

**Reading:**  
**Chapters 5&6 of Koller&Friedman**

# BN Semantics 3 – Now it's personal! Exact inference & Variable elimination

Graphical Models – 10708

Carlos Guestrin

Carnegie Mellon University

September 21<sup>st</sup>, 2005

# Announcements



- Let's talk about the Waiting List
  - Who wants to be registered?
  - Send us an email ASAP if you want in!!!!

# Perfect maps (P-maps)

- I-maps are not unique and often not simple enough
- Define “simplest”  $G$  that is I-map for  $P$ 
  - A BN structure  $G$  is a **perfect map** for a distribution  $P$  if  $I(P) = I(G)$
- Our goal:
  - Find a perfect map!
  - Must address equivalent BNs

# Inexistence of P-maps 1

- XOR (this is a hint for the homework)

$A, B, C$  binary :  $C = A \text{ XOR } B$

$(A \perp B)$

$A, B$  uniform (50/50)

$(A \perp C)$

$(B \perp C)$

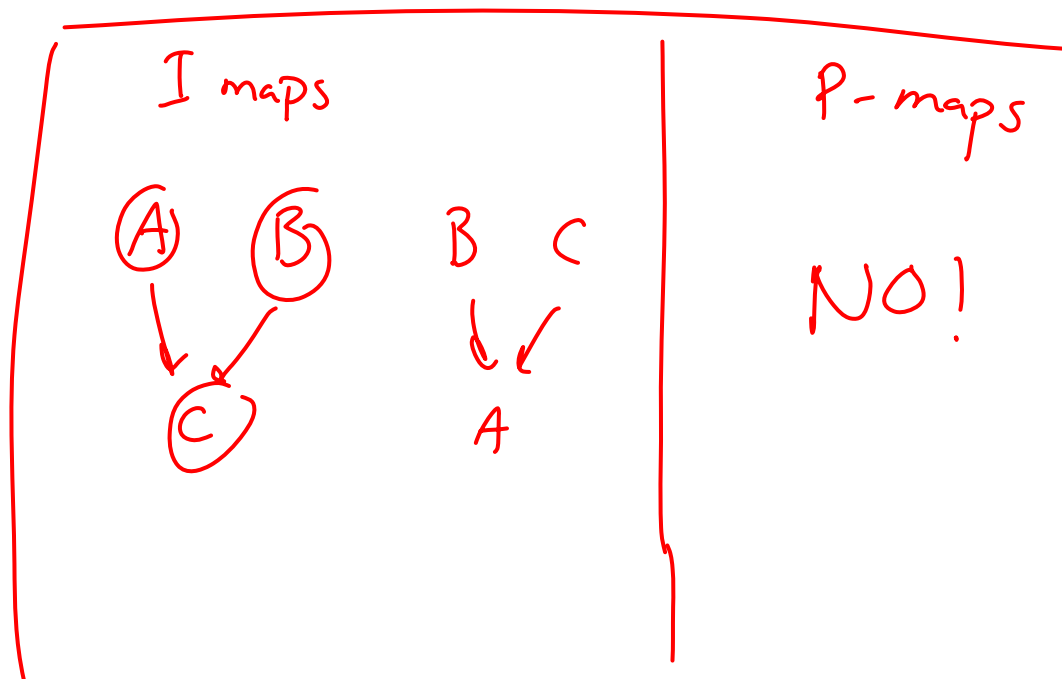
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not ind:

