

PROBABILISTIC MODELS – PART 4a: EXACT INFERENCE IN BAYESIAN NETWORKS

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and [Russell & Norvig, 2021], including the use of some figures from their books
and/or lecture slides.

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(pgm.stanford.edu; aima.cs.berkeley.edu).

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Goals of this Lecture

- ▶ Review the probabilistic query
- ▶ Describe the general Inference-by-Enumeration Algorithm for BNs
- ▶ Analyse the computational complexity of exact inference
- ▶ Optimisation: Introduce the basic idea of Variable Elimination
- ▶ The Variable Elimination Algorithm for Bayesian Networks
- ▶ Revisit the computational complexity of exact inference

Outline

- ① Probabilistic Queries
- ② Inference by Enumeration in BNs
 - The General Algorithm
 - Computational Complexity
- ③ Variable Elimination
 - A Simple Example
 - Deriving Insight from the Simple Example
 - The General Algorithm
 - Complexity

The Probabilistic Query

Remember:

We will be interested in answering questions of the following form

Definition

A **Probabilistic Query** involves computing the **conditional probability distribution**

$$P(\mathbf{X} \mid \mathbf{E} = e)$$

or $P(\mathbf{X} \mid e)$ for short

for some sets of variables $\mathbf{X}, \mathbf{E} \subseteq \mathcal{X}$ and a specific value assignment $\mathbf{E} = e$.

IN WORDS:

Given that we know or have observed the specific values e of the variables \mathbf{E} (the ‘**evidence variables**’), what are the probabilities for the different value combinations of the \mathbf{X} (the ‘**query variables**’)?

The Probabilistic Query: Special Cases

We might also be interested in computing

- ▶ the **probability of a specific value combination** x of the X :

$$P(X = x \mid e)$$

- ▶ or the **most likely value combination** of the X , given the evidence e :^a

$$x^* = \arg \max_x P(X = x \mid e)$$

^aThis is called a **MAP** (**M**aximal **A** Posteriori) Query.

Of course, these follow naturally once we have computed the full conditional distribution $P(X \mid e)$.

Computing a Conditional Distribution: Inference by Enumeration

Remember from last section:

By the definition of conditional probability, we have that

$$P(\mathbf{X} \mid e) = \frac{P(\mathbf{X}, e)}{P(e)} = \frac{1}{Z} P(\mathbf{X}, e)$$

IN WORDS:

The conditional distribution $P(\mathbf{X} \mid e)$ is equal to the *joint probabilities* $P(\mathbf{X}, e)$ (the probabilities of conjunctions $P(x, e)$), normalised by the *probability of the evidence* $P(e)$.

- 👉 Compute this for each possible assignment of values x of the query variables \mathbf{X} , and you have the full conditional distribution $P(\mathbf{X} \mid \mathbf{E} = e)$.
- 👉 $P(e)$ simply acts as a normalisation constant Z – compute only once.

Inference by Enumeration for Probabilistic Queries

Goal: Compute $P(\mathbf{X} \mid \mathbf{e})$ for some sets of variables $\mathbf{X}, \mathbf{E} \subseteq \mathcal{X}$ and some specific value assignment $\mathbf{E} = \mathbf{e}$.

Algorithm

- 1 Compute $P(\mathbf{X}, \mathbf{e})$ via *Inference by Enumeration*, $\mathbf{Z} = \mathcal{X} - \mathbf{X} - \mathbf{E}$

$$P(\mathbf{X}, \mathbf{e}) = \sum_{\mathbf{z} \in \text{Val}(\mathbf{Z})} P(\mathbf{X}, \mathbf{e}, \mathbf{z})$$

