Bayesian Networks II Monday, March 28, 2022



Materials

Great materials on BNs from Volodymyr Kuleshov and Stefano Ermon from Stanford:

https://ermongroup.github.io/cs228-notes/

Bayesian Network (The Graph)



Bayesian Network Distribution

Given a BN with a graph G, the BN induces the following distribution:



$$\mathbf{I} P_{X_i | Par(X_i)} \left(x_i | par_{\mathbf{X}}(X_i) \right) .$$

Definition (special case of 3 random variables X, Y, Z): **Definition 1:** X and Y are conditionally independent given Z if holds for all values x, y, z (using the alternative notation: $P_{X,Y|Z}(x,y|z) = P_{X|Z}(x|z) \cdot P_{Y|Z}(y|z)).$

Definition 2: X and Y are conditionally independent given Z if

holds for all values x, y, z (using the alternative notation: $P_{X|Y,Z}(x|y,z) = P_{X|Z}(x|z).$

Conditional Independence

- $P[X = x \land Y = y | Z = z] = P[X = x | Z = z] \cdot P[Y = y | Z = z]$

 - $P[X = x | Y = y \land Z = z] = P[X = x | Z = z]$

written:

Conditional Independence

Notation: The notation for X and Y are conditionally independent given Z is

 $X \perp Y \mid Z$

D-Separation

Given a Bayesian network and a set of variables \mathscr{C} that are conditioned on, we will want to detect those random variables that are conditionally independent given the values of the variables in \mathscr{C} .

Two variables X_1 and X_2 are conditionally independent given \mathscr{E} if there is no active path connecting them.

We will be checking all **undirected** paths between the two variables (i.e. ignoring the direction of the edges).

Terminology: Nodes which we condition on will be called **observed nodes** and the others unobserved nodes.

Active Path (1/3)



Active Path (2/3)

Blocked triples:



Definition: A path is active if all triples along it are active. Otherwise it is blocked.

EXAMPLES:



Active Path (3/3)

Part 2: Variable Elimination Algorithm (Intuition)

Marginal Inference

Problem: Given a BN on random variables X_1, X_2, \ldots, X_n , compute the the random variables X_1, X_2, \ldots, X_n .

Example: Compute $P_{X_1,X_5}(x_1,x_5)$ from the BN shown here:

probability $P_{X_{i_1}, X_{i_2}, \dots, X_{i_k}}(x_{i_1}, x_{i_2}, \dots, x_{i_k})$, where $X_{i_1}, X_{i_2}, \dots, X_{i_k}$ is a subset of



Let's Simplify Notation (1/2)

To simplify notation, we will assume that:

- We have a joint distribution, given by a BN, on random variables $Y_1, Y_2, \ldots, Y_k, Z_1, \ldots, Z_l$ (this is the same as was before X_1, X_2, \ldots, X_n).
- We want to compute the marginal probability $P_{Y_1,\ldots,Y_k}(y_1,\ldots,y_k)$.
- We will call Z_1, \ldots, Z_l unobserved random variables.

Let's Simplify Notation (2/2)

What we want to compute is now:

$$P_{Y_1,...,Y_k}(y_1,...,y_k) = \sum_{z_1} z_1$$

where $P(y_1, ..., y_k, z_1, ..., z_l)$ is the joint probability given by the Bayesian network.



Naive Approach

Naive idea (we won't be able to do better in the worst case):

Compute the following sum explicitly:

$$P_{Y_1}(y_1) = \sum_{z_1} \sum_{z_2} \sum_{z_3} P(y_1, z_1, z_2, z_3)$$

This will have exponential complexity in the number of random variables.

- (3).



Naive Approach: Example (1/2)

		Y ₁	Z_2	$P_{Y_1 Z_2}$	Z ₁	Z 2	$P_{Z_1 Z_2}$	Z ₁	Z ₂	P_{Z_2}
Z ₃	P_{Z_3}	0	0	0.2	0	0	0.5	0	0	0.
0	0.4	1	0	0.8	1	0	0.5	1	0	0.
1	0.6	0	1	0.9	0	1	0.1	0	1	0.
		1	1	0.1	1	1	0.9	1	1	0.
		Z_1		Р	$Y_1 = 11 =$	= <i>P_v</i> (1) = ?			



