

Variable Elimination: Algorithm

Sargur Srihari

srihari@cedar.buffalo.edu

Topics

1. Types of Inference Algorithms
2. Variable Elimination: the Basic ideas
3. Variable Elimination
 - Sum-Product VE Algorithm
 - Sum-Product VE for Conditional Probabilities
4. Variable Ordering for VE

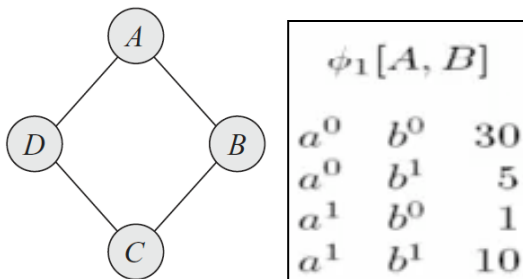
Variable Elimination: Use of Factors

- To formalize VE need concept of factors ϕ
- χ is a set of r.v.s, \mathbf{X} is a subset $\mathbf{X} \subseteq \chi$
- We say $Scope[\phi] = \mathbf{X}$
 - Factor associates a real value for each setting of its arguments $\phi: Val(\mathbf{X}) \rightarrow R$
- Factor in BN is a product term
 - say $\phi(A, B, C) = P(A/B, C)$

Factors in BNs and MNs

- Useful in both BNs and MNs
 - Factor in BN: product term, $\phi(A, B, C) = P(A/B, C)$
 - Factor in MN: Gibbs distribution, say $\phi(A, B)$
 - Definition of Gibbs:

- Example:



$$P_{\Phi}(X_1, \dots, X_n) = \frac{1}{Z} \tilde{P}(X_1, \dots, X_n)$$

where

$$\tilde{P}(X_1, \dots, X_n) = \prod_{i=1}^m \phi_i(D_i)$$

is an unnormalized measure and

$$Z = \sum_{X_1, \dots, X_n} \tilde{P}(X_1, \dots, X_n)$$

is a normalizing constant

called the partition function

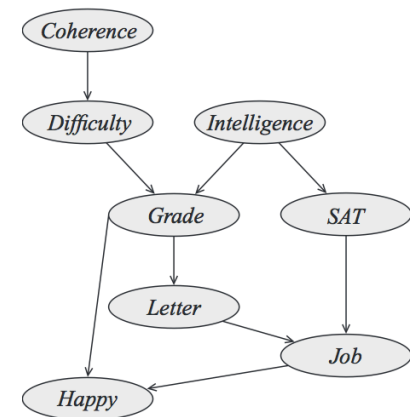
Role of Factor Operations

- The joint distribution is a product of factors

$$P(C,D,I,G,S,L,J,H) = P(C)P(D|C)P(I)P(G|I,D)P(S|I)P(L|G)P(J|L)P(H|G,J) = \phi_C(C) \phi_D(D,C) \phi_I(I) \phi_G(G,I,D) \phi_S(S,I) \phi_L(L,G) \phi_J(J,L,S) \phi_H(H,G,J)$$

- Inference is a task of marginalization

$$P(J) = \sum_L \sum_S \sum_G \sum_H \sum_I \sum_D \sum_C P(C,D,I,G,S,L,J,H)$$



- We wish to systematically eliminate all variables other than J

About Factors

- Inference Algorithms manipulate factors
- Occur in both directed and undirected PGMs
- Need two operations:
 - Factor Product: $\Phi_1(X,Y) \Phi_2(Y,Z)$
 - Factor Marginalization: $\psi(X) = \sum_Y \phi(X,Y)$

Factor Product

- Let X , Y and Z be three disjoint sets of variables and let $\phi_1(X, Y)$ and $\phi_2(Y, Z)$ be two factors.
- The factor product is the mapping $Val(X, Y, Z) \rightarrow R$ as follows

$$\psi(X, Y, Z) = \phi_1(X, Y) \phi_2(Y, Z)$$

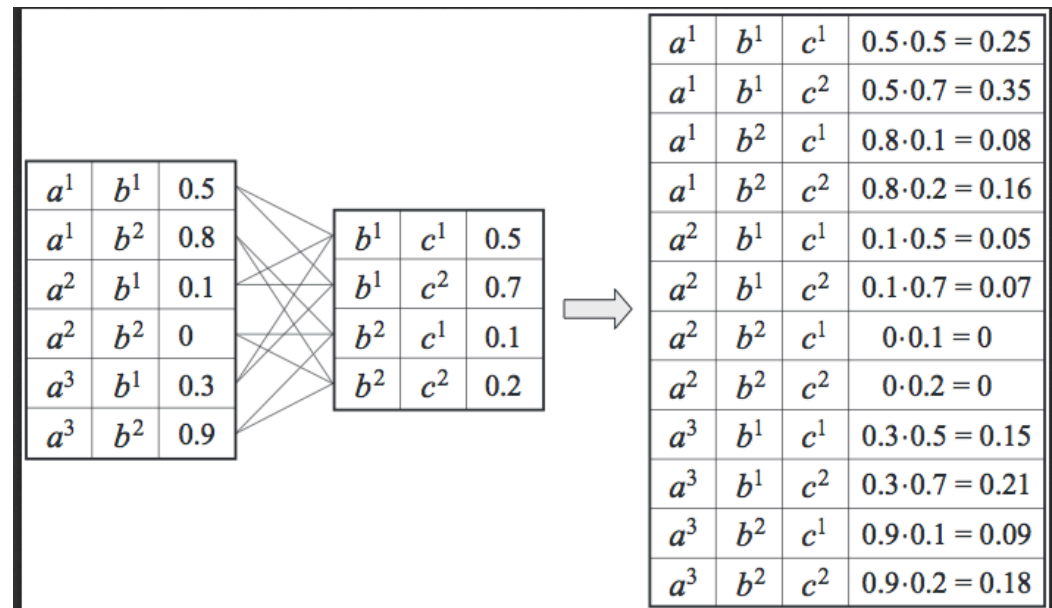
- An example:

$\phi_1: 3 \times 2 = 6$ entries

$\phi_2: 2 \times 2 = 4$ entries

yields

$\psi: 3 \times 2 \times 2 = 12$ entries



Factor Marginalization

- X is a set of variables and $Y \notin X$ is a variable
- $\phi(X, Y)$ is a factor
- We wish to eliminate Y
- Factor marginalization of Y is a factor ψ s.t.

$$\psi(X) = \sum_Y \phi(X, Y)$$

- Process is called summing out of Y in ϕ
- We sum up entities in the table only when the values of X match up
- If we sum out all variables we get a factor which is a single value of 1
- If we sum out all of the variables in an unnormalized distribution $\tilde{P}_\phi = \prod_{i=1}^N \phi_i(D_i)$ we get the partition function

a^1	b^1	c^1	0.25
a^1	b^1	c^2	0.35
a^1	b^2	c^1	0.08
a^1	b^2	c^2	0.16
a^2	b^1	c^1	0.05
a^2	b^1	c^2	0.07
a^2	b^2	c^1	0
a^2	b^2	c^2	0
a^3	b^1	c^1	0.15
a^3	b^1	c^2	0.21
a^3	b^2	c^1	0.09
a^3	b^2	c^2	0.18

$\phi(A, B, C)$

a^1	c^1	0.33
a^1	c^2	0.51
a^2	c^1	0.05
a^2	c^2	0.07
a^3	c^1	0.24
a^3	c^2	0.39

$\psi(A, C)$

Example of Factor Marginalization:
Summing-out $Y=B$ when $X=\{A, C\}$

Distributivity of product over sum

Example with nos.

