# Statistical Inference in Bayesian Networks

Wenhu Chen

Lecture 9

Readings: RN 13.4. PM 8.4.

## Outline

Learning Goals

Why Use the Variable Elimination Algorithm

The Variable Elimination Algorithm

Factors Affecting the Complexity of VEA

Approximate Inference

Revisiting Learning Goals

## Learning Goals

- Explain how we can perform probabilistic inference more efficiently using the variable elimination algorithm.
- ▶ Define factors. Manipulate factors using operations restrict, sum out, multiply and normalize.
- Describe/trace/implement the variable elimination algorithm for calculating a prior or a posterior probability given a Bayesian network.
- Explain how the elimination ordering affects the complexity of the variable elimination algorithm.
- Know about approximate statistical inference.

#### Learning Goals

## Why Use the Variable Elimination Algorithm

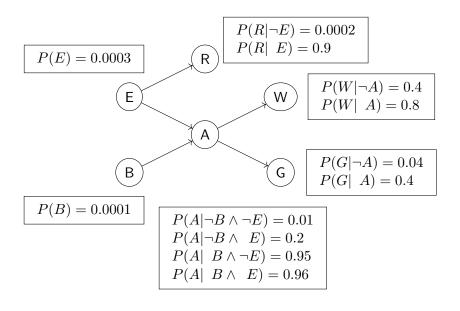
The Variable Elimination Algorithm

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# A Bayesian Network for the Holmes Scenario



## Answering a Question

What is the probability that a burglary is happening given that Dr. Watson and Mrs. Gibbon both call?

$$P(B|w \wedge g)$$

▶ Query variables: *B* 

Evidence variables: W and G

▶ Hidden variables: *E*, *A*, and *R*.

Notice the new notation: capital letters for random variables and lowercase letters for values.

## Answering the query using the joint distribution

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Evaluate  $P(B|w \wedge g)$  in terms of known distributions from the Bayesian network.

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# Answering the query using the joint distribution

Evaluate  $P(B|w \wedge g)$  in terms of known distributions from the Bayesian network.

→ Following the approach from Lecture 6:

$$\begin{split} P(B|w \wedge g) &= \frac{P(B \wedge w \wedge g)}{P(w \wedge g)} \\ &= \frac{P(B \wedge w \wedge g)}{P(b \wedge w \wedge g) + P(\neg b \wedge w \wedge g)} \\ &\propto P(B \wedge w \wedge g) \\ &\propto \sum_{e} \sum_{a} \sum_{r} P(B \wedge e \wedge a \wedge w \wedge g \wedge r) \\ &\propto \sum_{e} \sum_{a} \sum_{r} P(B)P(e)P(a|B \wedge e)P(w|a)P(g|a)P(r|e) \end{split}$$

# **Q** #1: Number of operations using the joint distribution

How many addition and multiplication operations do we need to calculate the expression below?

$$\sum_e \sum_a \sum_r P(B) P(e) P(a|B \wedge e) P(w|a) P(g|a) P(r|e)$$

- (A)  $\leq 10$
- (B) 11-20
- (C) 21-40
- (D) 41-60
- $(E) \geq 61$

# **Q** #1: Number of operations using the joint distribution

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- (A)  $\leq 10$
- (B) 11-20
- (C) 21-40
- (D) 41-60
- $(E) \geq 61$
- $\rightarrow$  Correct answer is (D). 47 operations.

## Is there any duplication?

- ightharpoonup P(B) appears in every single term, but it doesn't involve any of the three hidden variables.
- ightharpoonup P(B) can be thought of as a constant number.
- If you pull P(B) outside of the summation, you decrease 8 multiplication to 1 multiplication
- Push summation to as right as possible.

# Answering the query using variable elimination algorithm

$$\sum_{e} \sum_{a} \sum_{r} P(B)P(e)P(a|B \wedge e)P(w|a)P(g|a)P(r|e)$$

 $\rightarrow$  We should move the summations as much to the right of the expression as possible to reduce the overall # of operations.

$$\begin{split} &= \sum_{e} \sum_{a} \sum_{r} P(B) P(e) P(a|B \wedge e) P(w|a) P(g|a) P(r|e) \\ &= P(B) \sum_{e} P(e) \sum_{a} P(a|B \wedge e) P(w|a) P(g|a) \sum_{r} P(r|e) \\ &= P(B) \sum_{e} P(e) \sum_{a} P(a|B \wedge e) P(w|a) P(g|a) \end{split}$$