 Z_2

 Z_1

	Na	ive	Ap	proa	ach:		(am		$\left(\frac{2}{2}\right)$	2)
		Y_1	Z ₂	$P_{Y_1 Z_2}$	Z ₁	Z_2	$P_{Z_1 Z_2}$	Z ₁	Z 2	P_{Z_2}
7 3	P_{Z_2}	0	0	0.2	0	0	0.5	0	0	0
0	0.4	1	0	0.8	1	0	0.5	1	0	0
1	0.6	0	1	0.9	0	1	0.1	0	1	0
		1	1	0.1	1	1	0.9	1	1	0
	$\lfloor 2 \rfloor$			1 1 1						

 $P_{Y_1}(1) = \sum \sum P(1,z_1,z_2,z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $z_1 = 0 z_2 = 0 z_3 = 0$

We need $2^3 - 1 = 7$ additions and 24 multiplications...

 $\sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3)$

 $= 0.8 \cdot 0.5 \cdot 0.5 \cdot 0.4 + 0.8 \cdot 0.5 \cdot 0.1 \cdot 0.6 + 0.1 \cdot 0.1 \cdot 0.5 \cdot 0.4 + 0.4 + 0.8 \cdot 0.5 \cdot 0.5 \cdot 0.4 + 0.8 \cdot 0.5 \cdot 0.$ $+0.1 \cdot 0.1 \cdot 0.9 \cdot 0.6 + 0.8 \cdot 0.5 \cdot 0.5 \cdot 0.4 + 0.8 \cdot 0.5 \cdot 0.1 \cdot 0.6$ $+0.1 \cdot 0.9 \cdot 0.5 \cdot 0.4 + 0.1 \cdot 0.9 \cdot 0.9 \cdot 0.6 = 0.282$





Variable Elimination: Basic Idea (1/10) $z_1 = 0 z_2 = 0 z_3 = 0$

$P_{Y_1}(1) = \sum_{i=1}^{1} \sum_{j=1}^{1} \sum_{i=1}^{1} P(1,z_1,z_2,z_3) =$







Variable Elimination: Basic Idea (1/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$







 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) \sum P_{Z_1|Z_2}(z_1|z_2)$ $z_2 = 0 z_3 = 0$

Variable Elimination: Basic Idea (1/10) $z_1 = 0$ $=G(z_2)$ $G_1(0) = 0.5 + 0.5 = 1$ $G_1(1) = 0.1 + 0.9 = 1$







Variable Elimination: Basic Idea (2/10) $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum_{i=1}^{n} \sum_{Y_{1}|Z_{2}}^{i} (1|z_{2}) P_{Z_{2}|Z_{3}}(z_{2}|z_{3}) P_{Z_{3}}(z_{3}) \sum_{Y_{2}|Z_{2}}^{i} P_{Z_{1}|Z_{2}}(z_{1}|z_{2})$ $z_2 = 0 z_3 = 0$ $z_1 = 0$ $=G_1(z_2)$ $G_1(0) = 0.5 + 0.5 = 1$

 $G_1(1) = 0.1 + 0.9 = 1$







Variable Elimination: Basic Idea (3/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3)G_1(z_2)$ $z_2 = 0 z_3 = 0$









Variable Elimination: Basic Idea (4/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_2}(z_3)G_1(z_2)$ $z_2 = 0 z_3 = 0$









Variable Elimination: Basic Idea (5/10) $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$

 $= \sum P_{Z_3}(z_3) \sum P_{Y_1|Z_2}(1|z_2) P_{Z_2|Z_2}(z_2|z_3) G_1(z_2)$

 $z_3 = 0$

 $z_2 = 0$







Variable Elimination: Basic Idea (6/10) $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3) \sum P_{Y_1|Z_2}(1|z_2) P_{Z_2|Z_3}(z_2|z_3) G_1(z_2)$ $z_3 = 0$ $z_2 = 0$