$a \cdot b_1 + a \cdot b_2 = a(b_1 + b_2)$: product is distributive
 $(a + b_1) \cdot (a + b_2)$ ne. $a + (b_1 \cdot b_2)$: sum is not
 Product distributivity allows fewer operations

$$\psi(A, B) = \sum_{A=a_1}^{a_2} \sum_{B=b_1}^{b_2} A \cdot B = a_1 b_1 + a_1 b_2 + a_2 b_1 + a_2 b_2 \quad \text{requires 4 products, 3 sums}$$

Alternative formulation requires 2 sums, 2 products

$$\psi(A, B) = \sum_{A=a_1}^{a_2} A \cdot \tau(B)$$

$$\text{where } \tau(B) = \sum_{B=b_1}^{b_2} B = b_1 + b_2$$

$$\psi(A, B) = a_1 \tau(B) + a_2 \tau(B)$$

Sum first
 Product next
 Saves ops over
 Product first
 Sum next

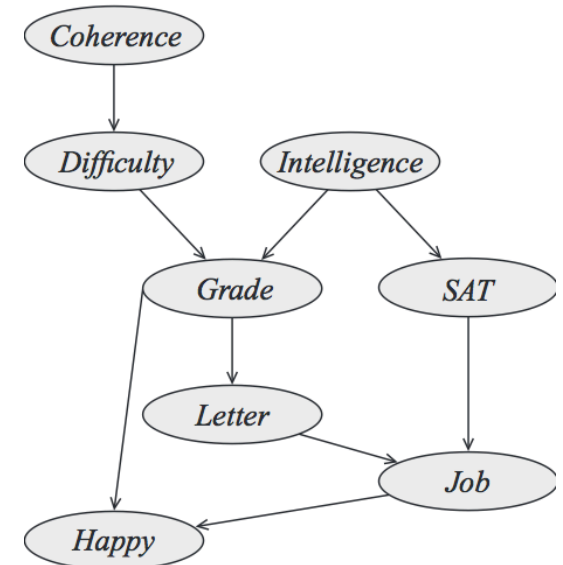
- Factor product and summation behave exactly like product and summation over nos.
- If $X \notin \text{Scope}(\phi_1)$ then $\sum_X (\phi_1 \cdot \phi_2) = \phi_1 \sum_X \phi_2$

Sum-Product Variable Elimination Algorithm

- Task of computing the value of an expression of the form
$$\sum_Z \prod_{\phi \in \Phi} \phi$$
- Called sum-product inference task
 - Sum of Products
- Key insight is that scope of the factors is limited
 - Allowing us to push in some of the *summations*, performing them over the product of only some of the factors
 - We sum out variables one at a time

Inference using Variable Elimination

- Example: Extended Student BN



- We wish to infer $P(J)$

$$P(J) = \sum_H \sum_L \sum_S \sum_G \sum_I \sum_D \sum_C P(C, D, I, G, S, L, J, H)$$

- By chain rule:

$$P(C, D, I, G, S, L, J, H) = P(C)P(D|C)P(I)P(G|I, D)P(S|I)P(L|G)P(J|L)P(H|G, J)$$

– Which is a Sum of Product of factors

Sum-product VE

$$P(J) = \sum_L \sum_S \sum_G \sum_H \sum_I \sum_D \sum_C P(C, D, I, G, S, L, J, H)$$

$$P(C, D, I, G, S, L, J, H) = P(C)P(D|C)P(I)P(G|I, D)P(S|I)P(L|G)P(J|L)P(H|G, J) = \phi_C(C) \phi_D(D, C) \phi_I(I) \phi_G(G, I, D) \phi_S(S, I) \phi_L(L, G) \phi_J(J, L, S) \phi_H(H, G, J)$$

Elimination ordering C, D, I, H, G, S, L

1. Eliminating C :

$$\psi_1(C, D) = \phi_C(C) \phi_D(D, C) \quad \tau_1(D) = \sum_C \psi_1(C, D)$$

Compute the factors

Each step involves factor product ψ and factor marginalization to obtain a new factor τ

2. Eliminating D :

$$\psi_2(G, I, D) = \phi_G(G, I, D) \tau_1(D) \quad \tau_2(G, I) = \sum_D \psi_2(G, I, D)$$

Note we already eliminated one factor with D , but introduced τ_1 involving D

3. Eliminating I :

$$\psi_3(G, I, S) = \phi_I(I) \phi_S(S, I) \tau_2(G, I) \quad \tau_3(G, S) = \sum_I \psi_3(G, I, S)$$

4. Eliminating H :

Note $\tau_4(G, J) = 1$

$$\psi_4(G, J, H) = \phi_H(H, G, J) \tau_3(G, S) \quad \tau_4(G, J) = \sum_H \psi_4(G, J, H)$$

5. Eliminating G :

$$\psi_5(G, J, L, S) = \tau_4(G, J) \tau_3(G, S) \phi_L(L, G) \quad \tau_5(J, L, S) = \sum_G \psi_5(G, J, L, S)$$

6. Eliminating S :

$$\psi_6(J, L, S) = \tau_5(J, L, S) \cdot \phi_J(J, L, S) \quad \tau_6(J, L) = \sum_S \psi_6(J, L, S)$$

7. Eliminating L :

$$\psi_7(J, L) = \tau_6(J, L) \quad \tau_7(J) = \sum_L \psi_7(J, L)$$

Computing $\tau(A,C) = \sum_B \psi(A,B,C) = \sum_B \phi(A,B)\phi(B,C)$

1. Factor product

$$\psi(A,B,C) = \phi(A,B)\phi(B,C)$$

2. Factor marginalization

a^1	b^1	0.5		b^1	c^1	0.5		a^1	b^1	c^1	$0.5 \cdot 0.5 = 0.25$
a^1	b^2	0.8		b^1	c^2	0.7		a^1	b^1	c^2	$0.5 \cdot 0.7 = 0.35$
a^2	b^1	0.1		b^2	c^1	0.1		a^1	b^2	c^1	$0.8 \cdot 0.1 = 0.08$
a^2	b^2	0		b^2	c^2	0.2		a^1	b^2	c^2	$0.8 \cdot 0.2 = 0.16$
a^3	b^1	0.3						a^2	b^1	c^1	$0.1 \cdot 0.5 = 0.05$
a^3	b^2	0.9						a^2	b^1	c^2	$0.1 \cdot 0.7 = 0.07$
								a^2	b^2	c^1	$0 \cdot 0.1 = 0$
								a^2	b^2	c^2	$0 \cdot 0.2 = 0$
								a^3	b^1	c^1	$0.3 \cdot 0.5 = 0.15$
								a^3	b^1	c^2	$0.3 \cdot 0.7 = 0.21$
								a^3	b^2	c^1	$0.9 \cdot 0.1 = 0.09$
								a^3	b^2	c^2	$0.9 \cdot 0.2 = 0.18$

$$\tau(A,C) = \sum_B \psi(A,B,C)$$

a^1	b^1	c^1	0.25		a^1	c^1	0.33
a^1	b^1	c^2	0.35		a^1	c^2	0.51
a^1	b^2	c^1	0.08		a^2	c^1	0.05
a^1	b^2	c^2	0.16		a^2	c^2	0.07
a^2	b^1	c^1	0.05		a^3	c^1	0.24
a^2	b^1	c^2	0.07		a^3	c^2	0.39
a^2	b^2	c^1	0				
a^2	b^2	c^2	0				
a^3	b^1	c^1	0.15				
a^3	b^1	c^2	0.21				
a^3	b^2	c^1	0.09				
a^3	b^2	c^2	0.18				