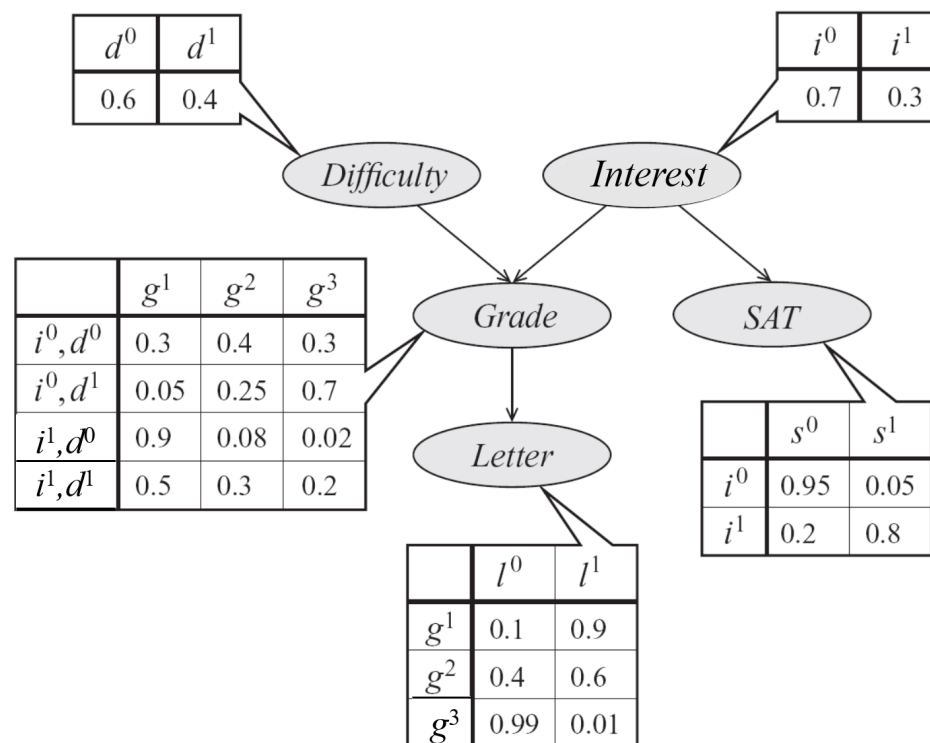
- 2 Compute normalisation constant Z from the above as

$$Z = P(\mathbf{e}) = \sum_{\mathbf{x}} P(\mathbf{x}, \mathbf{e})$$

- 3 Condition via renormalisation:

$$P(\mathbf{X} \mid \mathbf{e}) = \frac{1}{Z} P(\mathbf{X}, \mathbf{e})$$

Example: The Student Network



Example query:

$$P(D \mid g^3, s^1) = ?$$

Solving the Example Query (1)

$$\begin{aligned}
 \underline{P(d^0, g^3, s^1)} &= \sum_{i=\{i^0, i^1\}, l=\{l^0, l^1\}} P(i, d^0, g^3, l, s^1) \\
 &= \sum_{i=\{i^0, i^1\}, l=\{l^0, l^1\}} P(i)P(d^0)P(g^3|d^0, i)P(l|g^3)P(s^1|i) \\
 &= P(i^0)P(d^0)P(g^3|d^0, i^0)P(l^0|g^3)P(s^1|i^0) + \\
 &\quad P(i^0)P(d^0)P(g^3|d^0, i^0)P(l^1|g^3)P(s^1|i^0) + \\
 &\quad P(i^1)P(d^0)P(g^3|d^0, i^1)P(l^0|g^3)P(s^1|i^1) + \\
 &\quad P(i^1)P(d^0)P(g^3|d^0, i^1)P(l^1|g^3)P(s^1|i^1) \\
 &= 0.7 \cdot 0.6 \cdot 0.3 \cdot 0.99 \cdot 0.05 + \\
 &\quad 0.7 \cdot 0.6 \cdot 0.3 \cdot 0.01 \cdot 0.05 + \\
 &\quad 0.3 \cdot 0.6 \cdot 0.02 \cdot 0.99 \cdot 0.8 + \\
 &\quad 0.3 \cdot 0.6 \cdot 0.02 \cdot 0.01 \cdot 0.8 \\
 &= \underline{0.00918}
 \end{aligned}$$