$(A \perp B | C)$

$(A \perp C | B)$

$(B \perp C | A)$

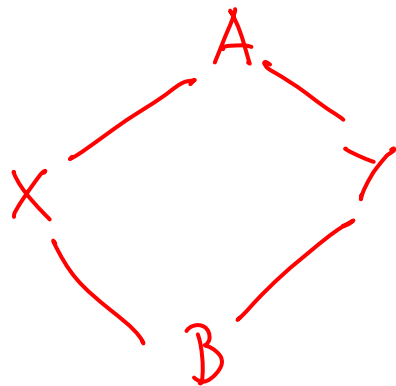


# Inexistence of P-maps 2

- (Slightly un-PC) swinging couples example

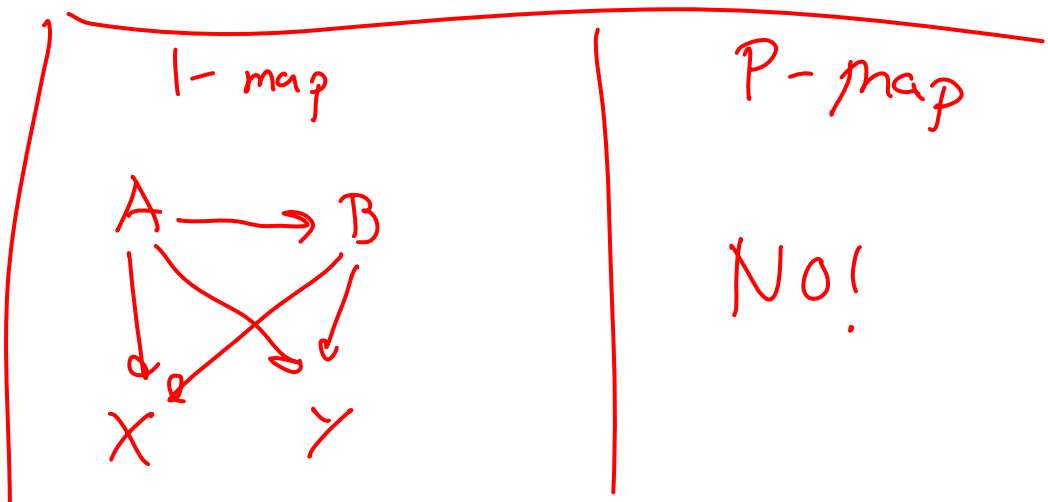
men  $A, B$

women  $X, Y$



$(A \perp B \mid X, Y)$

$(X \perp Y \mid A, B)$



# Obtaining a P-map

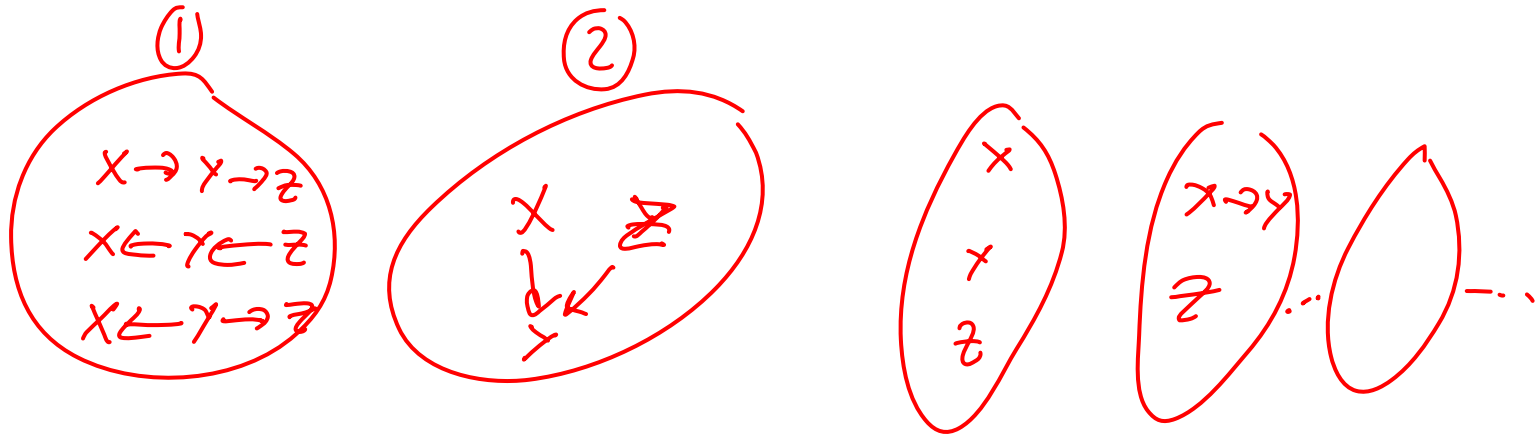
- Given the independence assertions that are true for  $P$
- Assume that there exists a perfect map  $G^*$ 
  - Want to find  $G^*$
- Many structures may encode same independencies as  $G^*$ , when are we done?
  - Find all equivalent structures simultaneously!