Sum-Product VE Algorithm

- To compute

$$\sum_Z \prod_{\phi \in \Phi} \phi$$

- First procedure specifies ordering of k variables Z_i

- Second procedure eliminates a single variable Z (contained in factors Φ') and returns factor τ

Procedure Sum-Product-VE (

Φ , // Set of factors

Z , // Set of variables to be eliminated

\prec // Ordering on Z

)

1 Let Z_1, \dots, Z_k be an ordering of Z such that

2 $Z_i \prec Z_j$ if and only if $i < j$

3 **for** $i = 1, \dots, k$

4 $\Phi \leftarrow \text{Sum-Product-Eliminate-Var}(\Phi, Z_i)$

5 $\phi^* \leftarrow \prod_{\phi \in \Phi} \phi$

6 **return** ϕ^*

Procedure Sum-Product-Eliminate-Var (

Φ , // Set of factors

Z // Variable to be eliminated

)

1 $\Phi' \leftarrow \{\phi \in \Phi : Z \in \text{Scope}[\phi]\}$

2 $\Phi'' \leftarrow \Phi - \Phi'$

3 $\psi \leftarrow \prod_{\phi \in \Phi'} \phi$

4 $\tau \leftarrow \sum_Z \psi$

5 **return** $\Phi'' \cup \{\tau\}$

Two runs of Variable Elimination

- Elimination Ordering: C, D, I, H, G, S, L

Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G, I, D), \tau_1(D)$	G, I, D	$\tau_2(G, I)$
3	I	$\phi_I(I), \phi_S(S, I), \tau_2(G, I)$	G, S, I	$\tau_3(G, S)$
4	H	$\phi_H(H, G, J)$	H, G, J	$\tau_4(G, J)$
5	G	$\tau_4(G, J), \tau_3(G, S), \phi_L(L, G)$	G, J, L, S	$\tau_5(J, L, S)$
6	S	$\tau_5(J, L, S), \phi_J(J, L, S)$	J, L, S	$\tau_6(J, L)$
7	L	$\tau_6(J, L)$	J, L	$\tau_7(J)$

- Elimination Ordering: G, I, S, L, H, C, D

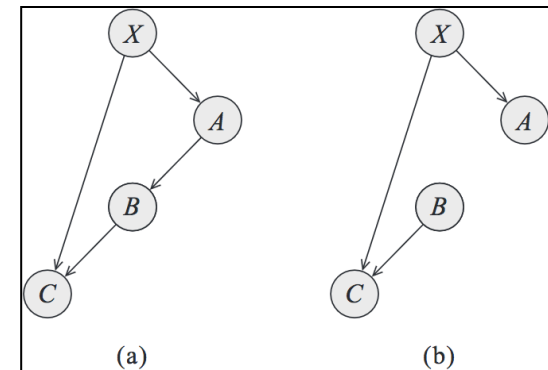
Step	Variable eliminated	Factors used	Variables involved	New factor
1	G	$\phi_G(G, I, D), \phi_L(L, G), \phi_H(H, G, J)$	G, I, D, L, J, H	$\tau_1(I, D, L, J, H)$
2	I	$\phi_I(I), \phi_S(S, I), \tau_1(I, D, L, S, J, H)$	S, I, D, L, J, H	$\tau_2(D, L, S, J, H)$
3	S	$\phi_J(J, L, S), \tau_2(D, L, S, J, H)$	D, L, S, J, H	$\tau_3(D, L, J, H)$
4	L	$\tau_3(D, L, J, H)$	D, L, J, H	$\tau_4(D, J, H)$
5	H	$\tau_4(D, J, H)$	D, J, H	$\tau_5(D, J)$
6	C	$\tau_5(D, J), \phi_C(C), \phi_D(D, C)$	D, J, C	$\tau_6(D, J)$
7	D	$\tau_6(D, J)$	D, J	$\tau_7(J)$

Factors with much larger scope

Semantics of Factors

- What are the intermediate factors?
- Sometimes they correspond to marginal or conditional probabilities in the network
- It is not always the case
- Result of eliminating X in (a) is

$$\tau(A, B, C) = \sum_X P(X) P(A|X) P(C|B, X)$$



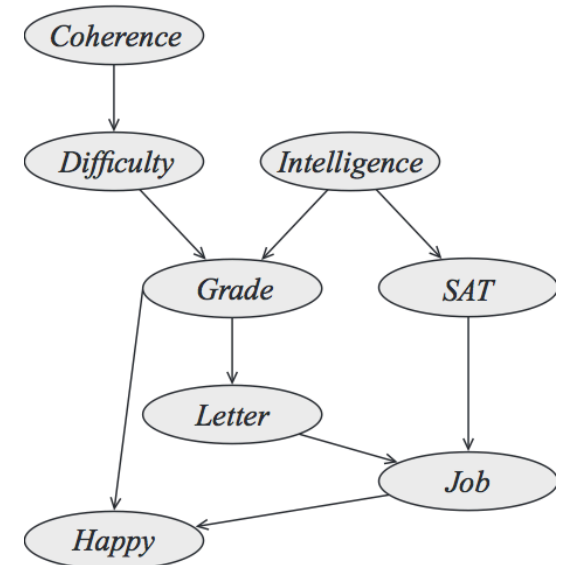
- It does *not* correspond to any probability or conditional probability in (a)
- It does correspond to a conditional probability $P(A, C|B)$ in (b)

Dealing with Evidence

- We observe student is intelligent (i^1) and is unhappy (h^0)
- What is the probability that student has a job?

$$P(J \mid i^1, h^0) = \frac{P(J, i^1, h^0)}{P(i^1, h^0)} \leftarrow \text{Probability of evidence}$$

- For this we need unnormalized distribution $P(J, i^1, h^0)$. Then we compute conditional distribution by renormalizing by $P(e) = P(i^1, h^0)$



BN with evidence e is Gibbs with $Z=P(e)$

Defined by original factors reduced to context $E=e$

Let \mathcal{B} be a BN over χ and $E=e$ an observation. Let $W=\chi-E$.