Solving the Example Query (2)

$$\begin{aligned}
 \underline{P(d^1, g^3, s^1)} &= \sum_{i=\{i^0, i^1\}, l=\{l^0, l^1\}} P(i, d^1, g^3, l, s^1) \\
 &= \sum_{i=\{i^0, i^1\}, l=\{l^0, l^1\}} P(i)P(d^1)P(g^3|d^1, i)P(l|g^3)P(s^1|i) \\
 &= P(i^0)P(d^1)P(g^3|d^1, i^0)P(l^0|g^3)P(s^1|i^0) + \\
 &\quad P(i^0)P(d^1)P(g^3|d^1, i^0)P(l^1|g^3)P(s^1|i^0) + \\
 &\quad P(i^1)P(d^1)P(g^3|d^1, i^1)P(l^0|g^3)P(s^1|i^1) + \\
 &\quad P(i^1)P(d^1)P(g^3|d^1, i^1)P(l^1|g^3)P(s^1|i^1) \\
 &= 0.7 \cdot 0.4 \cdot 0.7 \cdot 0.99 \cdot 0.05 + \\
 &\quad 0.7 \cdot 0.4 \cdot 0.7 \cdot 0.01 \cdot 0.05 + \\
 &\quad 0.3 \cdot 0.4 \cdot 0.2 \cdot 0.99 \cdot 0.8 + \\
 &\quad 0.3 \cdot 0.4 \cdot 0.2 \cdot 0.01 \cdot 0.8 \\
 &= \underline{0.029}
 \end{aligned}$$

Solving the Example Query (3)

$$P(d^0, g^3, s^1) = 0.00918$$

$$P(d^1, g^3, s^1) = 0.029$$

$$Z = P(g^3, s^1) = 0.00918 + 0.029 = 0.03818$$

$$\boxed{P(D \mid g^3, s^1)} = \frac{1}{Z} \times \begin{bmatrix} 0.00918 \\ 0.029 \end{bmatrix} = \begin{bmatrix} 0.24044 \\ 0.75956 \end{bmatrix}$$

$$\Rightarrow P(d^1 \mid g^3, s^1) = 75.96\%$$

The probability that the AI class was difficult, given that Joe got a C grade but has a high SAT score, is $\approx 76\%$.

(see last chapter, “Reasoning Patterns”)

The Complexity of Exact Inference

Consider

- ▶ a Bayesian Network \mathcal{B} over binary random variables $\mathcal{X} = \mathbf{X} \cup \mathbf{E} \cup \mathbf{Z}$
- ▶ a query $P(\mathbf{X} \mid \mathbf{E} = e)$

To compute

$$P(\mathbf{x}, e) = \sum_{\mathbf{z}} P(\mathbf{x}, e, \mathbf{z}) = \sum_{\mathbf{z}} \prod_{x_i \in \mathbf{x} \cup e \cup \mathbf{z}} P(x_i \mid \text{pa}(X_i))$$

for some specific assignment of values \mathbf{x} to \mathbf{X} ,

- ▶ we need to compute $P(\mathbf{x}, e, \mathbf{z})$ for every combination of values \mathbf{z} of the variables \mathbf{Z}
- ▶ If $|\mathbf{Z}| = k$, there are 2^k such assignments \mathbf{z}
- ▶ If we only have few evidence variables \mathbf{E} and few query variables \mathbf{X} , then $k \approx N$ and we must sum out over $O(2^N)$ terms $P(\mathbf{x}, e, \mathbf{z})$!
- ▶ Not feasible for networks of reasonable complexity ...

The Complexity of Exact Inference

The Bad News

- ▶ It can be shown that the problem of inference in graphical models is \mathcal{NP} -hard, and therefore requires **exponential time**, in the worst case.

