Probabilistic Graphical Models

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Lecture 5, February 22, 2012

Today's lecture

1. Worst-case complexity of probabilistic inference
2. Elimination algorithm
3. Running-time analysis of elimination algorithm (*treewidth*)

Probabilistic inference

- Today we consider exact inference in graphical models
- In particular, we focus on conditional probability queries,

$$p(\mathbf{Y}|\mathbf{E}=\mathbf{e}) = \frac{p(\mathbf{Y},\mathbf{e})}{p(\mathbf{e})}$$

  (e.g., the probability of a patient having a disease given some observed symptoms)

- Let $\mathbf{W} = \mathcal{X} - \mathbf{Y} - \mathbf{E}$ be the random variables that are neither the query nor the evidence. Each of these joint distributions can be computed by marginalizing over the other variables:

$$p(\mathbf{Y},\mathbf{e}) = \sum_{\mathbf{w}} p(\mathbf{Y},\mathbf{e},\mathbf{w}), \quad p(\mathbf{e}) = \sum_{\mathbf{y}} p(\mathbf{y},\mathbf{e})$$

- Naively marginalizing over all unobserved variables requires an exponential number of computations
- Does there exist a more efficient algorithm?

Computational complexity of probabilistic inference

- Here we show that, unless P=NP, there does *not* exist a more efficient algorithm
- We show this by reducing 3-SAT, which is NP-hard, to probabilistic inference in Bayesian networks
- 3-SAT asks about the *satisfiability* of a logical formula defined on n literals $Q_1, \ldots, Q_n$, e.g.

$$(\neg Q_3 \vee \neg Q_2 \vee Q_3) \wedge (Q_2 \vee \neg Q_4 \vee \neg Q_5) \cdots$$

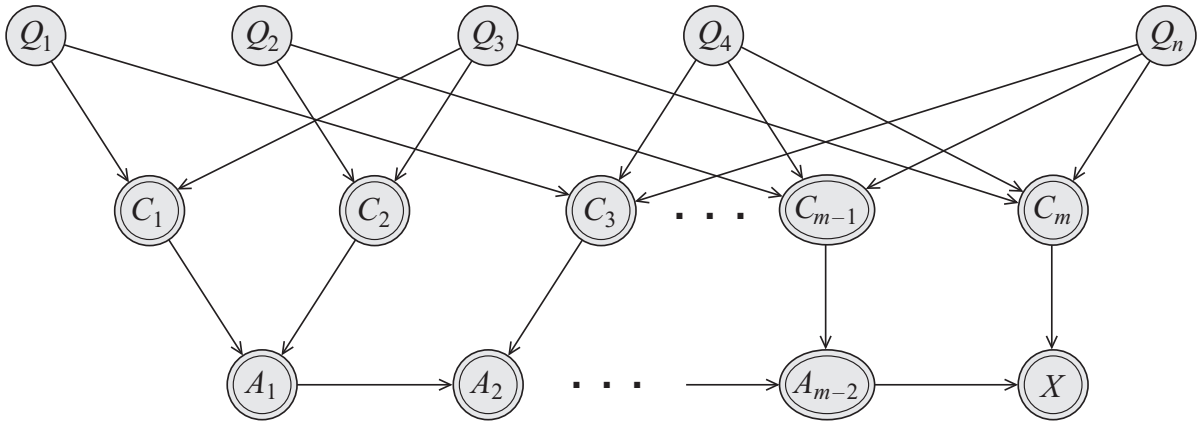
- Each of the disjunction terms is called a *clause*, e.g.

$$C_1(q_1, q_2, q_3) = \neg q_3 \vee \neg q_2 \vee q_3$$

  In 3-SAT, each clause is defined on at most 3 literals.
- Our reduction also proves that inference in Markov networks is NP-hard (why?)

Reducing satisfiability to MAP inference

- **Input:** 3-SAT formula with n literals $Q_1, \ldots Q_n$ and m clauses $C_1, \ldots, C_m$



- One variable $Q_i \in \{0, 1\}$ for each literal, $p(Q_i = 1) = 0.5$.
- One variable $C_i \in \{0, 1\}$ for each clause, whose parents are the literals used in the clause. $C_i = 1$ if the clause is satisfied, and 0 otherwise:

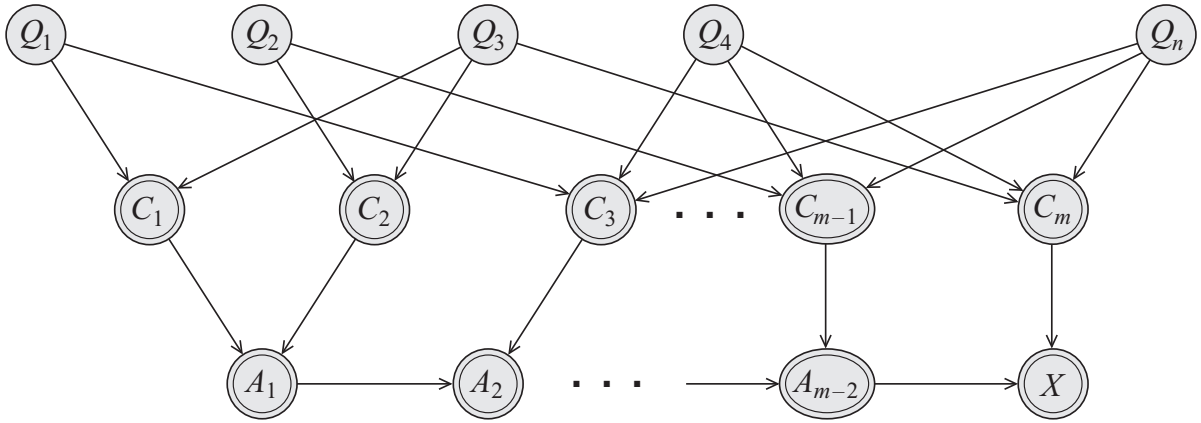
$$p(C_i = 1 \mid \mathbf{q}_{\mathrm{pa}(i)}) = 1[C_i(\mathbf{q}_{\mathrm{pa}(i)})]$$