# **Q #2:** Number of operations via the variable elimination algorithm

How many addition and multiplication operations do we need to calculate the expression below?

$$P(B)\sum_{e}P(e)\sum_{a}P(a|B\wedge e)P(w|a)P(g|a)$$

- $(A) \leq 10$
- (B) 11-20
- (C) 21-40
- (D) 41-60
- (E)  $\geq 61$

# **Q #2:** Number of operations via the variable elimination algorithm

How many addition and multiplication operations do we need to calculate the expression below?

$$P(B)\sum_{e}P(e)\sum_{a}P(a|B\wedge e)P(w|a)P(g|a)$$

- (A)  $\leq 10$
- (B) 11-20
- (C) 21-40
- (D) 41-60
- (E)  $\geq 61$
- $\rightarrow$  The inner term requires 1 add + 4 mul. It requires 1 mul + 1 add + (1 mul + 5 opss) \* 2 = 14 ops
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# **Q #2:** Number of operations via the variable elimination algorithm

How many addition and multiplication operations do we need to calculate the expression below?

$$P(B)\sum_{e}P(e)\sum_{a}P(a|B\wedge e)P(w|a)P(g|a)$$

- (A) < 10
- (B) 11-20
- (C) 21-40
- (D) 41-60
- (E)  $\geq 61$
- $\rightarrow$  Correct answer is (B) 11-20. 14 operations in total.

## Efficient Inference Algorithm

- ► To compute the posterior or prior distribution from a given Bayesian Network.
- Different orders will lead to different complexity.
- ▶ 14 operations vs 47 operations.
- We prefer to choose the most efficient inference algorithm.

Learning Goals

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## Introducing the Variable Elimination Algorithm

- ▶ Performing probabilistic inference is challenging.
  - → Computing the posterior distribution of one or more query variables given some evidence is #NP. Estimate the posterior probability in a Bayesian network within an absolute error is already NP-hard. No general efficient implementation.
- Exact and approximate inferences.
  - → Compute the probabilities exactly. Naive approach: enumerate all the worlds consistent with the evidence. Do better below.
- ► The variable elimination algorithm uses dynamic programming and exploits the conditional independence.
  - ightarrow Do the calculations once and save the results for later.

Factors and operations.

## Introducing the Variable Elimination Algorithm

- High-Level Idea: Reuse intermediate computation and exploits the conditional independence present in the Bayesian Network.
- Define Factors.
- Restrict Factors to reflect the evidence.
- Multiply factors with shared variables.
- Sum out hidden variables.
- Normalize to obtain probability.

#### **Factors**

- A function from some random variables to a number.
- $f(X_1, \ldots, X_j)$ : a factor f on variables  $X_1, \ldots, X_j$ .
- ▶ A factor can represent a joint or a conditional distribution. For example,  $f(X_1, X_2)$  can represent  $P(X_1 \wedge X_2)$ ,  $P(X_1|X_2)$  or  $P(X_1 \wedge X_3 = v_3|X_2)$ .
- Define a factor for every conditional probability distribution in the Bayes net.
- ightarrow Every conditional probability distribution in the Bayes net is a factor.

$$f(B), f(E), f(A, B, E), f(R, E), f(W, A), f(G, A)$$
 
$$P(B), P(E), P(A|B \land E), P(R|E), P(W|A), P(G|A)$$

$$P(B \wedge w \wedge g)$$

$$= P(B) \sum_{a} P(w|a) P(g|a) \sum_{a} P(e) P(a|B \wedge e)$$

### Restrict a variable

- ➤ To eliminate hidden variables, we need to find all factors containing the variable.
- We want to restrict the factor to the case where  $X_1 = v_1$ .
- ► This operation produces a new factor which only contains the variables without being restricted.

### Restrict a factor

#### Restrict a factor.

- Assign each evidence variable to its observed value.
- Restricting  $f(X_1, X_2, \dots, X_j)$  to  $X_1 = v_1$ , produces a new factor  $f(X_1 = v_1, X_2, \dots, X_j)$  on  $X_2, \dots, X_j$ .
- $f(X_1 = v_1, X_2 = v_2, \dots, X_j = v_j)$  is a number.
- $\rightarrow$  Restrict f(W,A) to W=t. Restrict f(G,A) to G=t.