The Good News:

- ▶ Many real-world problems seem to be far from the worst case ...
- ▶ ... and for many sparsely connected networks (i.e., networks where variables tend to have few parents), inference can be done quite efficiently with optimised algorithms (e.g., \rightarrow *Variable Elimination*)

Making Inference More Efficient (in the Average Case)

Problem with the Standard Approach:

- ▶ Computations are highly redundant
- ▶ Many terms are computed many (an exponential number of!) times ...

Consider example from above:

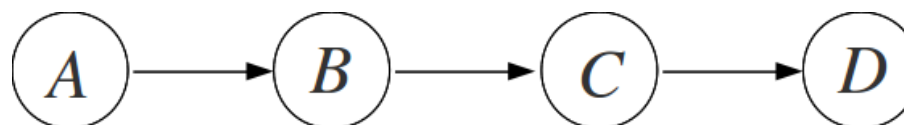
$$\begin{aligned} P(d^0, g^3, s^1) = & 0.7 \times 0.6 \times 0.3 \times 0.99 \times 0.05 + \\ & 0.7 \times 0.6 \times 0.3 \times 0.01 \times 0.05 + \\ & 0.3 \times 0.6 \times 0.02 \times 0.99 \times 0.8 + \\ & 0.3 \times 0.6 \times 0.02 \times 0.01 \times 0.8 \end{aligned}$$

In the following:

- ▶ Demonstrate the problem on a simple linear example network
- ▶ Explain basic idea of **Dynamic Programming**
- ▶ Show that inference on this simple network can be done in linear time
- ▶ Then: Generalise this process to general networks.

A Simple Example

Consider a simple linearly structured Bayesian network:

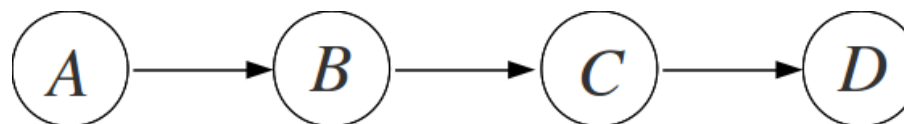


where each variable has k values

Task:

Compute $P(D)$.

A Simple Example



Standard Inference by Enumeration:

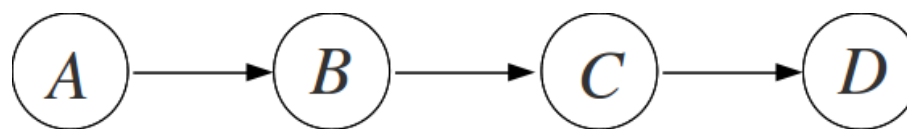
$$P(D) = \sum_c \sum_b \sum_a P(a, b, c, D) = \sum_c \sum_b \sum_a P(a)P(b|a)P(c|b)P(D|c)$$

- ▶ would repeatedly compute $P(a)$ for each b, c and d
- ▶ would repeatedly compute $\sum_a P(a)P(b|a) = P(b)$ for each c, d
- ▶ would repeatedly compute $\sum_b \sum_a P(a)P(b|a)P(c|b) = \sum_b P(b)P(c|b) = P(c)$ for each d .

👉 **Wasteful**

👉 **Idea:** Pre-compute these parts and store them for repeated use.

A Simple Example



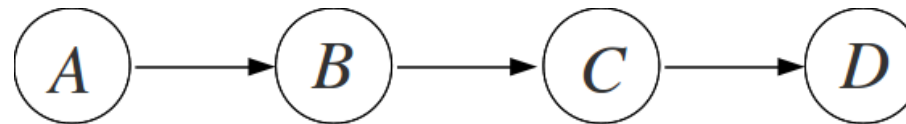
Step 1: Let's first compute $P(A)$:

\Rightarrow Trivial. The numbers $P(a^0), P(a^1), \dots$ are given by A 's CPD.

Computational complexity of this first step:

$O(1)$ (constant).