# I-Equivalence

$$x \rightarrow y \rightarrow z$$

$$x \leftarrow y \rightarrow z$$

- Two graphs  $G_1$  and  $G_2$  are **I-equivalent** if  $I(G_1) = I(G_2)$
- Equivalence class** of BN structures
  - Mutually-exclusive and exhaustive partition of graphs



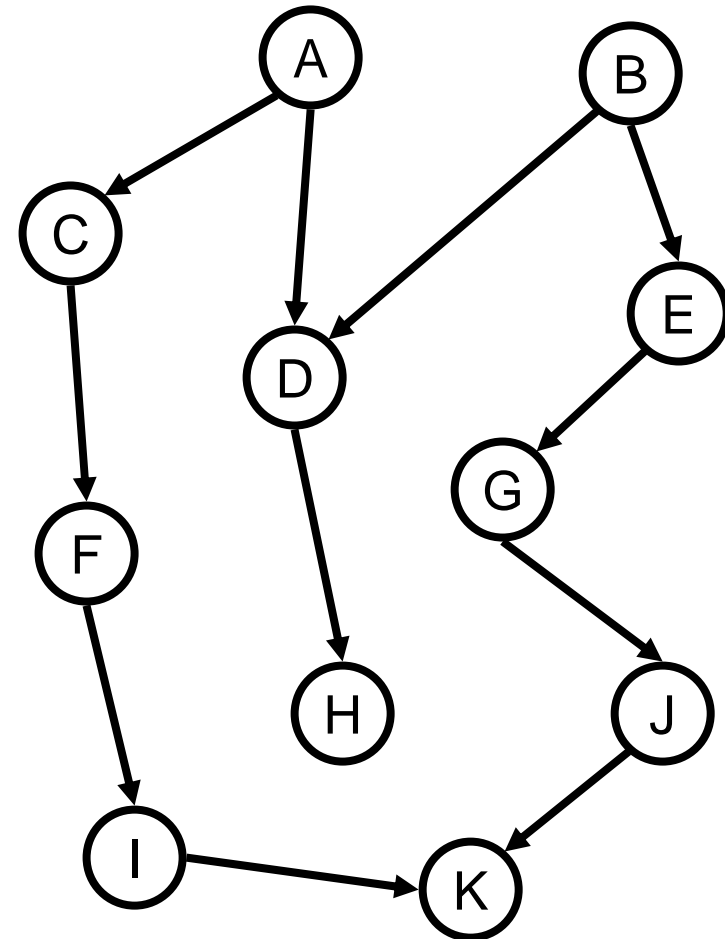
- How do we characterize these equivalence classes?

# Skeleton of a BN

- **Skeleton** of a BN structure  $G$  is an **undirected graph** over the same variables that has an edge  $X-Y$  for every  $X \rightarrow Y$  or  $Y \rightarrow X$  in  $G$

- (Little) **Lemma**: Two I-equivalent BN structures must have the same skeleton

*counter example*

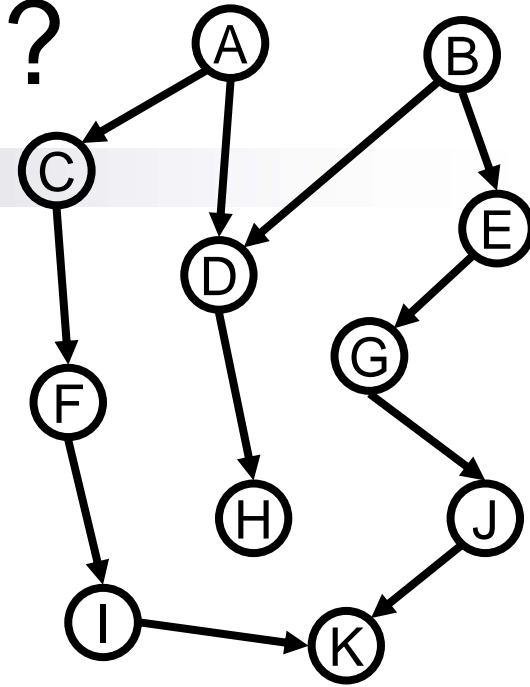




# What about V-structures?

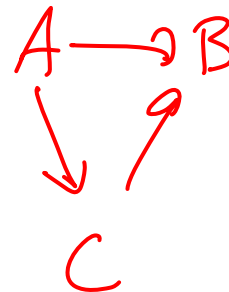
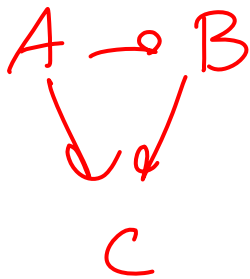
- V-structures are key property of BN structure

- **Theorem:** If  $G_1$  and  $G_2$  have the same skeleton and V-structures, then  $G_1$  and  $G_2$  are I-equivalent



# Same V-structures not necessary

- **Theorem:** If  $G_1$  and  $G_2$  have the same skeleton and V-structures, then  $G_1$  and  $G_2$  are I-equivalent
- Though sufficient, same V-structures not necessary



V-structures  $A \rightarrow C \leftarrow B$

$A \rightarrow B \leftarrow C$

diff. V-structures  
same indep. !