 $G_2(z_3)$ $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$









Variable Elimination: Basic Idea (7/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3)G_2(z_3)$ $z_3 = 0$

 $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$







Variable Elimination: Basic Idea (8/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3)G_2(z_3)$ $z_3 = 0$

 $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$





Variable Elimination: Basic Idea (9/10) $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3)G_2(z_3)$ $z_3 = 0$

 $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$





Variable Elimination: Basic Idea (10/10)

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_1|Z_2}(z_1|z_2)P_{Z_2|Z_3}(z_2|z_3)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3)G_2(z_3)$ $z_3 = 0$

 $P_{Y_1}(1) = 0.4 \cdot 0.45 + 0.6 \cdot 0.17 = 0.282$

 $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$





How Many Operations Did We Need?

 $G_2(0) = 0.8 \cdot 0.5 \cdot 1 + 0.1 \cdot 0.5 \cdot 1 = 0.45$ $G_2(1) = 0.8 \cdot 0.1 \cdot 1 + 0.1 \cdot 0.9 \cdot 1 = 0.17$

additions fot the naive approach!)

- $G_1(0) = 0.5 + 0.5 = 1$
- $G_1(1) = 0.1 + 0.9 = 1$
- $P_{Y_1}(1) = 0.4 \cdot 0.45 + 0.6 \cdot 0.17 = 0.282$

10 multiplications and 5 additions (we needed 24 multiplications and 7

 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3)$ $z_1 = 0 z_2 = 0 z_3 = 0$





 $P_{Y_1}(1) = \sum \sum P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum_{i=1}^{1} \sum_{Y_{1}|Z_{2}}^{1} (1|z_{2}) P_{Z_{3}}(z_{3}) \sum_{Y_{2}|Z_{1}}^{1} P_{Z_{1}}(z_{1}) P_{Z_{2}|Z_{1},Z_{3}}(z_{2}|z_{1},z_{3})$ $z_2 = 0 z_3 = 0$ $z_1 = 0$

Variable Elimination: Example II (2/8)



 $P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum_{i=1}^{1} \sum_{i=1}^{1} P_{Y_{1}|Z_{2}}(1|z_{2})P_{Z_{3}}(z_{3}) \sum_{i=1}^{1} P_{Z_{1}}(z_{1})P_{Z_{2}|Z_{1},Z_{3}}(z_{2}|z_{1},z_{3})$ $z_2 = 0 z_3 = 0$ $z_1 = 0$

 $G_1(0,0) = \dots, G_1(0,1) = \dots$ $G_1(1,0) = \dots, G_1(1,1) = \dots$

Variable Elimination: Example II (3/8)

 $=G_1(z_2,z_3)$



$P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Y_1|Z_2}(1|z_2)P_{Z_3}(z_3)G_1(z_2,z_3)$ $z_2 = 0 z_3 = 0$



$P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Y_1|Z_2}(1|z_2)P_{Z_3}(z_3)G_1(z_2,z_3)$ $z_2 = 0 z_3 = 0$


$P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3) \sum P_{Y_1|Z_2}(1|z_2)G_1(z_2,z_3)$ $z_3 = 0$ $z_2 = 0$

Variable Elimination: Example II (6/8)



 $P_{Y_1}(1) = \sum \sum P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3) \sum P_{Y_1|Z_2}(1|z_2)G_1(z_2,z_3)$ $z_3 = 0$ $z_2 = 0$

 $=G_{2}(z_{3})$

 $G_2(0) = ...,$ $G_2(1) = ...,$





$P_{Y_1}(1) = \sum_{Y_1}^{1} \sum_{Y_1}^{1} \sum_{Y_1}^{1} P(1, z_1, z_2, z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum \sum P_{Y_1|Z_2}(1|z_2)P_{Z_2|Z_1,Z_3}(z_2|z_1,z_3)P_{Z_1}(z_1)P_{Z_3}(z_3) =$ $z_1 = 0 z_2 = 0 z_3 = 0$ $= \sum P_{Z_3}(z_3)G_2(z_3)$ $z_3 = 0$



Factor Representation (1/2)

We will now abstract a bit... We will replace conditional probabilities in a BN by factors $\psi_i(x_i, x_{p_1}, \dots, x_{p_k})$. This is for now just a change of notation, which will simplify things.