$$P(B \land w \land g)$$

$$= P(B) \sum_{a} P(w|a) P(g|a) \sum_{e} P(e) P(a|B \land e)$$

## Restrict a factor

	X	Y	Z	val	l
	t	t	t	0.1	
	t	t	f	0.9	Ì
	t	f	t	0.2	Ì
$f_1(X,Y,Z)$ :	t	f	f	8.0	Ì
	f	t	t	0.4	Ì
	f	t	f	0.6	Ì
	f	f	t	0.3	Ì
	f	f	f	0.7	
'					

	Y	Z	val
	t	t	0.1
$f_2(Y,Z)$ :	t	f	0.9
	f	t	0.2
	f	f	0.8

	Y	val
$f_3(Y)$ :	t	0.9
	f	0.8

$$f_4() = 0.8$$

- ▶ What is  $f_2(Y, Z) = f_1(x, Y, Z)$ ?
- ▶ What is  $f_3(Y) = f_2(Y, \neg z)$ ?
- ▶ What is  $f_4() = f_3(\neg y)$ ?

## Sum out a variable

- ➤ To eliminate hidden variables, we need to find all factors containing the variable.
- Multiply the factors together, and sum out the variable from the product.
- The sum out operation is similar to the sum rule of probability.
- ▶ The rule will derive a new factor without the sum-out variable.

## Sum out a variable

Sum out a variable.

Summing out  $X_1$  with domain  $\{v_1,\ldots,v_k\}$  from factor  $f(X_1,\ldots,X_j)$ , produces a factor on  $X_2,\ldots,X_j$  defined by:

$$(\sum_{X_1} f)(X_2, \dots, X_j) = f(X_1 = v_1, \dots, X_j) + \dots + f(X_1 = v_k, \dots, X_j)$$

 $\rightarrow$  Sum out a and e.

$$P(B \land w \land g)$$
  
=  $P(B) \sum P(w|a)P(g|a) \sum P(e)P(a|B \land e)$ 

## Sum out a variable

## $f_1(X,Y,Z)$ :

X	Y	Z	val
t	t	t	0.03
t	t	f	0.07
t	f	t	0.54
t	f	f	0.36
f	t	t	0.06
f	t	f	0.14
f	f	t	0.48
f	f	f	0.32

$$\rightarrow f_2(X,Z)$$
:

X	Z	val
t	t	0.57
t	f	0.43
f	t	0.54
f	f	0.46

What is  $f_2(X, Z) = \sum_{Y} f_1(X, Y, Z)$ ?

# Multiplying factors

- ► To eliminate hidden variables, we need to find all factors containing the variable.
- Multiply the factors together, and sum out the variable from the product.
- ▶ Multiplication is the first step of the procedure.
- ▶ The new factor is a union of the two sets.

## Multiplying factors

Multiply two factors together.

The **product** of factors  $f_1(X,Y)$  and  $f_2(Y,Z)$ , where Y are the variables in common, is the factor  $(f_1 \times f_2)(X,Y,Z)$  defined by:

$$(f_1 \times f_2)(X, Y, Z) = f_1(X, Y) * f_2(Y, Z).$$

 $\rightarrow$ 

$$P(B \land w \land g)$$

$$= P(B) \sum_{a} P(w|a) P(g|a) \sum_{e} P(e) P(a|B \land e)$$

# Multiplying factors

	X	Y	val
	t	t	0.1
$f_1$ :	t	f	0.9
	f	t	0.2
	f	f	0.8

	Y	Z	val
	t	t	0.3
$f_2$ :	t	f	0.7
	f	t	0.6
	f	f	0.4

	X	Y	Z	val
	t	t	t	0.03
	t	t	f	0.07
	t	f	t	0.54
$f_1 \times f_2$ :	t	f	f	0.36
	f	t	t	0.06
	f	t	f	0.14
	f	f	t	0.48
	f	f	f	0.32

What is  $f_1(X,Y) \times f_2(Y,Z)$ ?

### Normalize a factor

- ► The purpose of normalization is to convert some numbers into a valid probability distribution
- Normalize is the last step of the variable elimination algorithm
- After normalizing the values, they will sum to 1 and represent valid probabilities

## Normalize a factor

- ► Convert it to a probability distribution.
- Divide each value by the sum of all the values.

	$\mid Y \mid$	val
$f_1$ :	t	0.2
	f	0.6

# Variable elimination algorithm

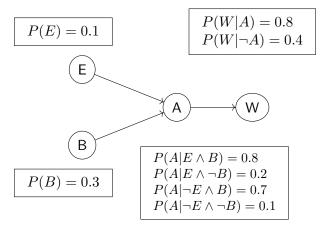
To compute 
$$P(X_q|X_{o_1}=v_1\wedge\ldots\wedge X_{o_j}=v_j)$$
:

- Construct a factor for each conditional probability distribution.
- **Restrict** the observed variables to their observed values.
- ▶ Eliminate each hidden variable  $X_{h_i}$ .
  - **Multiply** all the factors that contain  $X_{h_i}$  to get new factor  $g_j$ .
  - **Sum out** the variable  $X_{h_j}$  from the factor  $g_j$ .
- Multiply the remaining factors.
- Normalize the resulting factor.