– Then $P_{\mathcal{B}}(W|e)$ is a Gibbs distribution defined by the factors

$$\Phi = \{\phi_{X_i}\}_{X_i \in \chi} \text{ where } \phi_{X_i} = P_{\mathcal{B}}(X_i | Pa_{X_i})[E=e]$$

• Partition function for Gibbs distribution is $P(e)$. Proof follows:

$$P_{\mathcal{B}}(\chi) = \prod_{i=1}^N P_{\mathcal{B}}(X_i | Pa_{X_i})$$

$$P_{\mathcal{B}}(W | E=e) = \frac{P_{\mathcal{B}}(W)[E=e]}{P_{\mathcal{B}}(E=e)} = \frac{\prod_{i=1}^N P_{\mathcal{B}}(X_i | Pa_{X_i})[E=e]}{\sum_W P_{\mathcal{B}}(\chi)[E=e]} = \frac{\prod_{i=1}^N P_{\mathcal{B}}(X_i | Pa_{X_i})[E=e]}{\sum_W \prod_{i=1}^N P_{\mathcal{B}}(X_i | Pa_{X_i})[E=e]}$$

- Thus any BN conditioned on evidence can be regarded as a Markov network
 - and use techniques developed for MN analysis

Sum-Product for Conditional Probabilities

- Apply Sum-product VE to $\mathcal{X} - \mathbf{Y} - \mathbf{E}$
- Returned factor $\phi^*(\mathbf{Y})$ is $P(\mathbf{Y}, e)$
- To obtain $P(\mathbf{Y} | e)$
 - Renormalize $\phi^*(\mathbf{Y})$ by $P(e)$, sum over entries in the unnormalized distribution

Procedure Cond-Prob-VE (

\mathcal{K} , // A network over \mathcal{X}

\mathbf{Y} , // Set of query variables

$\mathbf{E} = e$ // Evidence

)

```

1   $\Phi \leftarrow$  Factors parameterizing  $\mathcal{K}$ 
2  Replace each  $\phi \in \Phi$  by  $\phi[\mathbf{E} = e]$ 
3  Select an elimination ordering  $\prec$ 
4   $\mathbf{Z} \leftarrow \mathcal{X} - \mathbf{Y} - \mathbf{E}$ 
5   $\phi^* \leftarrow$  Sum-Product-VE( $\Phi, \prec, \mathbf{Z}$ )
6   $\alpha \leftarrow \sum_{\mathbf{y} \in \text{Val}(\mathbf{Y})} \phi^*(\mathbf{y})$ 
7  return  $\alpha, \phi^*$ 
```

Run of Sum-Product VE

• Computing

$$P(J, i^1, h^0)$$

Step	Variable eliminated	Factors used	Variables involved	New factor
1'	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau'_1(D)$
2'	D	$\phi_G[I = i^1](G, D), \phi_I[I = i^1](), \tau'_1(D)$	G, D	$\tau'_2(G)$
5'	G	$\tau'_2(G), \phi_L(L, G), \phi_H[H = h^0](G, J)$	G, L, J	$\tau'_5(L, J)$
6'	S	$\phi_S[I = i^1](S), \phi_J(J, L, S)$	J, L, S	$\tau'_6(J, L)$
7'	L	$\tau'_6(J, L), \tau'_5(J, L)$	J, L	$\tau'_7(J)$

Compare with previous elimination ordering:

- Steps 3,4 disappear
- Since I and H need not be eliminated
- By not eliminating I we avoid step that correlates G and I

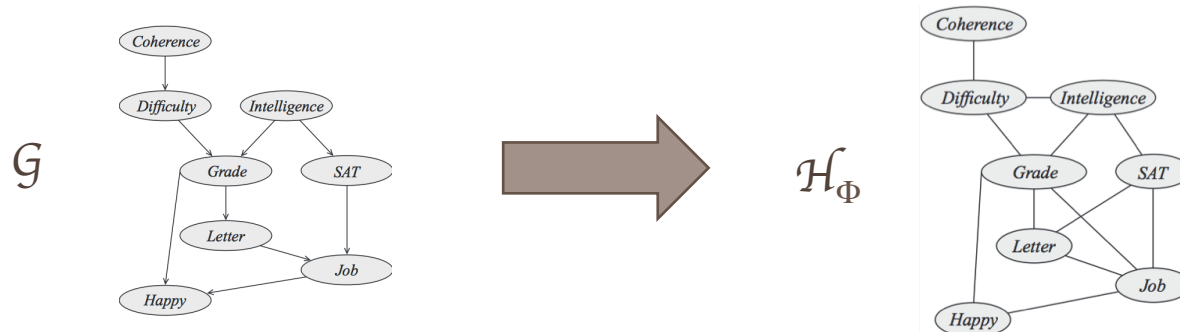
Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G, I, D), \tau_1(D)$	G, I, D	$\tau_2(G, I)$
3	I	$\phi_I(I), \phi_S(S, I), \tau_2(G, I)$	G, S, I	$\tau_3(G, S)$
4	H	$\phi_H(H, G, J)$	H, G, J	$\tau_4(G, J)$
5	G	$\tau_4(G, J), \tau_3(G, S), \phi_L(L, G)$	G, J, L, S	$\tau_5(J, L, S)$
6	S	$\tau_5(J, L, S), \phi_J(J, L, S)$	J, L, S	$\tau_6(J, L)$
7	L	$\tau_6(J, L)$	J, L	$\tau_7(J)$

Complexity of VE: Simple Analysis

- If n random variables and m initial factors:
 - We have $m=n$ in a BN
 - In a MN we may have more factors than variables
- VE picks a variable X_i then multiplies all factors involving that variable
 - Result is a single factor ψ_i
- If N_i is no. of entries in factor ψ_i and $N_{\max} = \max N_i$
 - Overall amount of work required is $O(mN_{\max})$
 - Inevitable exponential blowup is exponential growth in size of factors ψ_i

Complexity: Graph-Theoretic Analysis

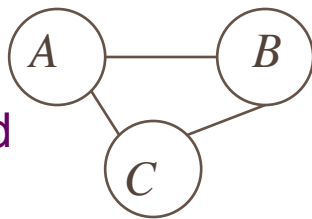
- VE doesn't care if input directed/undirected/combo
 - It can be viewed as operating on an undirected graph \mathcal{H} with factors Φ
 - Let P be defined by multiplying factors in $\Phi = \{\phi\}$
 - Defining $X = \text{Scope}[\Phi]$ $P(\mathbf{X}) = \frac{1}{Z} \prod_{\phi \in \Phi} \phi$ where $Z = \sum_{\mathbf{X}} \prod_{\phi \in \Phi} \phi$
 - Then \mathcal{H}_{Φ} is the minimal MN I-map for P and factors Φ are a parameterization of this network
 - For a BN \mathcal{G} , the undirected graph \mathcal{H}_{Φ} is precisely the Moralized BN



MN induced by context $E=e$

- Factor $\psi(A, B, C)$
- Variable C eliminated by context $C=c^1$

Moralized
BN



a^1	b^1	c^1	$0.5 \cdot 0.5 = 0.25$
a^1	b^1	c^2	$0.5 \cdot 0.7 = 0.35$
a^1	b^2	c^1	$0.8 \cdot 0.1 = 0.08$
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a^2	b^1	c^2	$0.1 \cdot 0.7 = 0.07$
a^2	b^2	c^1	$0 \cdot 0.1 = 0$
a^2	b^2	c^2	$0 \cdot 0.2 = 0$
a^3	b^1	c^1	$0.3 \cdot 0.5 = 0.15$
a^3	b^1	c^2	$0.3 \cdot 0.7 = 0.21$
a^3	b^2	c^1	$0.9 \cdot 0.1 = 0.09$
a^3	b^2	c^2	$0.9 \cdot 0.2 = 0.18$