- Variable X which is 1 if all clauses satisfied, and 0 otherwise:

$$\begin{aligned} p(A_i = 1 \mid \mathbf{pa}(A_i)) &= 1[\mathbf{pa}(A_i) = \mathbf{1}], \text{ for } i = 1, \ldots, m-2 \\ p(X = 1 \mid a_{m-2}, c_m) &= 1[a_{m-2} = 1, c_m = 1] \end{aligned}$$

Reducing satisfiability to MAP inference

- **Input:** 3-SAT formula with n literals $Q_1, \ldots Q_n$ and m clauses $C_1, \ldots, C_m$



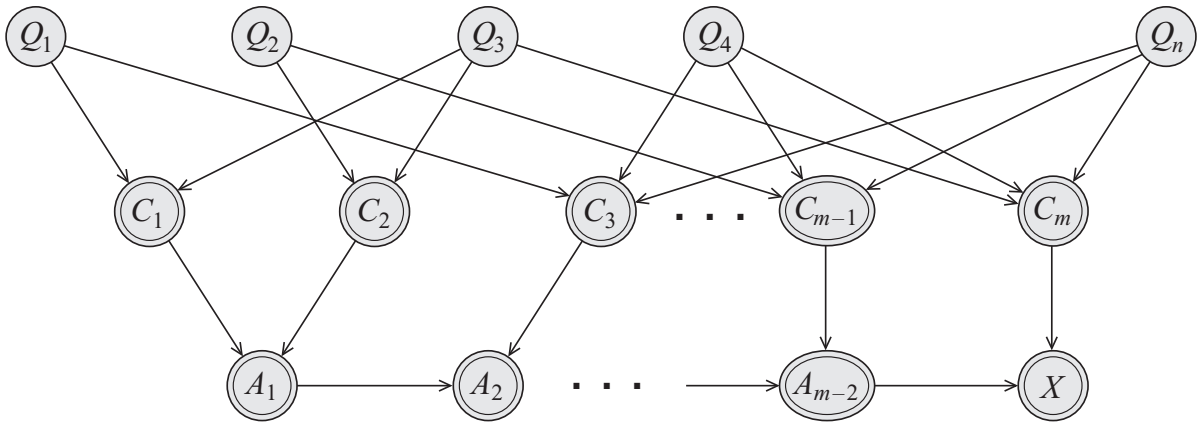
- $p(\mathbf{q}, \mathbf{c}, \mathbf{a}, X = 1) = 0$ for any assignment $\mathbf{q}$ which does not satisfy all clauses
- $p(\mathbf{Q} = \mathbf{q}, \mathbf{C} = \mathbf{1}, \mathbf{A} = \mathbf{1}, X = 1) = \frac{1}{2^n}$ for any satisfying assignment $\mathbf{q}$
- Thus, we can find a satisfying assignment (whenever one exists) by constructing this BN and finding the maximum a posteriori (MAP) assignment:

$$\operatorname*{argmax}_{\mathbf{q},\mathbf{c},\mathbf{a}} p(\mathbf{Q} = \mathbf{q}, \mathbf{C} = \mathbf{c}, \mathbf{A} = \mathbf{a} \mid X = 1)$$

- This proves that MAP inference in Bayesian networks and MRFs is NP-hard

Reducing satisfiability to marginal inference

- **Input:** 3-SAT formula with n literals $Q_1, \ldots Q_n$ and m clauses $C_1, \ldots, C_m$



- $p(X = 1) = \sum_{\mathbf{q},\mathbf{c},\mathbf{a}} p(\mathbf{Q} = \mathbf{q}, \mathbf{C} = \mathbf{c}, \mathbf{A} = \mathbf{a}, X = 1)$ is equal to the number of satisfying assignments times $\frac{1}{2^n}$
- Thus, $p(X = 1) > 0$ if and only if the formula has a satisfying assignment
- This shows that *marginal inference* is also NP-hard

Reducing satisfiability to approximate marginal inference

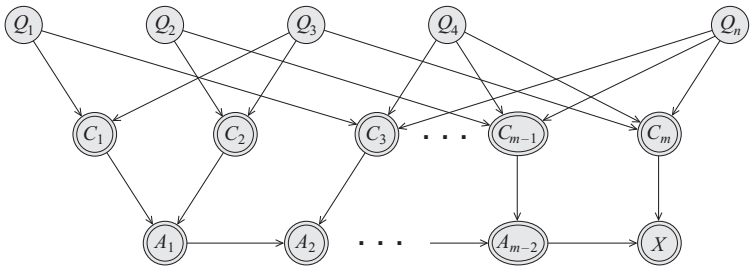
- Might there exist polynomial-time algorithms that can *approximately* answer marginal queries, i.e. for some ϵ, find ρ such that

$$\rho - \epsilon \leq p(\mathbf{Y} \mid \mathbf{E} = \mathbf{e}) \leq \rho + \epsilon \quad ?$$