So instead of

 $P(x_1, x_2, ..., x_n)$

we will write

 $P(x_1,\ldots,x_n)$

where each \mathbf{v}_i is a tuple consisting of a subset of $\{x_1, x_2, \dots, x_n\}$.

$$P_{X_i|Par(X_i)}\left(x_i|\operatorname{par}_{\mathbf{X}}(X_i)\right)$$

$$f_{n} = \prod_{i=1}^{n} \psi_{i}(\mathbf{v}_{i})$$

Factor Representation (2/2)

We will now abstract a bit... We will replace conditional probabilities in a BN by factors $\psi_i(x_i, x_{p_1}, \dots, x_{p_k})$. This is for now just a change of notation, which will simplify things.

So instead of

 $P(x_1, x_2, ..., x_n)$

we will write

 $P(x_1,\ldots,x_n)$

where each \mathbf{v}_i is a tuple consisting of a subset of $\{x_1, x_2, \dots, x_n\}$. This can simply be done by setting $\psi_i(\mathbf{v}_i) = P_{X_i | Par(X_i)}(x_i | par_{\mathbf{x}}(X_i)))$ and $\mathbf{v}_i = (x_i, x'_1, \dots, x'_{k_i})$ where $x'_1, x'_2, \dots, x'_{k_i}$ are the parents of X_i (more precisely, their values).

$$P_{X_i|Par(X_i)}\left(x_i|\operatorname{par}_{\mathbf{X}}(X_i)\right)$$

$$\psi_{i}(\mathbf{v}_{i}) = \prod_{i=1}^{n} \psi_{i}(\mathbf{v}_{i})$$

Two Operations: Product

Product:

Given factors $\psi_1(x_{i_1}, \dots, x_{i_k})$ and $\psi_2(x_{j_1}, \dots, x_{j_k})$, their product is defined simply as: $\psi_{1\times 2}(x_{h_1},\ldots,x_{h_k})=\psi_1(x_{i_1},\ldots,x_{i_k})\cdot\psi_2(x_{i_1},\ldots,x_{i_k}),$ where $\{x_{h_1}, \dots, x_{h_k}\} = \{x_{i_1}, \dots, x_{i_k}\} \cup \{x_{i_1}, \dots, x_{i_k}\}$. (Note that this will be represented as a table that will have a row for every possible combination of the values of the variables in it.)

Example:

 $\psi_1(x_1, x_2) = P_{X_1|X_2}(x_1|x_2), \psi_2(x_2, x_3) =$

=
$$P_{X_2|X_3}(x_2|x_3)$$
. Then

 $\psi_{1\times 2}(x_1, x_2, x_3) = P_{X_1|X_2}(x_1|x_2) \cdot P_{X_2|X_3}(x_2|x_3).$

Two Operations: Marginalization

Product:

Given a factor $\psi(x_{i_1}, \dots, x_{i_*}, \dots, x_{i_k})$ and a variable x_{i_*} , the marginalization is: $\tau_{i^*}(x_{i_1}, \dots, x_{i^*}, \dots, x_{i_k}) =$

Example:

Let us have a factor $\psi(x_1, x_2, x_3)$. Then $\tau_2(x_1, x_3) =$

Note: The operations product and marginalization are similar in spirit to join and projection operations from relational databases.

$$= \sum_{\substack{x_{i^*} \\ x_{i^*}}} \psi(x_{i_1}, \dots, x_{i^*}, \dots, x_{i_k}).$$

$$\sum_{x_2} \psi(x_1, x_2, x_3).$$

Variable Elimination: Algorithm

- Assume that the unobserved random variables of the BN are ordered as $Z_1, Z_2, ..., Z_n$
- For i = 1, ..., n:

Collect all factors containing Z_i and compute their product $\psi_{prod}^{(i)}$.