A Simple Example



Step 2: Let's compute $P(B)$:

$$P(B) = \sum_a P(a)P(B \mid a)$$

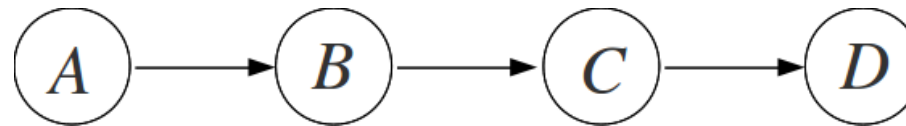
The numbers for $P(B \mid a)$ are in B 's CPD; $P(A)$ **has been computed before**.

Computational complexity (if both A and B have k values) is

$$O(k \times k) = O(k^2)$$

- ▶ k multiplications $P(a)P(b|a)$ (one for each value of A)
- ▶ $k - 1$ additions (the sum)
- ▶ Must compute this for all k values of B to get probability distribution $P(B)$.

A Simple Example



Step 3: Let's compute $P(C)$:

$$P(C) = \sum_b P(b)P(C \mid b)$$

The numbers for $P(C \mid b)$ are in C 's CPD; $P(B)$ has been computed before.

Complexity:

$$O(k \times k) = O(k^2).$$

Step 4: Compute $P(D)$: analogous to above, **using cached results for $P(C)$...**

Complexity of the Whole Process

Assume:

- ▶ A Bayesian network in the form of a strict chain $X_1 \rightarrow \dots \rightarrow X_N$
- ▶ where each variable X_i has k values.
- ▶ An algorithm that recursively computes $P(X_{i+1})$ from $P(X_i)$:

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

and **caches the result** $P(X_{i+1})$ as a table (list of values).

Complexity of the i^{th} step – computing $P(X_{i+1})$:

$$O(k \times k) = O(k^2)$$

Cost of the entire process:

$$O(N \times k^2)$$

👉 **For fixed k , this is **linear** in N !**

Complexity of the Whole Process

Notes:

- ▶ Example where inference can be done in **linear time**, despite the exponential size $O(k^N)$ of the joint distribution!
- ▶ This extreme reduction of complexity was made possible by the specific linear structure of the network
- ▶ Linear network is extremely **sparse**: every variable has only one parent
- ▶ Computed not single values, but *sets of values* (distributions over X_i)
- ▶ These are stored and then used to compute $P(X_{i+1})$.

👉 Algorithm needs to store **tables** as intermediate results (see *factors* τ below).

A somewhat more general view of what we just did

- Want to compute

$$P(D) = \sum_c \sum_b \sum_a P(a, b, c, D) = \sum_c \sum_b \sum_a P(a)P(b|a)P(c|b)P(D|c)$$

- **Step 1:** Push in summation over A :

$$P(D) = \sum_c \sum_b P(c|b)P(D|c) \sum_a P(a)P(b|a)$$

- **Step 2:** Compute innermost sum (“sum out A ”) for each value b^i of B :

$$\sum_a P(a)P(b^i|a) = \tau_A(b^i)$$

Store results as a function (table) $\tau_A(B)$ (holds a value $\tau_A(b^i)$ for each b^i)

- **Replace summation by table lookup:**

$$P(D) = \sum_c \sum_b P(c|b)P(D|c) \tau_A(b)$$

- **Now repeat the story: want to compute**

$$P(D) = \sum_c \sum_b P(c|b) P(D|c) \tau_A(b)$$

- **Step 1:** Push in the next summation (over B):

$$P(D) = \sum_c P(D|c) \sum_b P(c|b) \tau_A(b)$$

- **Step 2:** Compute innermost sum (“sum out B ”) for each value c^i of C :

$$\sum_b P(c^i|b) \tau_A(b) = \tau_B(c^i)$$

and store the results as table $\boxed{\tau_B(C)}$

- **Replace summation by table lookup:**

$$P(D) = \sum_c P(D|c) \tau_B(c)$$

which can be easily computed for each value d^i of D . □

Insights

Central Insights

- 1 **Sparse Connectivity:** Due to the structure of the Bayesian network, some subexpressions in the joint distribution depend only on a small number of variables.
- 2 **Caching:** By computing these expressions once and caching the results, we avoid computing them exponentially many times.