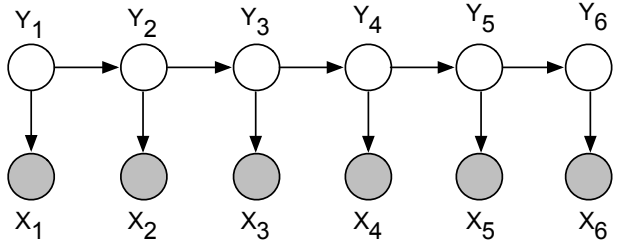
- Suppose such an algorithm exists, for any $\epsilon \in (0, \frac{1}{2})$. Consider the following:
  1. Start with $\mathbf{E} = \{ X = 1 \}$
  2. For $i = 1, \ldots, n$:
  3. Let $q_i = \arg\max_q \; p(Q_i = q \mid \mathbf{E})$
  4. $\mathbf{E} \leftarrow \mathbf{E} \cup (Q_i = q_i)$
- At termination, $\mathbf{E}$ is a satisfying assignment (if one exists). Pf by induction:
  - In iteration i, if $\exists$ satisfying assignment extending $\mathbf{E}$ for **both** $q_i = 0$ *and* $q_i = 1$, then choice in line 3 does not matter
  - Otherwise, suppose $\exists$ satisfying assignment extending $\mathbf{E}$ for $q_i = 1$ but not for $q_i = 0$. Then, $p(Q_i = 1 \mid \mathbf{E}) = 1$ and $p(Q_i = 0 \mid \mathbf{E}) = 0$
  - Even if approximate inference returned $p(Q_i = 1 \mid \mathbf{E}) = 0.501$ and $p(Q_i = 0 \mid \mathbf{E}) = .499$, we would still choose $q_i = 1$
- Thus, it is even NP-hard to *approximately* perform marginal inference!

Probabilistic inference in practice

- NP-hardness simply says that there **exist** difficult inference problems
- Real-world inference problems are not necessarily as hard as these worst-case instances
- The reduction from SAT created a very complex Bayesian network:



- Some graphs are **easy** to do inference in! For example, inference in hidden Markov models



and other tree-structured graphs can be performed in **linear time**

Variable elimination (VE)

- Exact algorithm for probabilistic inference in **any** graphical model
- Running time will depend on the *graph structure*
- Uses **dynamic programming** to circumvent enumerating all assignments
- First we introduce the concept for computing marginal probabilities, $p(X_i)$, in Bayesian networks
- After this, we will generalize to MRFs and conditional queries

Basic idea

- Suppose we have a simple chain, $A \to B \to C \to D$, and we want to compute $p(D)$
- $p(D)$ is a **set** of values, $\{p(D = d), d \in \mathrm{Val}(D)\}$. Algorithm computes sets of values at a time – an entire distribution
- By the chain rule and conditional independence, the joint distribution factors as

$$p(A, B, C, D) = p(A)p(B \mid A)p(C \mid B)p(D \mid C)$$

- In order to compute $p(D)$, we have to marginalize over A, B, C:

$$p(D) = \sum_{a,b,c} p(A = a, B = b, C = c, D)$$

Let's be a bit more explicit...

$$
\begin{array}{llll}
 & P(a^1) & P(b^1 \mid a^1) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
+ & P(a^2) & P(b^1 \mid a^2) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
+ & P(a^1) & P(b^2 \mid a^1) & P(c^1 \mid b^2) & P(d^1 \mid c^1) \\
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\end{array}
$$

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+ & P(a^2) & P(b^2 \mid a^2) & P(c^2 \mid b^2) & P(d^2 \mid c^2)
\end{array}
$$

- There is structure to the summation, e.g., repeated $P(c^1|b^1)P(d^1|c^1)$
- Let's modify the computation to first compute

$$P(a^1)P(b^1|a^1) + P(a^2)P(b^1|a^2)$$

Let's be a bit more explicit...

- Let's modify the computation to first compute

$$P(a^1)P(b^1|a^1) + P(a^2)P(b^1|a^2)$$

and

$$P(a^1)P(b^2|a^1) + P(a^2)P(b^2|a^2)$$

- Then, we get

$$\begin{array}{lll}
& (P(a^1)P(b^1 \mid a^1) + P(a^2)P(b^1 \mid a^2)) & P(c^1 \mid b^1) \quad P(d^1 \mid c^1) \\
+ & (P(a^1)P(b^2 \mid a^1) + P(a^2)P(b^2 \mid a^2)) & P(c^1 \mid b^2) \quad P(d^1 \mid c^1) \\
+ & (P(a^1)P(b^1 \mid a^1) + P(a^2)P(b^1 \mid a^2)) & P(c^2 \mid b^1) \quad P(d^1 \mid c^2) \\
+ & (P(a^1)P(b^2 \mid a^1) + P(a^2)P(b^2 \mid a^2)) & P(c^2 \mid b^2) \quad P(d^1 \mid c^2)
\end{array}$$

$$\begin{array}{lll}
& (P(a^1)P(b^1 \mid a^1) + P(a^2)P(b^1 \mid a^2)) & P(c^1 \mid b^1) \quad P(d^2 \mid c^1) \\
+ & (P(a^1)P(b^2 \mid a^1) + P(a^2)P(b^2 \mid a^2)) & P(c^1 \mid b^2) \quad P(d^2 \mid c^1) \\
+ & (P(a^1)P(b^1 \mid a^1) + P(a^2)P(b^1 \mid a^2)) & P(c^2 \mid b^1) \quad P(d^2 \mid c^2) \\
+ & (P(a^1)P(b^2 \mid a^1) + P(a^2)P(b^2 \mid a^2)) & P(c^2 \mid b^2) \quad P(d^2 \mid c^2)
\end{array}$$

- We define $\tau_1 : \mathrm{Val}(B) \to \Re, \quad \tau_1(b^i) = P(a^1)P(b^i|a^1) + P(a^2)P(b^i|a^2)$

Let's be a bit more explicit...