Marginalize out Z_i from $\psi_{prod}^{(i)}$ and call the result τ .

Remove all factors containing Z_i and add τ instead.

The Elimination Order Matters

The number of operations (~runtime) depends on the ordering of the unobserved variables that we use when eliminating them.

The runtime depends on the size of the intermediate factors and that depends on the order.

Finding the best ordering is an NP-hard problem (but there are heuristics).

Part 3: Approximate Methods

Approximate Methods

Variable elimination is an **exact method**.

Exact inference is computationally hard. Computing marginal probabilities in Bayesian networks is **#P-hard**.

Now we will take a look at approximate methods based on sampling.

Forward Sampling

Generating samples from a distribution given by a Bayesian network (without evidence) is easy...

Algorithm:

 $X'_{i}s$ parents must preceed X_{i} in this ordering.) Initialize: Sampled =

For i = 1, ..., n:

Let $X_{i_1}, X_{i_2}, \ldots, X_{i_l}$ be the parents of X_i and $P_{X_i, Par(X_i)}(x \mid x_{i_1}, \ldots, x_{i_l})$ be the conditional distribution of X_i .

Set Sampled[i] = x_i .

Let the nodes of X_1, X_2, \ldots, X_n be ordered topologically. (That is, for all i, all

Sample $x_i \sim P_{X_i | Par(X_i)}(. | Sampled[i_1], Sampled[i_2], ..., Sampled[i_l]).$

Forward Sampling: Example Topological ordering? ... X_1, X_2, X_3, X_4



Sampled = [0]



 X_2 X_{2}

Sampled = [0]

Sample $x_2 \sim P_{X_2}(.)$, e.g. $x_2 = 1$

Sampled = [0,1]



Sampled = [0]

Sample $x_2 \sim P_{X_2}(.)$, e.g. $x_2 = 1$

Sampled = [0,1]

Sample $x_3 \sim P_{X_3|X_1,X_2}(.|0,1)$, e.g. $x_3 = 1$ **Sampled** = [0,1,1]



Sampled = [0]Sample $x_2 \sim P_{X_2}(.)$, e.g. $x_2 = 1$ **Sampled** = [0,1]**Sampled** = [0,1,1]

- Sample $x_3 \sim P_{X_3|X_1,X_2}(.|0,1)$, e.g. $x_3 = 1$ Sample $x_4 \sim P_{X_4|X_3}(.|1)$, e.g. $x_4 = 1$
- **Sampled** = [0,1,1,1]

Monte Carlo Estimation

We can use **forward sampling to e** conditioning):

 $P_Y(\mathbf{y}) \approx \frac{1}{N}$

We can use forward sampling to estimate marginal probabilities (without

$$\sum_{(\mathbf{y}^{(i)},\mathbf{z}^{(i)})} \mathbb{I}(\mathbf{y}^{(i)} = \mathbf{y}).$$

Sampling with Evidence

How can we sample from a BN if there is evidence on some random variables?

 X_2 X_{Δ}

Evidence: e.g. $X_4 = 1$

Example: How can we sample $(x_1, x_2, x_3) \sim P_{X_1, X_2, X_3 | X_4}(..., | x_4)$?

Note: One possibility is to use marginal inference and to compute $P_{X_1,X_2,X_3|X_4}(x_1,x_2,x_3|x_4)$ for all tuples $(x_1,x_2,x_3) \in \{0,1\}^3$ as $P(x_1, x_2, x_3, 1)/P_{X_1}(1)$. However, that is something we want to avoid... after all we sample to do approximate marginal inference.







Rejection Sampling (1/2)

Basic idea:



Downside: What if $P[X_4 = 1]$ is small? Then we will need many samples from the unconditional distribution to get enough samples from the conditional one...