V-structures  
sufficient not  
necessary

# Immoralities & I-Equivalence

- Key concept not V-structures, but “immoralities” (unmarried parents 😊)
  - $X \rightarrow Z \leftarrow Y$ , with no arrow between X and Y
  - Important pattern: X and Y independent given their parents, but not given Z
  - (If edge exists between X and Y, we have *covered* the V-structure)
- **Theorem:**  $G_1$  and  $G_2$  have the same skeleton and immoralities if and only if  $G_1$  and  $G_2$  are I-equivalent

# Obtaining a P-map

- Given the independence assertions that are true for  $P$ 
  - Obtain skeleton
  - Obtain immoralities
- From skeleton and immoralities, obtain every (and any) BN structure from the equivalence class

# Identifying the skeleton 1



- When is there an edge between  $X$  and  $Y$ ?
  
  
  
  
  
  
  
  
  
  
- When is there no edge between  $X$  and  $Y$ ?

# Identifying the skeleton 2

- Assume  $d$  is max number of parents ( $d$  could be  $n$ )
- For each  $X_i$  and  $X_j$ 
  - $E_{ij} \leftarrow \text{true}$
  - For each  $\mathbf{U} \subseteq \mathbf{X} - \{X_i, X_j\}$ ,  $|\mathbf{U}| \leq 2d$ 
    - Is  $(X_i \perp X_j \mid \mathbf{U})$  ?
      - $E_{ij} \leftarrow \text{true}$
  - If  $E_{ij}$  is true
    - Add edge  $X - Y$  to skeleton

# Identifying immoralities

- Consider  $X - Z - Y$  in skeleton, when should it be an immorality?
- Must be  $X \rightarrow Z \leftarrow Y$  (immorality):
  - When  $X$  and  $Y$  are **never independent** given  $\mathbf{U}$ , if  $Z \in \mathbf{U}$
- Must **not** be  $X \rightarrow Z \leftarrow Y$  (not immorality):
  - When there exists  $\mathbf{U}$  with  $Z \in \mathbf{U}$ , such that  $X$  and  $Y$  are **independent** given  $\mathbf{U}$

# From immoralities and skeleton to BN structures

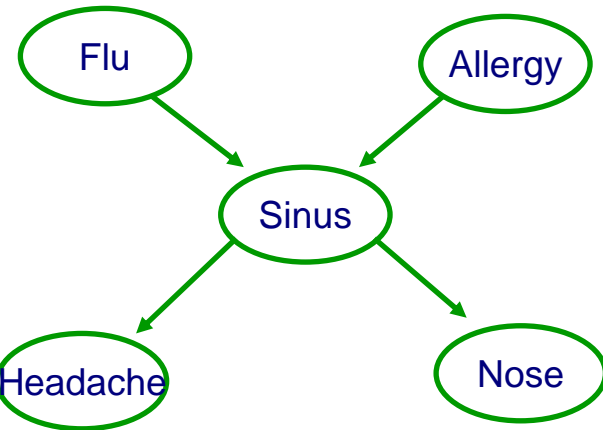
- Representing BN equivalence class as a **partially-directed acyclic graph (PDAG)**
  
- **Immoralities force direction on other BN edges**
- Full (polynomial-time) procedure described in reading



# What you need to know about BN semantics

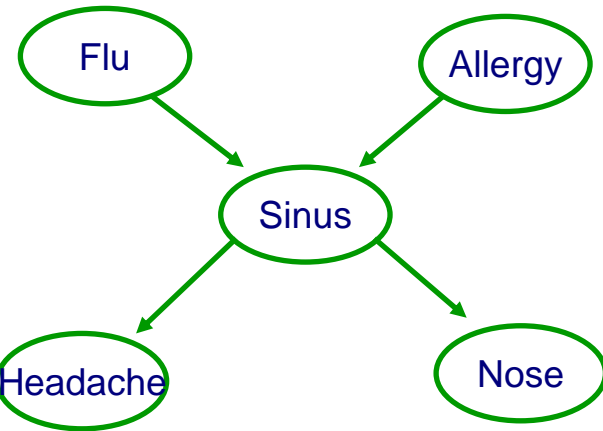
- Definition of a BN
- Local Markov assumption
- The representation theorem:  $G$  is an I-map for  $P$  if and only if  $P$  factorizes according to  $G$
- d-separation – sound and complete procedure for finding independencies
  - (almost) all independencies can be read directly from graph without looking at CPTs
- Minimal I-map
  - every  $P$  has one, but usually many
- Perfect map
  - better choice for BN structure
  - not every  $P$  has one
  - can find one (if it exists) by considering I-equivalence
  - Two structures are I-equivalent if they have same skeleton and immoralities