Value of C determines
the factor $\tau(A, B)$

a^1	b^1	c^1	0.25
a^1	b^2	c^1	0.08
a^2	b^1	c^1	0.05
a^2	b^2	c^1	0
a^3	b^1	c^1	0.15
a^3	b^2	c^1	0.09



$$C=c^1$$

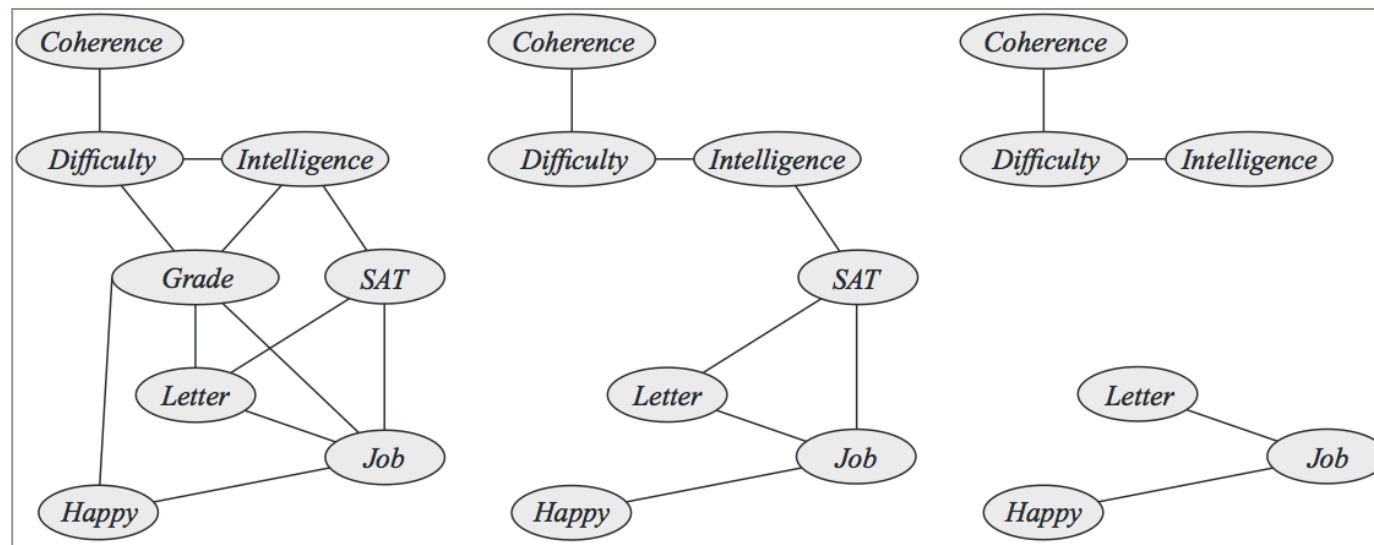
$$\tau(A, B) = \sum_{C=c^1} \psi(A, B, C)$$



Initial Set of Factors

Context $G=g$

Context $G=g, S=s$

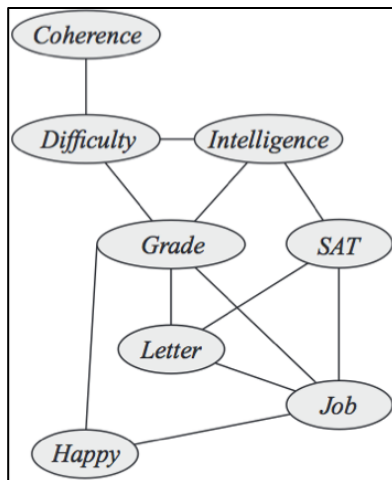


VE as graph transformation

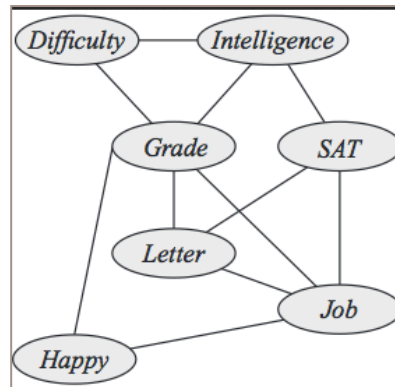
When a variable X is eliminated from Φ ,

Fill edges are introduced in Φ_X

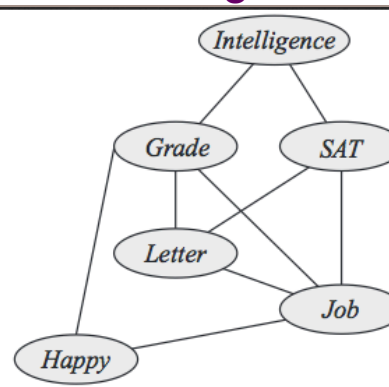
Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G, I, D), \tau_1(D)$	G, I, D	$\tau_2(G, I)$
3	I	$\phi_I(I), \phi_S(S, I), \tau_2(G, I)$	G, S, I	$\tau_3(G, S)$
4	H	$\phi_H(H, G, J)$	H, G, J	$\tau_4(G, J)$
5	G	$\tau_4(G, J), \tau_3(G, S), \phi_L(L, G)$	G, J, L, S	$\tau_5(J, L, S)$
6	S	$\tau_5(J, L, S), \phi_J(J, L, S)$	J, L, S	$\tau_6(J, L)$
7	L	$\tau_6(J, L)$	J, L	$\tau_7(J)$



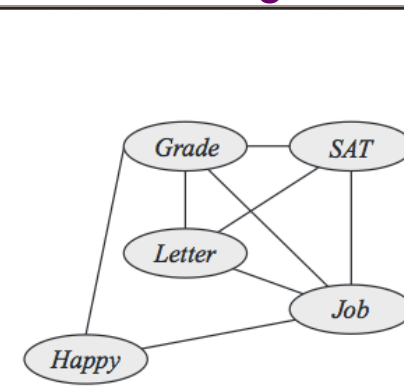
After eliminating C



After eliminating D
No fill edges



After eliminating I
Fill edge $G-S$



Induced Graph

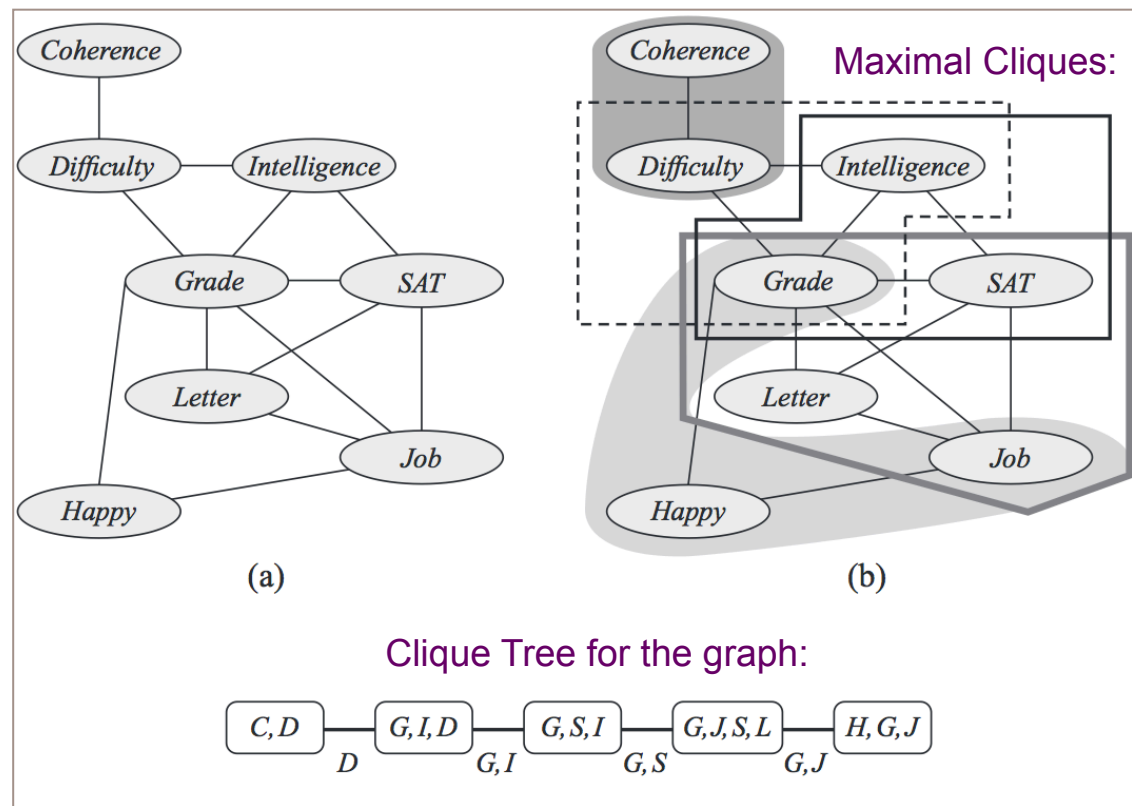
- Union of all graphs generated by VE
- Every factor generated is a clique
- Every maximal clique is the scope of some intermediate factor