Evidence: e.g. $X_4 = 1$

- We know how to sample without evidence (forward sampling). Let $(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, x_4^{(1)}), (x_1^{(2)}, x_2^{(2)}, x_3^{(2)}, x_4^{(2)}), \dots, (x_1^{(N)}, x_2^{(N)}, x_3^{(N)}, x_4^{(N)})$ be samples from the BN without taking evidence into account.
- To get samples from the distribution conditioned on $X_4 = 1$, we just need to filter out those samples where $x_{A}^{(i)} \neq 1$.





Rejection Sampling (2/2) Monte Carlo Estimation with rejection sampling: We are interested in estimating $P[\mathbf{Y} = \mathbf{y} | \mathbf{E} = \mathbf{e}] = P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} | \mathbf{e})$, e.g., (1 | 1).

$$P[X_2 = 1 | X_4 = 1] = P_{X_2 | X_4}($$

Algorithm Rejection MC(BN, Y, E, y, e): YES := 0, NO := 0For i = 1, ..., N: $(x_1^{(i)}, \dots, x_n^{(i)}) := \text{ForwardSampling(BN)}$ if $(x_1^{(i)}, \ldots, x_n^{(i)})$ is consistent with evidence **e** on **E**: if $(x_1^{(i)}, \ldots, x_n^{(i)})$ is consistent with $\mathbf{Y} = \mathbf{y}$ YES := YES + 1else NO = NO + 1return YES/(YES + NO)

 X_4

Importance Sampling: Basic Idea (1/3)

Problem: Estimate

 $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} \,|\, \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})}.$

Importance Sampling: Basic Idea (2/3) We have $P_{Y|E}(y | e) = \sum_{z} \frac{P(y, z, e)}{P_{E}(e)}$

 $P(\mathbf{y}, \mathbf{z}, \mathbf{e}) > 0 \Rightarrow Q(\mathbf{y}, \mathbf{z}, \mathbf{e}) > 0$

 $W_{\mathbf{e}}(\mathbf{y}, \mathbf{z}) = \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}$

Importance Sampling: Basic Idea (2/3) We have $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} \mid \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})} = \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{\sum_{\mathbf{v}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e})} =$



Importance Sampling: Basic Idea (2/3) We have $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} | \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})} = \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e})} =$ $= \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}', \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}', \mathbf{z}, \mathbf{e})}}$



Importance Sampling: Basic Idea (2/3) We have $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} | \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})} = \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e})} =$ $= \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}}{\sum_{\mathbf{z}} Q(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}}$ $\sum_{\mathbf{v}',\mathbf{z}} P(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{Q(\mathbf{y}',\mathbf{z},\mathbf{e})}{O(\mathbf{v}',\mathbf{z},\mathbf{e})} \qquad \sum_{\mathbf{v}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{O(\mathbf{v}',\mathbf{z},\mathbf{e})}$

 $W_{\mathbf{e}}(\mathbf{y}, \mathbf{z}) = \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}$

Importance Sampling: Basic Idea (2/3) We have $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} | \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})} = \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e})} =$ $\frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}', \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}', \mathbf{z}, \mathbf{e})}} = \frac{\sum_{\mathbf{z}} Q(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}}{\sum_{\mathbf{y}', \mathbf{z}} Q(\mathbf{y}', \mathbf{z}, \mathbf{e}) \frac{P(\mathbf{y}', \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}', \mathbf{z}, \mathbf{e})}}$ $\sum_{\mathbf{y}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \cdot \mathbb{I}(\mathbf{y}=\mathbf{y}') \cdot \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{O(\mathbf{v}',\mathbf{z},\mathbf{e})}$ $\sum_{\mathbf{y}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{Q(\mathbf{y}',\mathbf{z},\mathbf{e})}$

 $W_{\mathbf{e}}(\mathbf{y}, \mathbf{z}) = \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}$