# Inference in graphical models: Typical queries 1



- Conditional probabilities
  - Distribution of some var(s). given evidence

# Inference in graphical models: Typical queries 2 – Maximization



- Most probable explanation (MPE)
  - Most likely assignment to all hidden vars given evidence
- Maximum a posteriori (MAP)
  - Most likely assignment to some var(s) given evidence

# Complexity of conditional probability queries 1

- How hard is it to compute  $P(X|\mathbf{E}=\mathbf{e})$ ?


Reduction – 3-SAT

$$(\bar{X}_1 \vee X_2 \vee X_3) \wedge (\bar{X}_2 \vee X_3 \vee X_4) \wedge \dots$$

# Complexity of conditional probability queries 2

- How hard is it to compute  $P(X|\mathbf{E}=\mathbf{e})$ ?
  - At least NP-hard, but even harder!

# Inference is #P-hard, hopeless?



- Exploit structure!
- Inference is hard in general, but easy for many (real-world relevant) BN structures

# What about the maximization problems?

## First, most probable explanation (MPE)

- What's the complexity of MPE?

# What about maximum a posteriori?



- At least, as hard as MPE!
  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
- Actually, much harder!!! NP<sup>PP</sup>-complete!



# Can we exploit structure for maximization?



- For MPE

- For MAP

# Exact inference is hard, what about approximate inference?

- Must define approximation criterion!
- Relative error of  $\varepsilon > 0$
  
- Absolute error of  $\varepsilon > 0$



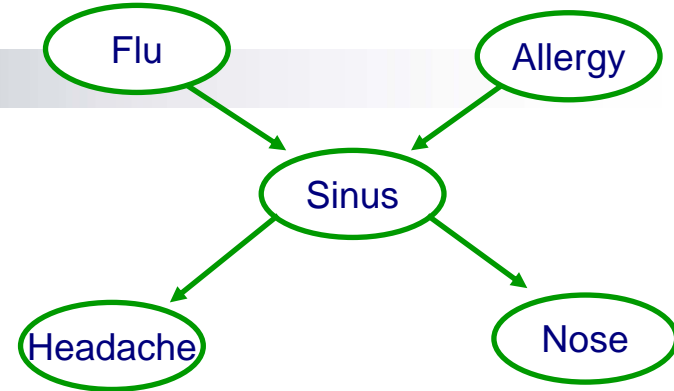
# Inference in BNs hopeless?



- In general, yes!
  - Even approximate!
  
- In practice
  - Exploit structure
  - Many effective approximation algorithms (some with guarantees)
  
- For now, we'll talk about exact inference
  - Approximate inference later this semester

# General probabilistic inference

■ Query:  $P(X | e)$



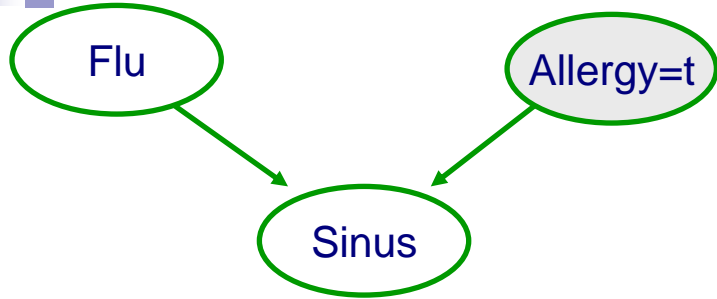
■ Using Bayes rule:

$$P(X | e) = \frac{P(X, e)}{P(e)}$$

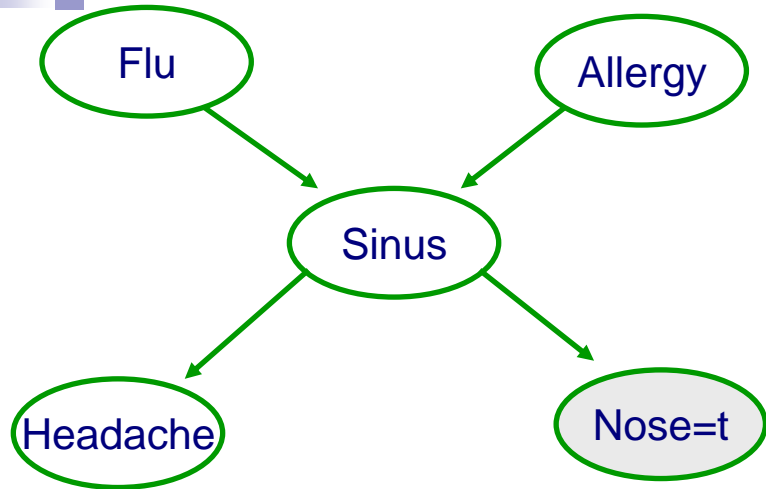
■ Normalization:

$$P(X | e) \propto P(X, e)$$

# Marginalization

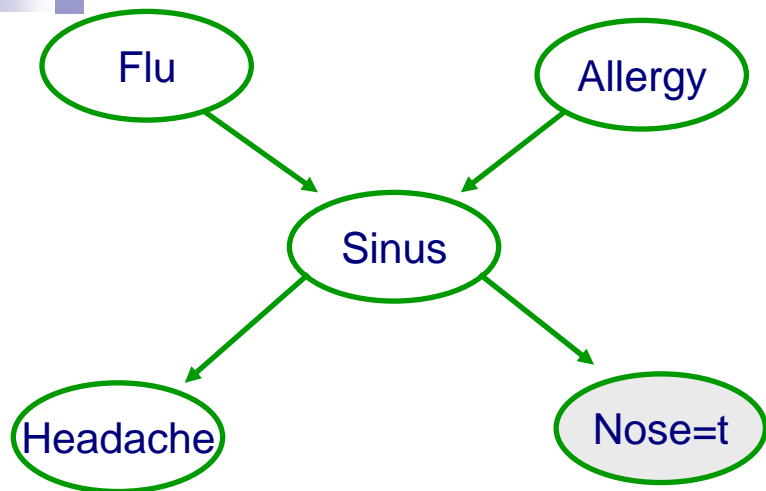


# Probabilistic inference example



**Inference seems exponential in number of variables!**

# Fast probabilistic inference example – Variable elimination



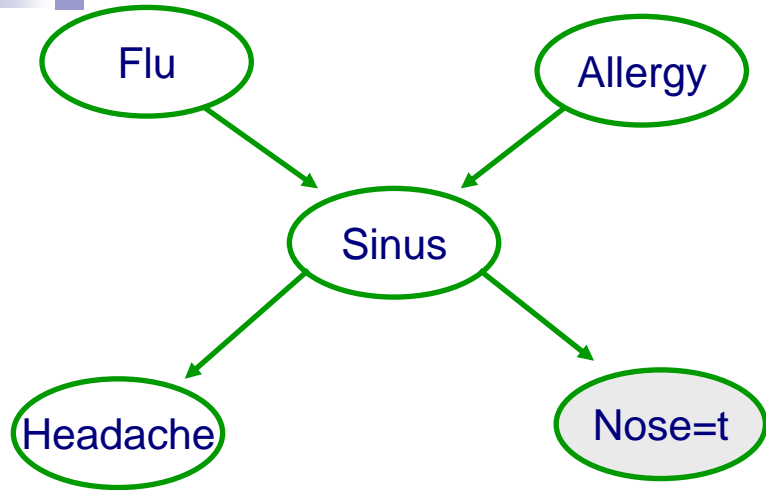
**(Potential for) Exponential reduction in computation!**



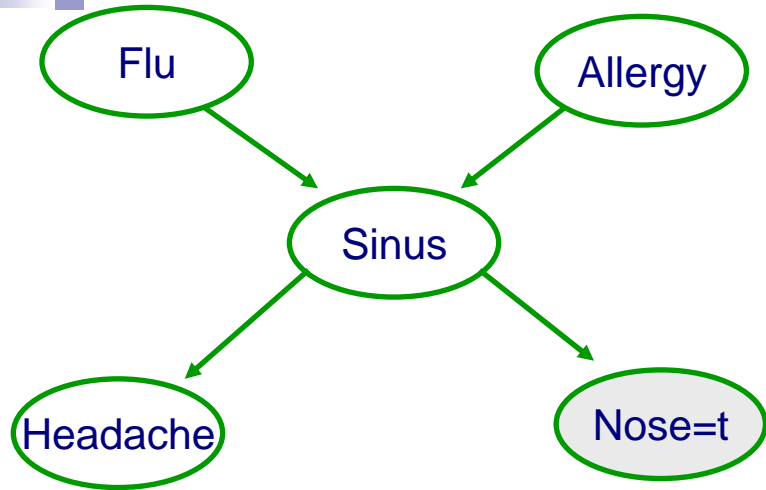
# Understanding variable elimination – Exploiting distributivity