## Example of VEA

Given a portion of the Holmes network below, calculate  $P(B|\neg a)$  using the variable elimination algorithm.

Eliminate the hidden variables in reverse alphabetical order.



## Example of VEA

- ▶ B is the query variable, and A is the evidence variable.
- ▶ To calculate  $P(B|\neg a)$ , it suffices to compute the joint distribution of  $P(B, \neg a)$
- Step 0: Define all the factors.
- ▶ Step 1: Restrict A = false.
- ightharpoonup Step 2: Sum out E and W.
- Step 3: Multiply remaining factors.
- Step 4: Normalizing the resulting factor.

# More Efficiency

The joint distribution can be written as:

$$P(B \land \neg a) = \sum_{e} \sum_{w} P(B)p(e)P(\neg a|B \land e)P(w| \land \neg a)$$

Simplify this term:

$$P(B \wedge \neg a) = P(B)(\sum_{e} p(e)P(\neg a|B \wedge e))(\sum_{w} P(w| \wedge \neg a))$$

## Define factors

$$P(B), P(E), P(A|B \land E), P(W|A)$$
  
  $\to f_1(B), f_2(E), f_3(A, B, E), f_4(W, A)$ 

r	(D)	
T.	1 6	•
/ 1	(D)	

B	val
t	0.3
f	0.7

# $f_2(E)$ :

L	vai
t	0.1
f	0.9

## $f_3(A,B,E)$ :

J3(A,D,E).				
A	B	E	val	
t	t	t	8.0	
t	t	f	0.7	
t	f	t	0.2	
t	f	f	0.1	
f	t	t	0.2	
f	t	f	0.3	
f	f	t	8.0	
f	f	f	0.9	

## $f_4(W,A)$ :

J4(**, 21)·				
W	A	val		
t	t	8.0		
t	f	0.4		
f	t	0.2		
f	f	0.6		

### Restrict factors

$$f_1(B), f_2(E), f_3(\neg a, B, E), f_4(W, \neg a)$$
  
 $\to f_1(B), f_2(E), f_5(B, E), f_6(W)$ 

# $f_1(B)$ :

B	val	
t	0.3	
f	0.7	

## $f_2(E)$ :

E	val
t	0.1
f	0.9

### $f_5(B,E)$ :

$J_{\mathfrak{I}}(\mathcal{L})$	$, L_{j}$ .	
B	E	val
t	t	0.2
t	f	0.3
f	t	8.0
f	f	0.9

### $f_6(W)$ :

16 (VV	):
W	val
t	0.4
f	0.6

### Sum out E and W

$$f_1(B), f_2(E), f_5(B, E), f_6(W)$$
  
 $\rightarrow f_1(B), f_2(E), f_5(B, E), f_7() = 1.0$ 

$f_1(B)$ :	
B	val
t	0.3
f	0.7

$f_2(E)$ :	
E	val
t	0.1
f	0.9

$f_5(B$	,E):	
B	E	val
t	t	0.2
t	f	0.3
f	t	8.0
f	f	0.9

f(D)

$f_7()$ :
val
1.0

### Sum out E and W

$$f_1(B), f_2(E), f_5(B, E), f_7() = 1.0$$
  
 $\rightarrow f_1(B), f_8(B, E), f_7() = 1.0$ 

	$f_8(B$	B, E)	$= f_5(B, E) \times f_2(E):$
	B	E	val
ĺ	t	t	0.2 * 0.1 = 0.02 0.3 * 0.9 = 0.27 0.8 * 0.1 = 0.08
	t	f	0.3 * 0.9 = 0.27
	f	t	0.8 * 0.1 = 0.08
	f	f	0.9 * 0.9 = 0.81

$f_7()$ :
val
1.0

### Sum out E and W

$$f_1(B), f_8(B, E), f_7() = 1.0$$
  
 $\rightarrow f_1(B), f_9(B), f_7() = 1.0$ 

$f_1(B$	):
B	val
t	0.3
f	0.7

$$\begin{array}{c|cccc} f_9(B) & = & \sum_E f_8(B,E) \text{:} \\ \hline B & \text{val} \\ \hline t & 0.02 + 0.27 = 0.29 \\ f & 0.81 + 0.08 = 0.89 \\ \hline \end{array}$$