Importance Sampling: Basic Idea (2/3) We have $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} | \mathbf{e}) = \sum_{\mathbf{z}} \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{P_{\mathbf{E}}(\mathbf{e})} = \frac{\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{\sum_{\mathbf{y}', \mathbf{z}} P(\mathbf{y}', \mathbf{z}, \mathbf{e})} =$ $\sum_{\mathbf{z}} P(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})} \qquad \sum_{\mathbf{z}} Q(\mathbf{y}, \mathbf{z}, \mathbf{e}) \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}$ $\frac{\sum_{\mathbf{y}',\mathbf{z}} P(\mathbf{y}',\mathbf{z},\mathbf{e})}{\sum_{\mathbf{y}',\mathbf{z}} P(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{Q(\mathbf{y}',\mathbf{z},\mathbf{e})}{O(\mathbf{v}',\mathbf{z},\mathbf{e})}} = \frac{\sum_{\mathbf{v}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e})}{\sum_{\mathbf{v}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{O(\mathbf{v}',\mathbf{z},\mathbf{e})}}$ $\sum_{\mathbf{y}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \cdot \mathbb{I}(\mathbf{y}=\mathbf{y}') \cdot \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{Q(\mathbf{y}',\mathbf{z},\mathbf{e})} \qquad \mathbb{E}_{\mathbf{Y},\mathbf{Z}\sim Q} \left[\mathbb{I}(\mathbf{y}=\mathbf{y}') \cdot W_{\mathbf{e}}(\mathbf{Y},\mathbf{Z})\right]$ $\sum_{\mathbf{y}',\mathbf{z}} Q(\mathbf{y}',\mathbf{z},\mathbf{e}) \frac{P(\mathbf{y}',\mathbf{z},\mathbf{e})}{Q(\mathbf{y}',\mathbf{z},\mathbf{e})}$ $\mathbb{E}_{\mathbf{Y},\mathbf{Z}\sim O} \left| W_{\mathbf{e}}(\mathbf{Y},\mathbf{Z}) \right|$ $W_{\mathbf{e}}(\mathbf{y}, \mathbf{z}) = \frac{P(\mathbf{y}, \mathbf{z}, \mathbf{e})}{Q(\mathbf{y}, \mathbf{z}, \mathbf{e})}$

Importance Sampling: Basic Idea (3/3)

We have

$$P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} \mid \mathbf{e}) = \frac{\mathbb{E}_{\mathbf{Y}, \mathbf{Z} \sim Q} \left[\mathbb{I}(\mathbf{y} = \mathbf{y}') \cdot W_{\mathbf{e}}(\mathbf{Y}, \mathbf{Z}) \right]}{\mathbb{E}_{\mathbf{Y}, \mathbf{Z} \sim Q} \left[W_{\mathbf{e}}(\mathbf{Y}, \mathbf{Z}) \right]} \approx \frac{\sum_{(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) \in \mathcal{D}} \mathbb{I}(\mathbf{y} = \mathbf{y}^{(i)}) \cdot W_{\mathbf{e}}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})}{\sum_{(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) \in \mathcal{D}} W_{\mathbf{e}}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})}$$

where \mathscr{D} is a collection of samples which Q.

The trick: Pick Q for which sampling is easy! (We will see one particular choice of Q next, which will lead to a method called likelihood weighting.)

where \mathscr{D} is a collection of samples which were sampled according to the distribution

Likelihood Weighting (1/4)

We want to find a Q from which it is easy to sample (we want to use forward sampling) and such that $P(\mathbf{y}, \mathbf{z}, \mathbf{e})/Q(\mathbf{y}, \mathbf{z}, \mathbf{e})$ is easy to compute.





Likelihood Weighting (2/4)

We want to find a Q from which it is easy to sample (we want to use forward sampling) and such that $P(\mathbf{y}, \mathbf{z}, \mathbf{e})/Q(\mathbf{y}, \mathbf{z}, \mathbf{e})$ is easy to compute.

Method: For every node from E (i.e. for every node on which we are conditioning), remove all edges that end in it.