- We now have

$$\begin{array}{lll} & \tau_1(b^1) & P(c^1 \mid b^1) \quad P(d^1 \mid c^1) \\ + & \tau_1(b^2) & P(c^1 \mid b^2) \quad P(d^1 \mid c^1) \\ + & \tau_1(b^1) & P(c^2 \mid b^1) \quad P(d^1 \mid c^2) \\ + & \tau_1(b^2) & P(c^2 \mid b^2) \quad P(d^1 \mid c^2) \end{array}$$

$$\begin{array}{lll} & \tau_1(b^1) & P(c^1 \mid b^1) \quad P(d^2 \mid c^1) \\ + & \tau_1(b^2) & P(c^1 \mid b^2) \quad P(d^2 \mid c^1) \\ + & \tau_1(b^1) & P(c^2 \mid b^1) \quad P(d^2 \mid c^2) \\ + & \tau_1(b^2) & P(c^2 \mid b^2) \quad P(d^2 \mid c^2) \end{array}$$

- We can once more reverse the order of the product and the sum and get

$$\begin{array}{ll} & (\tau_1(b^1)P(c^1 \mid b^1) + \tau_1(b^2)P(c^1 \mid b^2)) \quad P(d^1 \mid c^1) \\ + & (\tau_1(b^1)P(c^2 \mid b^1) + \tau_1(b^2)P(c^2 \mid b^2)) \quad P(d^1 \mid c^2) \end{array}$$

$$\begin{array}{ll} & (\tau_1(b^1)P(c^1 \mid b^1) + \tau_1(b^2)P(c^1 \mid b^2)) \quad P(d^2 \mid c^1) \\ + & (\tau_1(b^1)P(c^2 \mid b^1) + \tau_1(b^2)P(c^2 \mid b^2)) \quad P(d^2 \mid c^2) \end{array}$$

- There are still other repeated computations!

Let's be a bit more explicit...

- We define $\tau_2 : \mathrm{Val}(C) \to \Re$, with

$$\begin{aligned} \tau_2(c^1) &= \tau_1(b^1)P(c^1|b^1) + \tau_1(b^2)P(c^1|b^2) \\ \tau_2(c^2) &= \tau_1(b^1)P(c^2|b^1) + \tau_1(b^2)P(c^2|b^2) \end{aligned}$$

- Now we can compute the marginal $p(D)$ as

$$\begin{array}{lll} & \tau_2(c^1) & P(d^1 \mid c^1) \\ + & \tau_2(c^2) & P(d^1 \mid c^2) \end{array}$$

$$\begin{array}{lll} & \tau_2(c^1) & P(d^2 \mid c^1) \\ + & \tau_2(c^2) & P(d^2 \mid c^2) \end{array}$$

What did we just do?

- Our goal was to compute

$$p(D) = \sum_{a,b,c} p(a,b,c,D) = \sum_{a,b,c} p(a)p(b \mid a)p(c \mid b)p(D \mid c)$$
$$= \sum_{c}\sum_{b}\sum_{a} p(D \mid c)p(c \mid b)p(b \mid a)p(a)$$

- We can push the summations inside to obtain:

$$p(D) = \sum_{c} p(D \mid c) \sum_{b} p(c \mid b) \underbrace{\sum_{a} \underbrace{p(b \mid a)p(a)}_{\psi_1(a,b)}}_{\tau_1(b)}$$

- Let's call $\psi_1(A,B) = P(A)P(B|A)$. Then, $\tau_1(B) = \sum_a \psi_1(a,B)$
- Similarly, let $\psi_2(B,C) = \tau_1(B)P(C|B)$. Then, $\tau_2(C) = \sum_b \psi_1(b,C)$
- This procedure is dynamic programming: computation is inside out instead of outside in

Inference in a chain

- Generalizing the previous example, suppose we have a chain $X_1 \to X_2 \to \cdots \to X_n$ where each variable has k states
- In Problem Set 1, you gave an algorithm to compute $p(X_i)$, for $k = 2$
- For $i = 1$ up to $n - 1$, compute (and cache)

$$p(X_{i+1}) = \sum_{x_i} p(X_{i+1} \mid x_i) p(x_i)$$

- Each update takes k^2 time (why?)
- The total running time is $\mathcal{O}(nk^2)$
- In comparison, naively marginalizing over all latent variables has complexity $\mathcal{O}(k^n)$
- We did inference over the joint without ever explicitly constructing it!