$f_7()$ :
val
1.0

# Multiply all factors

$$f_1(B), f_9(B), f_7() = 1.0$$
  
  $\to f_{10}(B)$ 

$$f_{10}(B) = f_9(B) \times f_1(B) \times f_7()$$
:

B	val	
t	0.29 * 0.3 = 0.087	
f	0.89 * 0.7 = 0.623	

### Normalization

#### Normalization for the factor:

$$p(B|\neg a) = f_{10}(B)$$
:

	I (   10 )
B	val
t	0.087 / (0.087 + 0.623) = 0.1225
f	0.623 / (0.087 + 0.623) = 0.8775

Learning Goals

Why Use the Variable Elimination Algorithm

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## Effect of The Elimination Ordering

In general, VEA is exponential in space and time.

The complexity of VEA depends on:

- The size of the CPT in the Bayesian network.
- ▶ The size of the largest factor during algorithm execution.

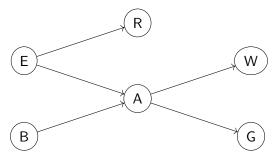
Effect of the elimination ordering on algorithm complexity:

- Every order yields a valid algorithm.
- Different orderings yields different intermediate factors.

Suppose that we want to calculate P(G). What factors do we produce if we

- ▶ Eliminate  $R \to W \to E \to B \to A$ ?
- ▶ Eliminate  $A \rightarrow B \rightarrow E \rightarrow R \rightarrow W$ ?

Which ordering leads to worse complexity for VEA?



Eliminate  $R \to W \to E \to B \to A$ ?

$$f_1(E), f_2(E, R), f_3(B), f_4(E, B, A), f_5(W, A), f_6(G, A)$$

Eliminate  $R \to W \to E \to B \to A$ ?

$$f_1(E), f_2(E, R), f_3(B), f_4(E, B, A), f_5(W, A), f_6(G, A)$$

- ►  $f_2(E,R) \to f_7(E)$ : 1 \* 2 = 2 ops
- $f_5(W,A) \to f_8(A)$ : 1 \* 2 = 2 ops
- $f_1(E)f_7(E)f_4(E,B,A) \to f_9(B,A)$ : (4 + 1) \* 4 = 20 ops
- $ightharpoonup f_9(B,A)f_8(A) o f_{10}(A)$ : (2 + 1) \* 2 = 6 ops
- $ightharpoonup f_{10}(A)f_6(G,A) \to f_{11}(G)$ : (2 + 1) \* 2 = 6 ops
- ► Total: 36 ops including additions and multiplication

Eliminate  $A \to B \to E \to R \to W$ 

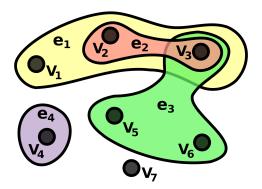
$$f_1(E), f_2(E, R), f_3(B), f_4(E, B, A), f_5(W, A), f_6(G, A)$$

Eliminate  $A \to B \to E \to R \to W$ 

$$f_1(E), f_2(E, R), f_3(B), f_4(E, B, A), f_5(W, A), f_6(G, A)$$

- $f_4(E,B,A)f_5(W,A)f_6(G,A) \to f_7(E,B,W,G)$ : (4 + 1) \* 16 = 80 ops
- $ightharpoonup f_7(E,B,W,G)f_3(B) o f_8(E,W,G)$ : (2 + 1) \* 8 = 24 ops
- $f_1(E)f_8(E,W,G)f_2(E,R) \to f_9(W,G,R)$ : (4 + 1) \* 8 = 24 ops
- $f_9(W,G,R) \to f_{10}(W,G)$ : 1 \* 4 = 4 ops
- $ightharpoonup f_{10}(W,G) o f_{11}(G)$ : 1 \* 2 = 2 ops
- ► Total: 134 ops including additions and multiplication

# Hypergraph



- ▶ A generalization graph, which contains vertices and a set of hyperedges. A hyperedge connects multiple vertices.
- A hyperedge is a clique of several vertices.
- ► A Bayesian Network can be seen as a hypergraph, where each factor is basically a hyperedge.