Notes:

- ▶ This is a form of **Dynamic Programming** – doing summations inside out, storing intermediate results for re-use
- ▶ Computing $P(D) = \sum_c \sum_b \sum_a P(a)P(b|a)P(c|b)P(D|c)$ in the naive way would have us compute every $\sum_a P(a)P(b|a) = P(b)$ many times (once for every value of C and D)
- ▶ In general: in a chain of length N , we would compute this internal sum *exponentially many times*!

The Variable Elimination Algorithm for Bayesian Networks

Comments:

- ▶ The linear network above was *extremely* simple and ‘nice’
- ▶ Generally, a Bayesian network does not have a simple linear structure
- ▶ A variable usually depends on *several* other variables
- ▶ Intermediate factors to be cached become multi-dimensional
- ▶ Not clear what the optimal order of variables is for summing out.

The Variable Elimination Algorithm for Bayesian Networks

Variable Elimination Algorithm for Bayesian Networks

Given:

- ▶ A Bayesian network \mathcal{B} over variables $\mathcal{X} = \mathbf{X} \cup \mathbf{E} \cup \mathbf{Z}$
- ▶ A query $P(\mathbf{X} \mid \mathbf{E} = e)$
- ▶ Some ordering Z_1, \dots, Z_k of the non-query variables \mathbf{Z}

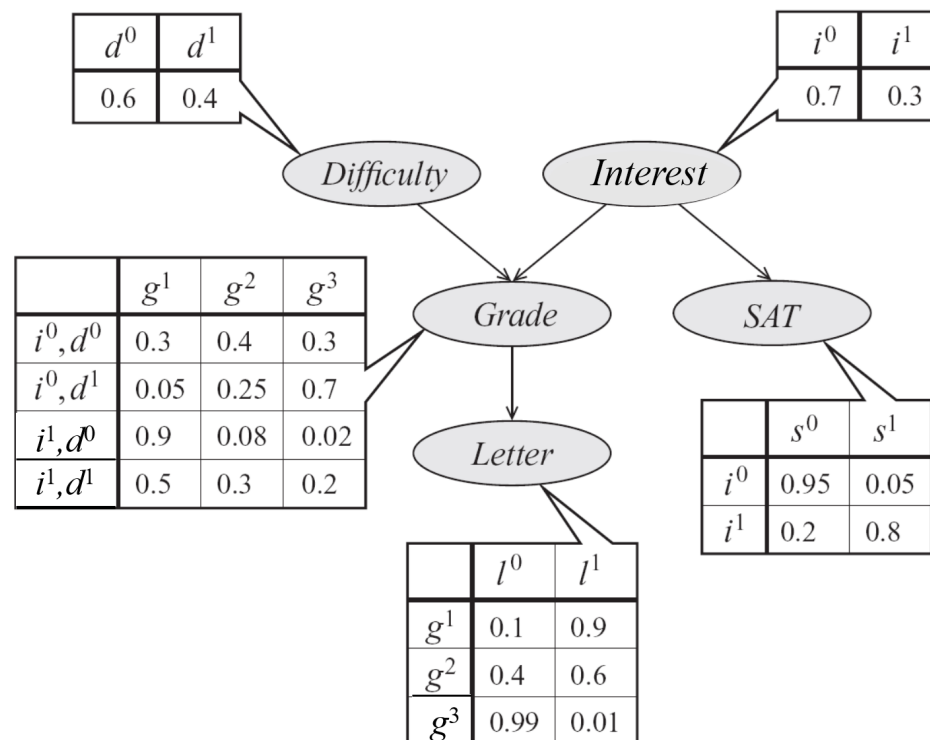
Eliminate Variables \mathbf{Z} : for $i = 1, \dots, k$ do