Induced Graph due to
VE using elimination order:

Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C), \phi_D(D, C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G, I, D), \tau_1(D)$	G, I, D	$\tau_2(G, I)$
3	I	$\phi_I(I), \phi_S(S, I), \tau_2(G, I)$	G, S, I	$\tau_3(G, S)$
4	H	$\phi_H(H, G, J)$	H, G, J	$\tau_4(G, J)$
5	G	$\tau_4(G, J), \tau_3(G, S), \phi_L(L, G)$	G, J, L, S	$\tau_5(J, L, S)$
6	S	$\tau_5(J, L, S), \phi_J(J, L, S)$	J, L, S	$\tau_6(J, L)$
7	L	$\tau_6(J, L)$	J, L	$\tau_7(J)$

Width of induced graph=
no. of nodes in largest clique minus 1

Minimal induced width over all
orderings is bound on VE performance

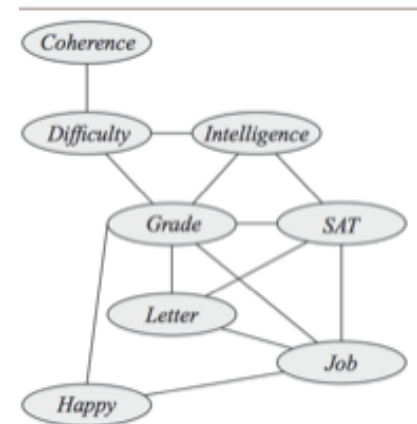


Finding Elimination Orderings

- Which ordering C, D, I, H, G, S, L or G, I, S, L, H, C, D ?
 - How can we compute minimal induced width of the graph and the elimination ordering achieving that width?
 - Given graph \mathcal{H} and some bound K , determine whether there exists an elimination ordering achieving induced width $\leq K$

1. Max-cardinality Search

- Induced graphs are chordal
 - Every minimal loop is of length 3
 - $G \rightarrow L \rightarrow J \rightarrow H$ is cut by chord $G \rightarrow J$



2. Greedy Search

Max-Cardinality Search

- **Procedure** Max-Cardinality (
 \mathcal{H} // An undirected graph over \mathcal{X}
)

```

1  Initialize all nodes in  $\mathcal{X}$  as unmarked
2  for  $k = |\mathcal{X}| \dots 1$ 
3       $X \leftarrow$  unmarked variable in  $\mathcal{X}$  with largest number of marked neighbors
4       $\pi(X) \leftarrow k$ 
5      Mark  $X$ 
6  return  $\pi$ 
  
```



Select S first
 Next is a neighbor, say J
 Largest no of marked neighbors are H and I

Greedy Search

• Procedure Greedy- Ordering(

\mathcal{H} // An undirected graph over \mathcal{X}

s // An evaluation metric

)

```

1  Initialize all nodes in  $\mathcal{X}$  as unmarked
2  for  $k = 1 \dots |\mathcal{X}|$ 
3      Select an unmarked variable  $X \in \mathcal{X}$  that minimizes  $s(\mathcal{H}, X)$ 
4       $\pi(X) \leftarrow k$ 
5      Introduce edges in  $\mathcal{H}$  between all neighbors of  $X$ 
6      Mark  $X$ 
7  return  $\pi$ 

```

Evaluation metric $s(\mathcal{H}, X)$:

- Min-neighbors: no. of neighbors it has in current graph
- Min-weight: product of weights (domain-cardinality) of its neighbors
- Min-fill: no. of edges that need to be added to the graph due to its elimination
- Weighted min-fill: sum of weights of edges that need to be added where weight of edge is product of weights of constituent vertices

Comparison of VE Orderings

- Different heuristics for variable orderings
- Testing data:
 - 8 standard BNs ranging from 8 to 1,000 nodes
- Methods:
 - Simulated annealing, BN package
 - Four heuristics