# Understanding variable elimination – Order can make a HUGE difference

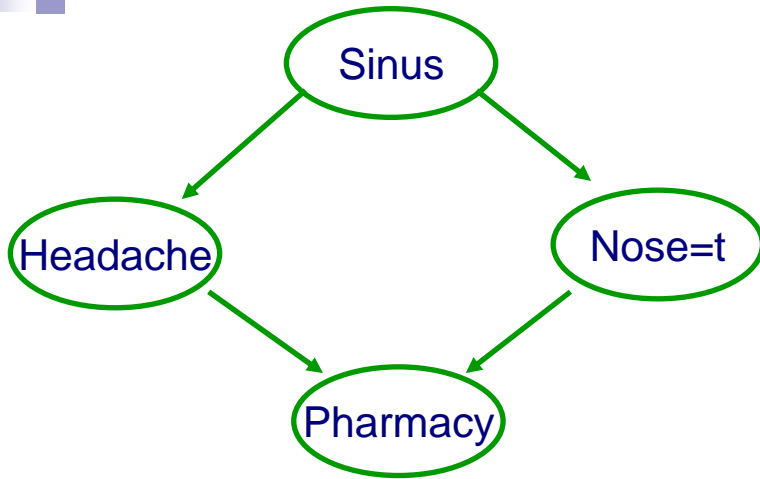


# Understanding variable elimination – Intermediate results

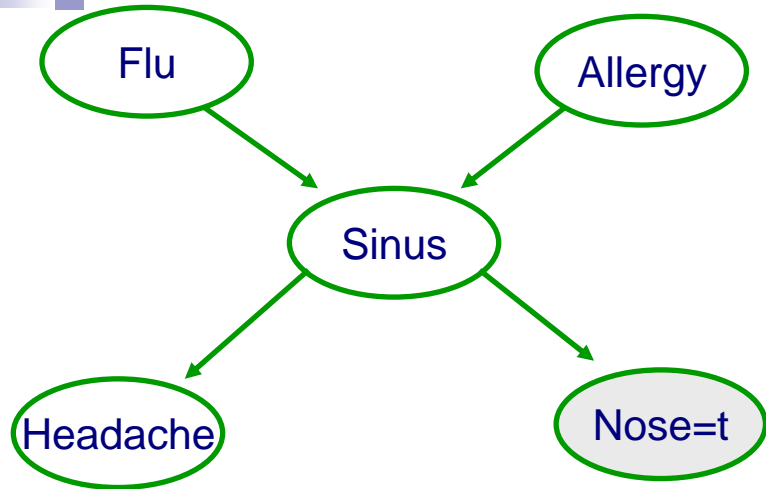


**Intermediate results are probability distributions**

# Understanding variable elimination – Another example



# Pruning irrelevant variables



**Prune all non-ancestors of query variables**  
**More generally:** prune all nodes not on active trail between evidence and query vars

# Variable elimination algorithm

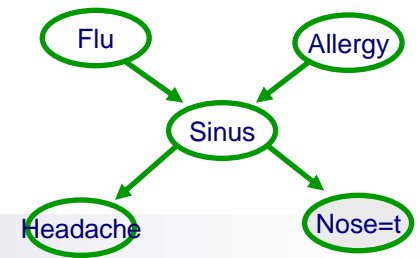
- Given a BN and a query  $P(X|e) \propto P(X,e)$
- Instantiate evidence  $e$
- Prune non-active vars for  $\{X,e\}$
- Choose an ordering on variables, e.g.,  $X_1, \dots, X_n$
- Initial *factors*  $\{f_1, \dots, f_n\}$ :  $f_i = P(X_i | \mathbf{Pa}_{X_i})$  (CPT for  $X_i$ )
- For  $i = 1$  to  $n$ , If  $X_i \notin \{X,e\}$ 
  - Collect factors  $f_1, \dots, f_k$  that include  $X_i$
  - Generate a new factor by eliminating  $X_i$  from these factors

**IMPORTANT!!!**

$$g = \sum_{X_i} \prod_{j=1}^k f_j$$

- Variable  $X_i$  has been eliminated!
- Normalize  $P(X,e)$  to obtain  $P(X|e)$