- 1 Push in summation over Z_i as far as possible.
Let \mathbf{U} = all variables that appear in this inner sum, except Z_i
- 2 Compute the product of terms in this inner sum, for all possible combinations of values of $Z_i \cup \mathbf{U} \Rightarrow$ temporary table \mathcal{T}
- 3 ... and sum out over Z_i (i.e., for each value combination \mathbf{u} , sum over all z_i)
- 4 Store resulting table (of dimensionality $|\mathbf{U}|$) as intermediate “factor” $\tau_{Z_i}(\mathbf{U})$

Simplify: Multiply out whatever factors are left; the result is a table $P(\mathbf{X}, e)$

Renormalise $P(\mathbf{X}, e)$ to obtain $P(\mathbf{X} \mid e)$.

An Example



Example query:

$$P(I \mid g^3) = ?$$

Solving the Query via Variable Elimination

Query:

$$P(I \mid g^3) = ?$$

Variable subsets (see algorithm above):

$$X = \{I\}$$

$$E = \{G\} \quad (e = \{g^3\})$$

$$Z = \{D, L, S\}$$

Assume some variable ordering over Z

(variables to be eliminated in this order):

$$D, L, S$$

Solving the Query via Variable Elimination

Starting Point:

$$P(I, g^3) = \sum_{D=d^0, d^1} \sum_{L=l^0, l^1} \sum_{S=s^0, s^1} P(D)P(I)P(g^3|D, I)P(L|g^3)P(S|I)$$

1. Eliminate D ($Z_1 = D$):

- Push in summation over D :

$$P(I, g^3) = \sum_L \sum_S P(I)P(L|g^3)P(S|I) \sum_D \underbrace{P(D)P(g^3|D, I)}_{\mathcal{T}}$$

- Compute $\mathcal{T} = P(D)P(g^3|D, I)$ for all values of D, I
(see next slide)
- $U = \{I\}$ (variables in the inner expression other than D)

Solving the Query via Variable Elimination

- Compute $\mathcal{T} = P(D)P(g^3|D, I)$ for all values of D, I :

D	I	$P(D)P(g^3 D, I)$
d^0	i^0	$0.6 \times 0.3 = 0.18$
d^0	i^1	$0.6 \times 0.02 = 0.012$
d^1	i^0	$0.4 \times 0.7 = 0.28$
d^1	i^1	$0.4 \times 0.2 = 0.08$

- Sum out D :

I	$\sum_D P(D)P(g^3 D, I)$
i^0	$0.18 + 0.28 = 0.46$
i^1	$0.012 + 0.08 = 0.092$

- Store result as table $\tau_D(I)$:

$$\tau_D(I) = \begin{bmatrix} 0.46 \\ 0.092 \end{bmatrix}$$

Solving the Query via Variable Elimination

New Target:

$$P(I, g^3) = \sum_L \sum_S P(I) P(L|g^3) P(S|I) \tau_D(I)$$

2. Eliminate L ($Z_2 = L$):

- Push in summation over L :

$$P(I, g^3) = \sum_S P(I) P(S|I) \tau_D(I) \sum_L \underbrace{P(L|g^3)}_{\mathcal{T}}$$

- Compute $\mathcal{T} = P(L|g^3)$ for all values of L
(see next slide)
- $U = \{\}$ (variables in the inner expression other than L)

Solving the Query via Variable Elimination

- Compute $\mathcal{T} = P(L|g^3)$ for all values of L :

L	$P(L g^3)$	(from L 's CPD)
l^0	0.99	
l^1	0.01	

- Sum out L :

$$\tau_L = 0.99 + 0.01 = 1.0$$

(the function τ_L has no arguments because $U = \{\}$)

\Rightarrow is a **constant**.

