g(e) m_f(a,e)$$

- Messages can be reused

From Elimination to Message Passing

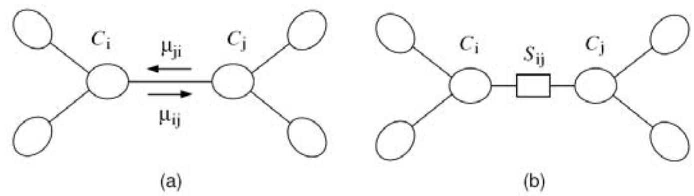
- Elimination ≡ message passing on a **clique tree**
  - **Another query ...**



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

The Shafer Shenoy Algorithm

- 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

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

A Sketch of the Junction Tree Algorithm

- **The algorithm**
  - Construction of junction trees --- a special **clique tree**
  - Propagation of probabilities --- a 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
- Many well-known algorithms are special cases of JT
  - Forward-backward, Kalman filter, Peeling, Sum-Product ...