Summary so far

- Worst-case analysis says that marginal inference is NP-hard
- Even approximating it is NP-hard
- In practice, due to the structure of the Bayesian network, we can cache computations that are otherwise computed exponentially many times
- This depends on our having a good **variable elimination ordering**

Sum-product inference task

- We want to give an algorithm to compute $p(\mathbf{Y})$ for BNs and MRFs
- This can be reduced to the following **sum-product** inference task:

$$\text{Compute} \quad \tau(\mathbf{y}) = \sum_{\mathbf{z}} \prod_{\phi \in \Phi} \phi(\mathbf{z}_{\text{Scope}[\phi] \cap \mathbf{Z}}, \mathbf{y}_{\text{Scope}[\phi] \cap \mathbf{Y}}) \quad \forall \mathbf{y},$$

  where Φ is a set of factors or potentials

- For a BN, Φ is given by the conditional probability distributions for all variables,

$$\Phi = \{\phi_{X_i}\}_{i=1}^n = \{p(X_i \mid \mathbf{X}_{\text{Pa}(X_i)})\}_{i=1}^n,$$

  and where we sum over the set $\mathbf{Z} = \mathcal{X} - \mathbf{Y}$

- For Markov networks, the factors Φ correspond to the set of potentials which we earlier called C
  - Sum-product returns an unnormalized distribution, so we divide by $\sum_{\mathbf{y}} \tau(\mathbf{y})$

Factor marginalization

- Let $\phi(\mathbf{X}, Y)$ be a factor where $\mathbf{X}$ is a set of variables and $Y \notin \mathbf{X}$
- **Factor marginalization** of ϕ over Y (also called "summing out Y in ϕ") gives a new factor:

$$\tau(\mathbf{X}) = \sum_{Y} \phi(\mathbf{X}, Y)$$

For example,

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

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

Sum-product variable elimination

- Order the variables $\mathbf{Z}$ (called the **elimination ordering**)
- Iteratively marginalize out variable Z_i, one at a time
- For each i,
  1. Multiply all factors that have Z_i in their scope, generating a new product factor
  2. Marginalize this product factor over Z_i, generating a smaller factor
  3. Remove the old factors from the set of all factors, and add the new one

Algorithm 9.1 Sum-Product Variable Elimination algorithm

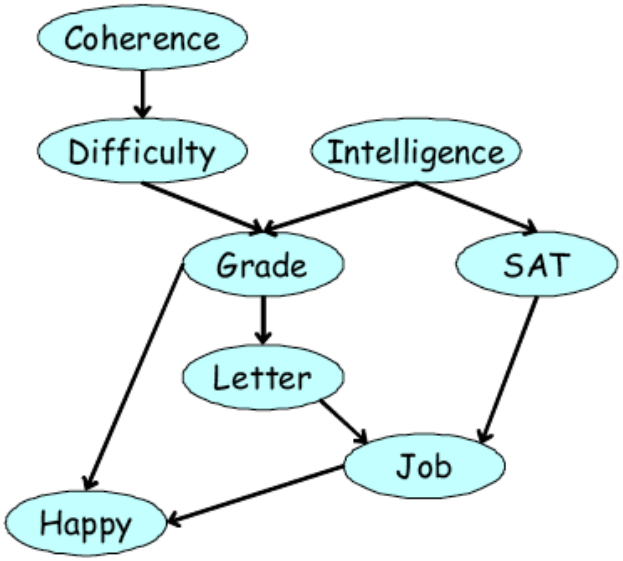
Procedure Sum-Product-Variable-Elimination (
  Φ, // Set of factors
  $\boldsymbol{Z}$, // Set of variables to be eliminated
  $\prec$ // Ordering on $\boldsymbol{Z}$
)

Let $Z_1, \ldots, Z_k$ be an ordering of $\boldsymbol{Z}$ such that
  $Z_i \prec Z_j$ iff $i < j$
for $i = 1, \ldots, k$
  $\Phi \leftarrow$ Sum-Product-Eliminate-Var(Φ, Z_i)
$\phi^* \leftarrow \prod_{\phi \in \Phi} \phi$
return ϕ^*

Procedure Sum-Product-Eliminate-Var (
  Φ, // Set of factors
  Z // Variable to be eliminated
)

$\Phi' \leftarrow \{\phi \in \Phi : Z \in Scope[\phi]\}$
$\Phi'' \leftarrow \Phi - \Phi'$
$\psi \leftarrow \prod_{\phi \in \Phi'} \phi$
$\tau \leftarrow \sum_Z \psi$
return $\Phi'' \cup \{\tau\}$

Example



- What is $p(\text{Job})$? Joint distribution factorizes as:

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

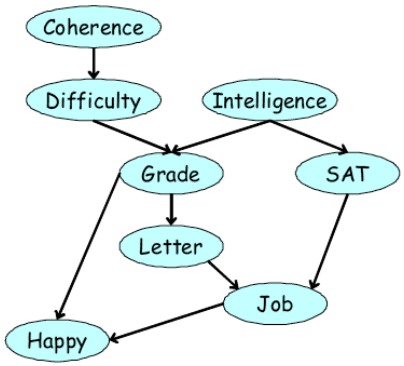
with factors

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

- Let's do variable elimination with ordering $\{C, D, I, H, G, S, L\}$ on the board!

Elimination ordering

- We can pick any order we want, but some orderings introduce factors with much larger scope



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	$\tau_7(J)$

- Alternative ordering...

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	$\tau_5(D,J)$, $\phi_D(D,C)$	D,J,C	$\tau_6(D,J)$
7	D	$\tau_6(D,J)$	D,J	$\tau_7(J)$

How to introduce evidence?