Comparison of VE variable ordering algorithms

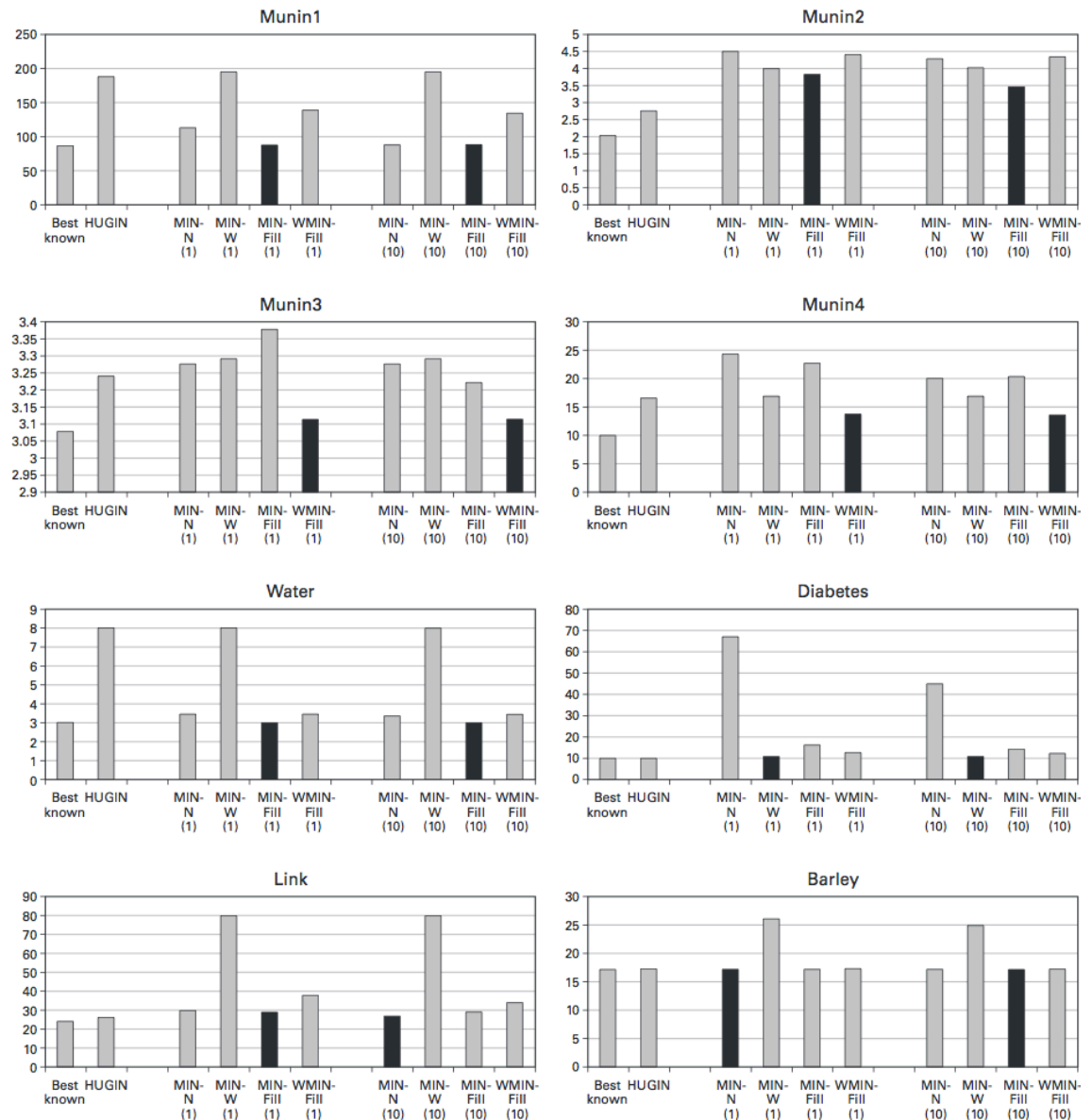
- Evaluation metric

$$s(\mathcal{H}, X):$$

- Min-neighbors (MIN-N)
 - Min-weight (MIN-W)
 - Min-fill (MIN-Fill)
 - Weighted min-fill (WMIN-Fill)
- Best of 4 is black bar

- For large networks

- worthwhile to run several heuristic algorithms to find best ordering

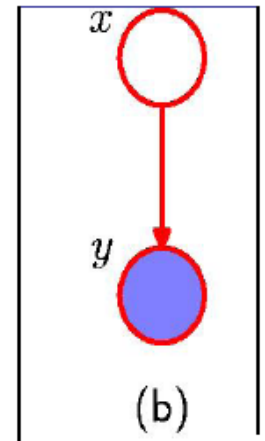
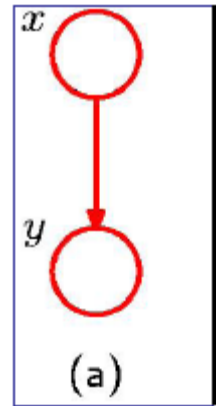


Two Simple Inference Cases

- Same ideas as before, as discussed in HMM literature
 1. Bayes theorem as inference
 2. Inference on a chain

1. Bayes Theorem as Inference

- Joint distribution $p(x,y)$ over two variables x and y
 - Factors $p(x,y)=p(x)p(y|x)$
 - represented as directed graph (a)
 - We are given CPDs $p(x)$ and $p(y|x)$
- If we observe value of y as in (b)
 - Can view marginal $p(x)$ as prior
 - Over latent variable x
- Analogy to 2-class classifier
 - Class $x \in \{0,1\}$ and feature y is continuous
 - Wish to infer a posteriori distribution $p(x|y)$



Inferring posterior using Bayes

- Using sum and product rules, we can evaluate marginal

$$p(y) = \sum_{x'} p(y | x') p(x')$$

– Need to evaluate a summation

- Which is then used in Bayes rule to calculate

$$p(x | y) = \frac{p(y | x) p(x)}{p(y)}$$

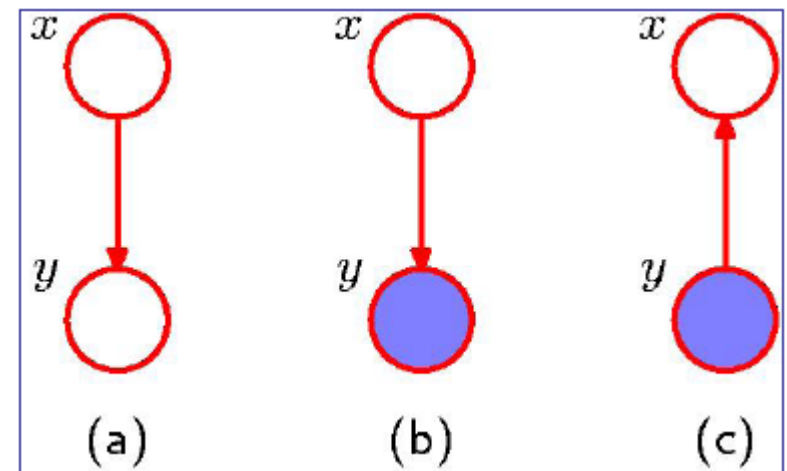
- Observations

– Joint is now expressed as

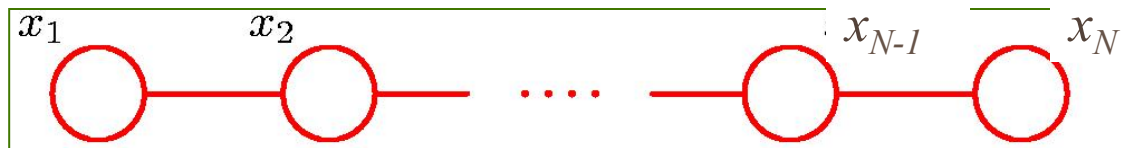
$$p(x, y) = p(y) p(x | y)$$

- Which is shown in (c)

– Thus knowing value of y
we know distribution of x



2. Inference on a Chain



- Graphs of this form are known as Markov chains
 - Example: $N = 365$ days and x is weather (cloudy,rainy,snow..)
- Analysis more complex than previous case
- In this case directed and undirected are exactly same since there is only one parent per node (no additional links needed)
- Joint distribution has form

$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)$$

Product of
potential functions
over pairwise cliques

- Specific case of N discrete variables
 - Potential functions are $K \times K$ tables
 - Joint distribution has $(n-1)K^2$ parameters

Inferring marginal of a node



- Wish to evaluate marginal distribution $p(x_n)$
 - What is the weather on November 11?
- For specific node x_n part way along chain
- As yet there are no observed nodes
- Required marginal obtained summing joint distribution over all variables except x_n

$$p(x_n) = \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_N} p(\mathbf{x})$$

By application of sum rule

Naïve Evaluation of marginal



$$p(x_n) = \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_N} p(\mathbf{x})$$

$$= \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_N} \underbrace{\frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)}_{\text{Joint}}$$

1. Evaluate joint distribution
2. Perform summations explicitly
 - Joint can be expressed as set of numbers one for each value of \mathbf{x}
 - There are N variables with K states
 - K^N values for \mathbf{x}
 - Evaluation of both joint and marginal
 - Exponential with length N of chain
 - Impossible with $K=10$ and $N=365$

Efficient Evaluation

$$p(x_n) = \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_N} \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)$$

- We are adding a bunch of products
- But multiplication is distributive over addition

$$ab + ac = a(b + c)$$

- Perform summation first and then do product
- LHS involves 3 arithmetic ops,
- RHS involves 2
- Sum-of-products evaluated as sums first

Efficient evaluation: exploiting conditional independence properties

$$p(x_n) = \sum_{x_1} \dots \sum_{x_{n-1}} \sum_{x_{n+1}} \dots \sum_{x_N} \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \dots \psi_{N-1,N}(x_{N-1}, x_N)$$