Likelihood Weighting (3/4)

We want to find a Q from which it is easy to sample (we want to use forward sampling) and such that $W_{\mathbf{e}}(\mathbf{y}, \mathbf{z}) = P(\mathbf{y}, \mathbf{z}, \mathbf{e})/Q(\mathbf{y}, \mathbf{z}, \mathbf{e})$ is easy to compute.

Method:

1. For every node from E (i.e. for every node on which we are conditioning), remove all edges that end in it.

- 2. Use forward sampling (keeping the values of nodes which are in **E** fixed to construct N samples from the modified BN. Store them in \mathcal{D} .
- 3. For every sample $(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})$, compute $W_e(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})$ as follows (here we are using the origonal set of the origonal set of the set of the origonal set of the set of $W_{e}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) = \prod P_{E_{i}|Par(E_{i})} \left(e_{i} | \mathsf{par}_{\mathbf{y}^{(i)}, \mathbf{z}^{(i)}}(E_{i}) \right).$ $E_i \in \mathbf{E}$









Likelihood Weighting (4/4)

Method:

it.

- 2. Use forward sampling (keeping the values of nodes which are in **E** fixed to construct N samples from the modified BN. Store them in \mathscr{D} .
- 3. For every sample $(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})$, compute $W_{\rho}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})$ $W_e(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) = \prod P$ $E_i \in \mathbf{E}$
- 4. Compute estimate of $P_{\mathbf{Y}|\mathbf{E}}(\mathbf{y} \mid \mathbf{e})$ as

1. For every node from E (i.e. for every node on which we are conditioning), remove all edges that end in

$$\mathbf{z}^{(i)}, \text{ compute } W_{e}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) \text{ as follows:}$$

$$W_{e}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) = \prod_{E_{i} \in \mathbf{E}} P_{E_{i} | Par(E_{i})} \left(e_{i} | \text{par}_{\mathbf{y}^{(i)}, \mathbf{z}^{(i)}}(E_{i}) \right).$$

$$P_{\mathbf{Y} | \mathbf{E}}(\mathbf{y} | \mathbf{e}) \text{ as}$$

$$P_{\mathbf{Y} | \mathbf{E}}(\mathbf{y} | \mathbf{e}) \approx \frac{\sum_{(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) \in \mathcal{D}} \mathbb{I}(\mathbf{y} = \mathbf{y}^{(i)}) \cdot W_{\mathbf{e}}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})}{\sum_{(\mathbf{y}^{(i)}, \mathbf{z}^{(i)}) \in \mathcal{D}} W_{\mathbf{e}}(\mathbf{y}^{(i)}, \mathbf{z}^{(i)})}.$$







Part 4: Requisite Network



Exploiting Conditional Independence

- Do we need to perform inference on the whole network in order to compute
- $P[X_3 = 1 | X_2 = 0, X_1 = 1]$?

- We can check that $X_3 \perp \{X_5, X_6, X_7\} \mid X_1, X_2$.
- Therefore we can do inference on a smaller

Exploiting Conditional Independence Do we need to perform inference on the whole X_7 network in order to compute $P[X_3 = 1 | X_2 = 0, X_1 = 1]$? X_6 X_5 No! We can check that $X_3 \perp \{X_5, X_6, X_7\} \mid X_1, X_2$. X_{2} Therefore we can do inference on a smaller network... X_4
Exploiting Conditional Independence Do we need to perform inference on the whole X_7 network in order to compute $P[X_3 = 1 | X_2 = 0, X_1 = 1]$? X_6 X_5 No! We can check that $X_3 \perp \{X_5, X_6, X_7\} \mid X_1, X_2$. X_{2} Therefore we can do inference on a smaller network... This can be done more efficiently than by checking all paths (whether they are active) by so-called **Bayes-Ball Algorithm.** X_{4}



Part 5: What we did not cover...

What we did not cover...

Inference: Join-tree algorithm, Gibbs sampling, variational inference...

Other inference problem: MAP-inference, MPE-inference

- **Learning:** Maximum-likelihood learning (for fully-observable data, this is just estimation of conditional probability tables from frequencies), EM algorithm (when we have missing data or latent random variables), structure learning...