- Recall that our original goal was to answer *conditional* probability queries,

$$p(\mathbf{Y}|\mathbf{E}=\mathbf{e}) = \frac{p(\mathbf{Y},\mathbf{e})}{p(\mathbf{e})}$$

- Apply variable elimination algorithm to the task of computing $P(\mathbf{Y},\mathbf{e})$
- Replace each factor $\phi \in \Phi$ that has $\mathbf{E} \cap \mathrm{Scope}[\phi] \neq \emptyset$ with

$$\phi'(\mathbf{x}_{\mathrm{Scope}[\phi]-\mathbf{E}}) = \phi(\mathbf{x}_{\mathrm{Scope}[\phi]-\mathbf{E}}, \mathbf{e}_{\mathbf{E}\cap\mathrm{Scope}[\phi]})$$

- Then, eliminate the variables in $\mathcal{X} - \mathbf{Y} - \mathbf{E}$. The returned factor $\phi^*(\mathbf{Y})$ is $p(\mathbf{Y},\mathbf{e})$
- To obtain the conditional $p(\mathbf{Y} \mid \mathbf{e})$, normalize the resulting product of factors – the normalization constant is $p(\mathbf{e})$

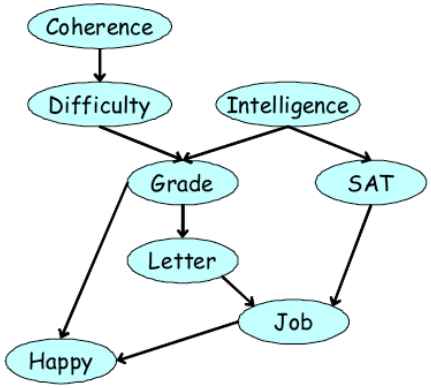
Sum-product VE for conditional distributions

Algorithm 9.2 Using Sum-Product-Variable-Elimination for computing conditional probabilities.

Procedure Cond-Prob-VE (
  $\mathcal{K}$, // A network over $\mathcal{X}$
  $\boldsymbol{Y}$, // Set of query variables
  $\boldsymbol{E} = \boldsymbol{e}$ // Evidence
)

$\Phi \leftarrow$ Factors parameterizing $\mathcal{K}$
Replace each $\phi \in \Phi$ by $\phi[\boldsymbol{E} = \boldsymbol{e}]$
Select an elimination ordering $\prec$
$\boldsymbol{Z} \leftarrow = \mathcal{X} - \boldsymbol{Y} - \boldsymbol{E}$
$\phi^* \leftarrow$ Sum-Product-Variable-Elimination$(\Phi, \prec, \boldsymbol{Z})$
$\alpha \leftarrow \sum_{\boldsymbol{y} \in Val(\boldsymbol{Y})} \phi^*(\boldsymbol{y})$
return α, ϕ^*

Running time of variable elimination

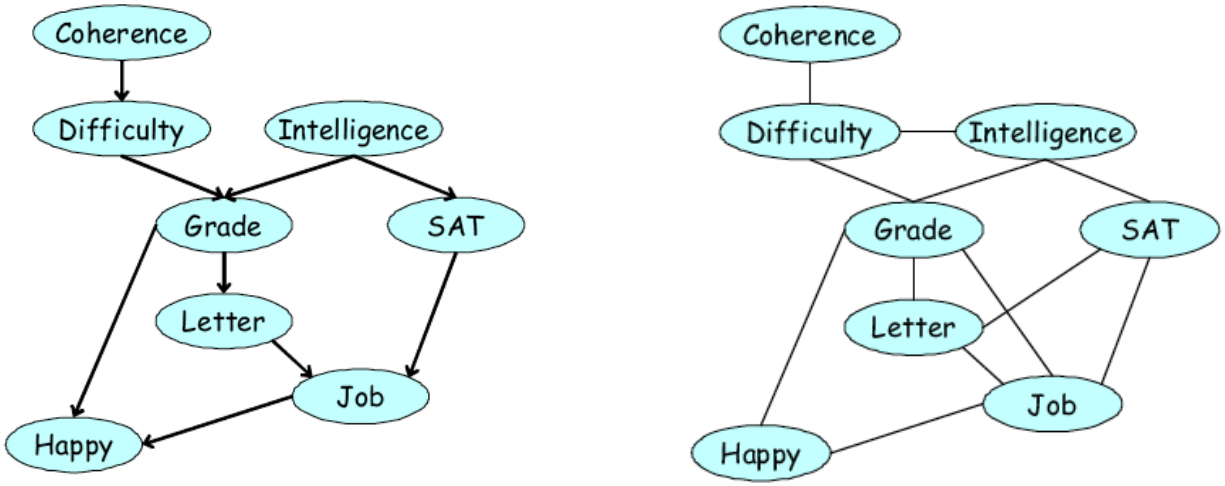


Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C)$, $\phi_D(D,C)$	C,D	$\tau_1(D)$
2	D	$\phi_G(G,I,D)$, $\tau_1(D)$	G,I,D	$\tau_2(G,I)$
3	I	$\phi_I(I)$, $\phi_S(S,I)$, $\tau_2(G,I)$	G,S,I	$\tau_3(G,S)$
4	H	$\phi_H(H,G,J)$	H,G,J	$\tau_4(G,J)$
5	G	$\tau_4(G,J)$, $\tau_3(G,S)$,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

- Let n be the number of variables, and m the number of initial factors
- At each step, we pick a variable X_i and multiply all factors involving X_i, resulting in a single factor ψ_i
- Let N_i be the number of entries in the factor ψ_i, and let $N_{max} = \max_i N_i$
- The running time of VE can be shown to be $O(mN_{max})$
- The primary concern is that N_{max} can potentially be exponential in n

Running time in graph-theoretic concepts

- Let's try to analyze the complexity in terms of the graph structure
- G_Φ is the undirected graph with one node per variable, where there is an edge (X_i, X_j) if these appear together in the scope of some factor ϕ
- Ignoring evidence, this is either the original MRF (for sum-product VE on MRFs) or the moralized Bayesian network:



Elimination as graph transformation

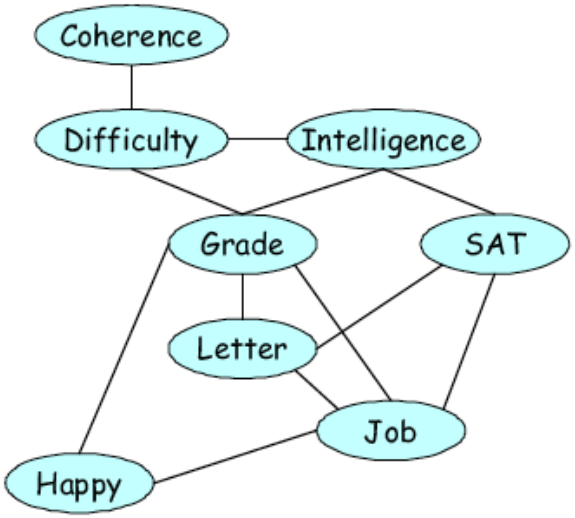
When a variable X is eliminated,

- We create a single factor ψ that contains X and all of the variables $\mathbf{Y}$ with which it appears in factors
- We eliminate X from ψ, replacing it with a new factor τ that contains all of the variables $\mathbf{Y}$, but not X. Let's call the new set of factors Φ_X

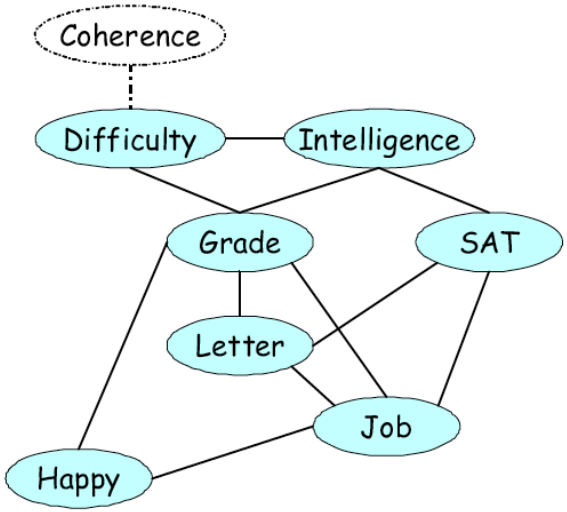
How does this modify the graph, going from G_Φ to G_{Φ_X}?

- Constructing ψ generates edges between all of the variables $Y \in \mathbf{Y}$
- Some of these edges were already in G_Φ, some are new
- The new edges are called **fill edges**
- The step of removing X from Φ to construct Φ_X removes X and all its incident edges from the graph

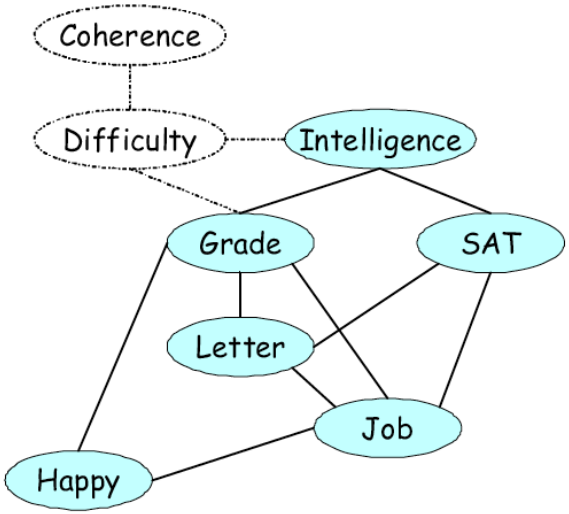
Example



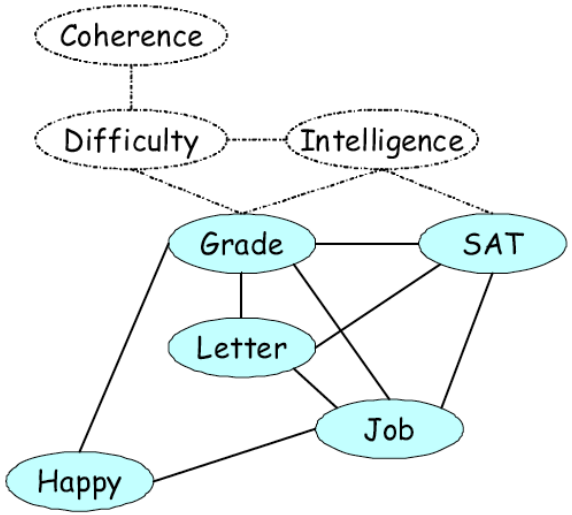
(Graph)



(Elim. C)



(Elim. D)

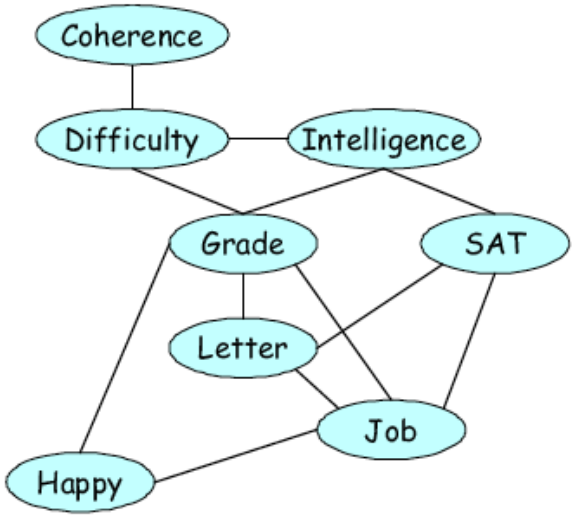


(Elim. I)