### Elimination Width

▶ Given an ordering  $\pi$  of the variables and an initial hypergraph  $\mathcal{H}$ , eliminating these variables yields a sequence of hypergraphs:

$$\mathcal{H} \to H_0, H_1, \cdots, H_n$$

- $\blacktriangleright$  where  $H_n$  contains only one vertex
- ▶ The elimination width is the maximum size of any hyperedge in any of the hypergraphs  $H_0, H_1, \dots, H_n$ .
- ▶ The elimination width is 4 for the hypergraph  $f_7(E, B, W, G)$ .

### Elimination Width

- ▶ If the elimination width of an ordering  $\pi$  is k, then the complexity of VE using that order is  $2^{O(k)}$
- Elimination width k means that at some stage in the elimination process, a factor involving k variables was generated.
- ▶ That factor will require  $2^{O(k)}$  space to store.
- ▶ And it will require  $2^{O(k)}$  operations to process.
- ► The time and space complexity of VE are both exponential w.r.t elimination width.

#### Tree Width

- ▶ Given a hypergraph  $\mathcal{H}$  with vertices  $\{X_1, X_2, \cdots, X_n\}$  the tree width of  $\mathcal{H}$  is the MINIMUM elimination width of any orderings  $\pi$  of these variables.
- ▶ Thus VE has best case complexity of  $2^{O(\omega)}$  where  $\omega$  is the tree width of the initial Bayes Net.
- In the worst case the treewidth can be equal to the number of variables.

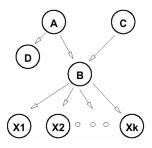
#### Tree Width

- VE complexity is exponential in the treewidth.
- Finding an ordering that has an elimination width equal to treewidth is NP-hard.
- Heuristics are used to find good orderings with low elimination widths.
- ▶ In practice, this can be very successful. Elimination widths can be often relatively small, 8-10 even when the network has 1000s of variables.
- ► Thus VE can be much more efficient than simply summing up the probability of all the possible events.

# Finding Good Orderings

- ► A **polytree** is a single-connected network in which there is at most one undirected path between any two nodes.
- A node can have multiple parents, but they have no cycles.
- Good orderings are easy to find for polytrees.
  - At each stage, eliminate a singly connected node.
  - Because we have a polytree, we are assured that a singly connected node will always exist.
  - ► The size of the factors never increases.

# Finding Good Orderings



- ► Treewidth of the polytree is equal to the maximum number of parents among all the nodes.
- ► Eliminating singly connected nodes allows VE to run the time linear in size of the network.
  - e.g. Eliminating D, A, C, X1, etc.
  - ▶ Results: No factor ever larger than original CPTs.

### Learning Goals

Why Use the Variable Elimination Algorithm

The Variable Elimination Algorithm

Factors Affecting the Complexity of VEA

Approximate Inference

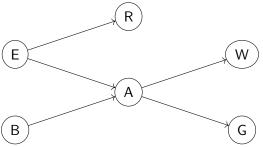
Revisiting Learning Goals

## Approximate Inference

We cannot make exact inferences in many cases where the graph is too large. Instead, we use approximate inferences with sampling to understand the distribution of different variables.

- Forward Sampling
- Rejection Sampling

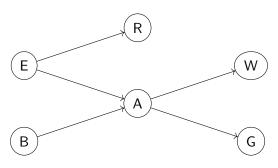
Forward Sampling



### Estimating p(G):

- ightharpoonup Loop for i in  $1 \cdots n$ , do
  - ▶ Sample  $e_i \sim P(E)$
  - ▶ Sample  $b_i \sim P(B)$
  - Sample  $a_i \sim P(A|E=e,B=b)$
  - ▶ Sample  $g_i \sim p(G|A=a)$
- $ightharpoonup p(G = True) = \frac{\sum_i g_i}{n}$

# Rejection Sampling



### Estimating $p(G|\neg b)$

- ightharpoonup Loop for i in  $1 \cdots n$ , do
  - ► Sample  $e_i, b_i, a_i, g_i$  as before.
  - Reject  $b_i$  = True, only take accepted  $\tilde{g}_i$ .
- $p(G = True) = \frac{\sum_{i} \tilde{g}_{i}}{n}$

## Revisiting Learning Goals

- Explain how we can perform probabilistic inference more efficiently using the variable elimination algorithm.
- ▶ Define factors. Manipulate factors using operations restrict, sum out, multiply and normalize.
- Describe/trace/implement the variable elimination algorithm for calculating a prior or a posterior probability given a Bayesian network.
- Explain how the elimination ordering affects the complexity of the variable elimination algorithm.
- Know about approximate statistical inference.