- Rearrange order of summations/multiplications
 - to allow marginal to be evaluated more efficiently
- Consider summation over x_N
 - Potential $\psi_{N-1,N}(x_{N-1}, x_N)$ is only one that depends on x_N
 - So we can perform $\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$
 - To give a function of x_{N-1}
- Use this to perform summation over x_{N-1}
- Each summation removes a variable from distribution or removal of node from graph

Marginal Expression

- Group potentials and summations together to give marginal

$$p(x_n) = \frac{1}{Z}$$

$$\underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \dots \left[\sum_{x_2} \psi_{2,3}(x_2, x_3) \left[\sum_{x_1} \psi_{1,2}(x_1, x_2) \right] \dots \right] \right]}_{\mu_\alpha(x_n)}$$

$$\underbrace{\left[\sum_{x_{n-1}} \psi_{n,n+1}(x_n, x_{n+1}) \dots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \dots \right]}_{\mu_\beta(x_n)}$$

Key concept:
 Multiplication is distributive over addition
 $ab + ac = a(b + c)$
 LHS involves 3 arithmetic ops,
 RHS involves 2

Computational cost

- Evaluation of marginal using reordered expression
- $N-1$ summations
 - Each with K states
 - Each a function of 2 variables
 - Summation over x_1 involves only $\psi_{1,2}(x_1, x_2)$
 - A table of $K \times K$ numbers
 - Sum table over x_1 for each x_2
 - $O(K^2)$ cost
- Total cost is $O(NK^2)$
- Linear in chain length vs. exponential cost of naïve approach
 - Able to exploit many conditional independence properties of simple graph

Interpretation as Message Passing

- Calculation viewed as message passing in graph
- Expression for marginal decomposes into

$$p(x_n) = \frac{1}{Z} \mu_\alpha(x_n) \mu_\beta(x_n)$$

- Interpretation
 - Message passed forwards along chain from node x_{n-1} to x_n is $\mu_\alpha(x_n)$
 - Message passed backwards from node x_{n+1} to x_n is $\mu_\beta(x_n)$
 - Each message comprises of K values one for each choice of x_n

Recursive evaluation of messages

- Message $\mu_\alpha(x_n)$ can be evaluated as

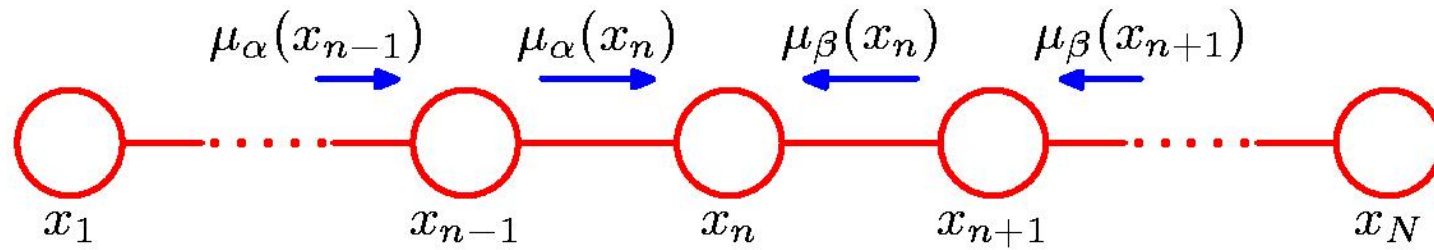
$$\begin{aligned}\mu_\alpha(x_n) &= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \left[\sum_{x_{n-2}} \dots \right] \\ &= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \mu_\alpha(x_{n-1})\end{aligned}\quad (1)$$

- Therefore first evaluate

$$\mu_\alpha(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2)$$

- Apply (1) repeatedly until we reach desired node
- Note that outgoing message $\mu_\alpha(x_n)$ in (1) is obtained by
 - multiplying incoming message $\mu_\alpha(x_{n-1})$ by the local potential involving the node variable and
 - the outgoing variable
 - and summing over node variable

Recursive message passing



- Similarly message $\mu_b(x_n)$ can be evaluated recursively starting with node x_n

$$\begin{aligned}\mu_\beta(x_n) &= \sum_{x_{n+1}} \psi_{n+1,n}(x_{n+1}, x_n) \left[\sum_{x_{n+2}} \dots \right] \\ &= \sum_{x_{n+1}} \psi_{n+1,n}(x_{n+1}, x_n) \mu_\beta(x_{n+1})\end{aligned}$$

Message passing equations known as *Chapman-Kolmogorov* equations for Markov processes

- Normalization constant Z is easily evaluated
 - By summing $\frac{1}{Z} \mu_\alpha(x_n) \mu_\beta(x_n)$ over all state of x_n
 - An $O(K)$ computation

Evaluating marginals for every node

- Evaluate $p(x_n)$ for every node $n = 1, \dots, N$
- Simply applying above procedure is $O(N^2 M^2)$
- Computationally wasteful with duplication
 - To find $p(x_1)$ we need to propagate message $m_b(.)$ from node x_N back to x_2
 - To evaluate $p(x_2)$ we need to propagate message $m_b(.)$ from node x_N back to x_3
- Instead
 - launch message $m_b(x_{N-1})$ starting from node x_N and propagate back to x_1
 - launch message $m_a(x_2)$ starting from node x_2 and propagate forward to x_N
 - Store all intermediate messages along the way
 - Then any node can evaluate its marginal by $p(x_n) = \frac{1}{Z} \mu_\alpha(x_n) \mu_\beta(x_n)$
 - Computational cost is only twice as finding marginal of single node instead of N times

Joint distribution of neighbors

- Wish to calculate joint distribution $p(x_{n-1}, x_n)$ for neighboring nodes
- Similar to previous computation
- Required joint distribution can be written as

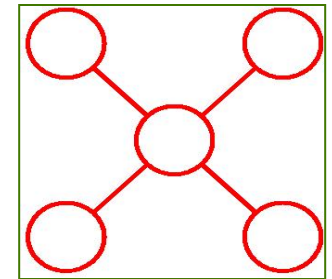
$$p(x_{n-1}, x_n) = \frac{1}{Z} \mu_\alpha(x_{n-1}) \psi_{n-1, n}(x_{n-1}, x_n) \mu_\beta(x_n)$$

- Obtained once message passing for marginals is completed
- Useful result if we wish to use parametric forms for conditional distributions

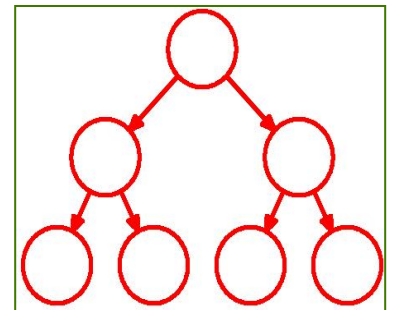
Tree structured graphs

- Local message passing can be performed efficiently on trees
- Message passing can be generalized to give *sum-product algorithm*
- Tree
 - a graph with only one path between any pair of nodes
 - Such graphs have no loops
 - In directed graphs a tree has a single node with no parents called a *root*
 - Directed to undirected will not add moralization links since every node has only one parent
- Polytree
 - A directed graph has nodes with more than one parent but there is only one path between nodes (ignoring arrow direction)
 - Moralization will add links

Undirected tree



Directed tree



Directed polytree