Induced graph

- We can summarize the computation cost using a single graph that is the union of all the graphs resulting from each step of the elimination
- We call this the **induced graph** $\mathcal{I}_{\Phi,\prec}$, where $\prec$ is the elimination ordering

Example



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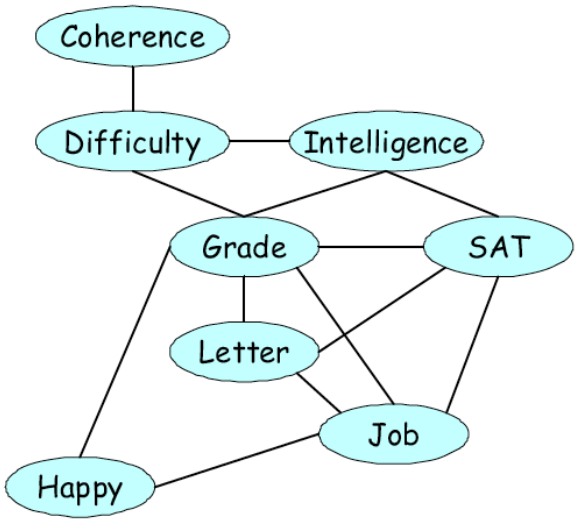
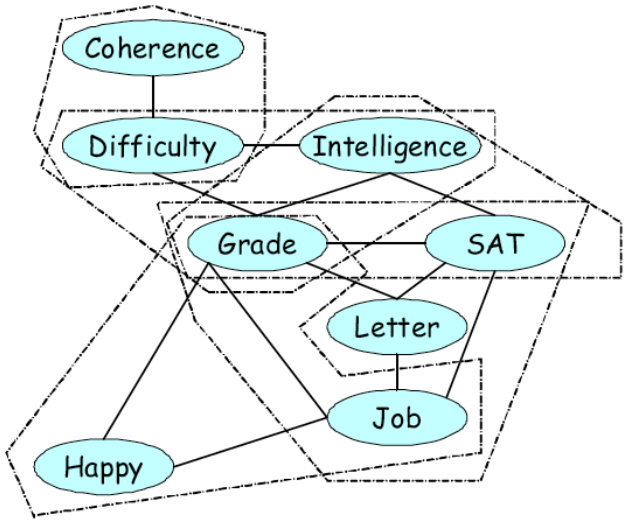


(Induced graph)



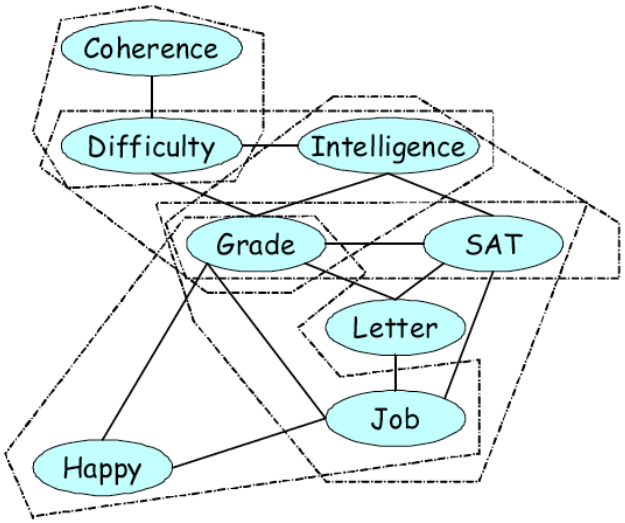
(Maximal Cliques)

Properties of the induced graph

- **Theorem**: Let $\mathcal{I}_{\Phi,\prec}$ be the induced graph for a set of factors Φ and ordering $\prec$, then
  1. Every factor generated during VE has a scope that is a clique in $\mathcal{I}_{\Phi,\prec}$
  2. Every maximal clique in $\mathcal{I}_{\Phi,\prec}$ is the scope of some intermediate factor in the computation

  (see book for proof)
- Thus, N_{max} is equal to the size of the largest clique in $\mathcal{I}_{\Phi,\prec}$
- The running time, $O(mN_{max})$, is exponential in the size of the largest clique of the induced graph

Example



(Maximal Cliques)

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(VE)

- The maximal cliques in $\mathcal{I}_{G,\prec}$ are

$$\begin{aligned} \mathbf{C}_1 &= \{C, D\} \\ \mathbf{C}_2 &= \{D, I, G\} \\ \mathbf{C}_3 &= \{G, L, S, J\} \\ \mathbf{C}_4 &= \{G, J, H\} \end{aligned}$$

Induced width

- We define the **width** of an induced graph to be the number of nodes in the largest clique in the graph, minus 1
- We define the **induced width** $w_{\mathcal{K},\prec}$ to be the width of the graph $\mathcal{I}_{\mathcal{K},\prec}$ induced by applying VE to $\mathcal{K}$ using ordering $\prec$
- The **minimal induced width** of a graph $\mathcal{K}$ is $w^*_{\mathcal{K}} = \min_{\prec} w_{\mathcal{K},\prec}$

  (also known as the **treewidth** of graph $\mathcal{K}$)
- The minimal induced width provides a bound on the best running time achievable by VE on a distribution that factorizes over $\mathcal{K}$
- Unfortunately, finding the **best** elimination ordering (equivalently, computing the minimal induced width) for a graph is NP-hard
- In practice, heuristics (e.g., min-fill) are used to find a good elimination ordering