Solving the Query via Variable Elimination

New Target:

$$P(I, g^3) = \sum_S P(I) P(S|I) \tau_D(I) \tau_L$$

3. Eliminate S ($Z_3 = S$):

- Push in summation over S :

$$P(I, g^3) = P(I) \tau_D(I) \tau_L \sum_S \underbrace{P(S|I)}_{\mathcal{T}}$$

- Compute $\mathcal{T} = P(S|I)$ for all values of S, I
(see next slide)
- $U = \{I\}$ (variables in the inner expression other than S)

Solving the Query via Variable Elimination

- Compute $\mathcal{T} = P(S|I)$ for all values of S, I :

S	I	$P(S I)$
s^0	i^0	0.95
s^0	i^1	0.2
s^1	i^0	0.05
s^1	i^1	0.8

(= CPD of S)

- Sum out S :

I	$\sum_S P(S I)$
i^0	$0.95 + 0.05 = 1.0$
i^1	$0.2 + 0.8 = 1.0$

- Store result as table $\tau_S(I)$:

$$\tau_S(I) = \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix}$$

Solving the Query via Variable Elimination

New Target:

$$\begin{aligned}
 P(I, g^3) &= P(I) \tau_D(I) \tau_L \tau_S(I) \\
 &= \begin{bmatrix} 0.7 \\ 0.3 \end{bmatrix} \times \begin{bmatrix} 0.46 \\ 0.092 \end{bmatrix} \times 1 \times \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix} \\
 &= \begin{bmatrix} 0.7 \times 0.46 \times 1.0 \\ 0.3 \times 0.092 \times 1.0 \end{bmatrix} \\
 &= \begin{bmatrix} 0.322 \\ 0.0276 \end{bmatrix}
 \end{aligned}$$

$$Z = 0.322 + 0.0276 = 0.3496$$

$$\boxed{P(I \mid g^3)} = \frac{1}{Z} \cdot \begin{bmatrix} 0.322 \\ 0.0276 \end{bmatrix} \approx \begin{bmatrix} 0.92105 \\ 0.07895 \end{bmatrix}$$

The probability that Joe is highly motivated, given that he got a C grade (and given that we know nothing else about him) is $\approx 7.9\%$.

Computational Complexity of Variable Elimination

Consider

- ▶ a Bayesian network with N variables $\mathcal{X} = \{X_1, \dots, X_N\}$
- ▶ let $M =$ maximum number of entries in any of the intermediate factors $\tau_{Z_i}(U)$ that are generated during variable elimination.

Then

- ▶ the number of arithmetic operations performed by the variable elimination algorithm is $O(N \cdot M)$
(easy to show; proof omitted)

The Bad News:

Have not gotten rid of the problem of exponential complexity (of course):
The intermediate factors $\tau_{Z_i}(U)$ (and thus M) can grow to **exponential size**
(the number of entries is exponential in the number of the variables U).

Computational Complexity of Variable Elimination

More detailed analysis:

- ▶ Real complexity depends on specific structure of the given network graph, and the ordering of the variables in the elimination process
- ▶ ... but systematic analysis of this is extremely complex.
- ▶ Not treated in this class.

General Conclusion:

- ▶ Exact inference can be feasible in **very sparse** networks (if we happen to guess a good variable ordering)
- ▶ but is still **exponential** (and thus **intractable**) in general!

Advanced Topics (not treated here)

A lot ...

Enhancements of variable elimination algorithms:

- ▶ Methods for finding good variable elimination orderings; Conditioning; ...

Alternative classes of algorithms for efficient inference:

- ▶ Clique Trees, Factor Graphs, Message Passing and Belief Update Algorithms,

What you should remember of this section

- ▶ The General Inference-by-Enumeration Algorithm for BNs
- ▶ The complexity of exact inference
- ▶ The basic strategy in variable elimination
- ▶ That even with such optimisations, exact inference is generally intractable
- ▶ That this is only a small part of a large field of inference algorithms for Bayesian Networks.

Literature

Koller, Daphne and Friedman, Nir (2009).

Probabilistic Graphical Models: Principles and Techniques. Cambridge, MA: MIT Press.