# Operations on factors



$$g = \sum_{X_i} \prod_{j=1}^k f_j$$

**Multiplication:**

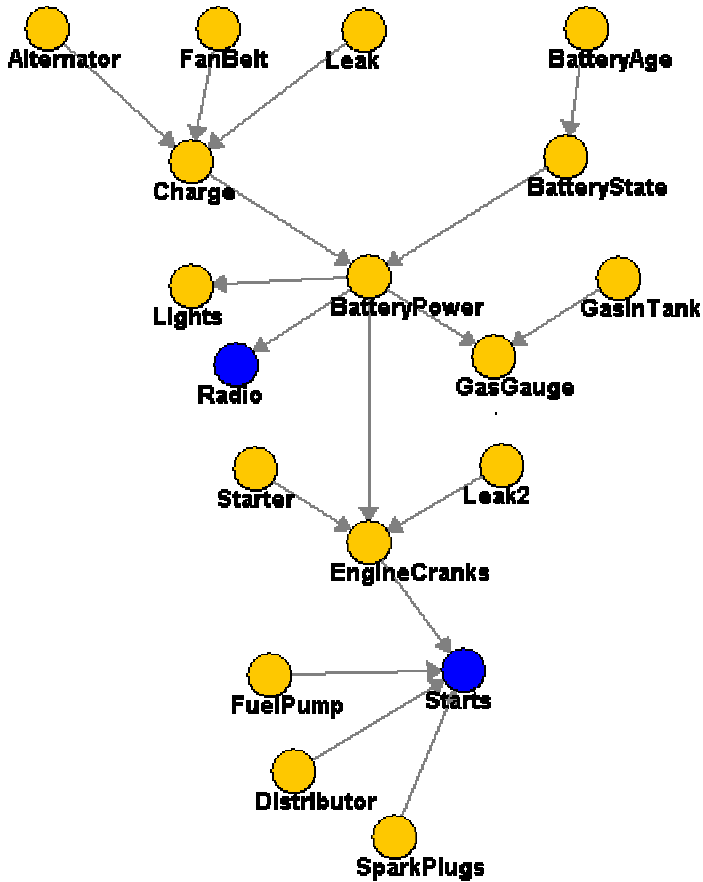
**Marginalization:**

# Complexity of variable elimination – (Poly)-tree graphs

## Variable elimination order:

Start from “leaves” in –

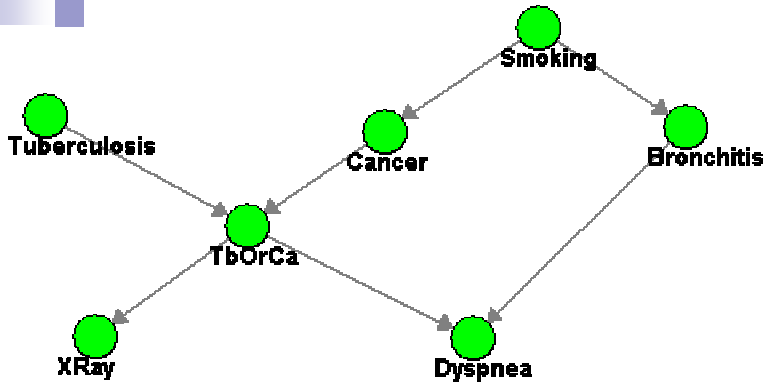
- Start from skeleton!
- Choose a “root”, any node
- Find topological order for root
- Eliminate variables in reverse order



**Linear in CPT sizes!!! (versus exponential)**

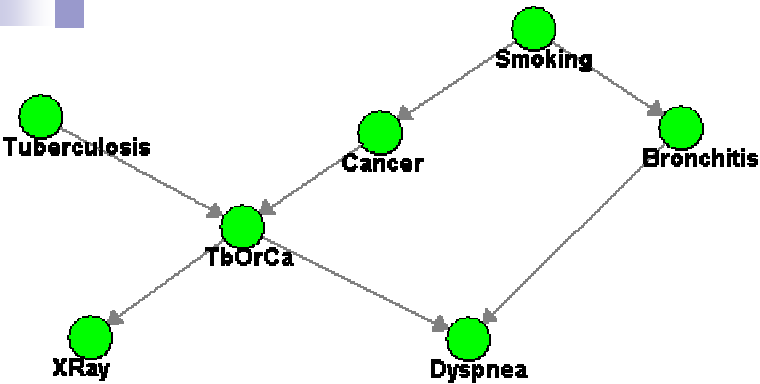


# Complexity of variable elimination – Graphs with loops



**Exponential in number of variables in largest factor generated**

# Complexity of variable elimination – Tree-width



## Moralize graph:

Connect parents  
into a clique and  
remove edge directions

**Complexity of VE elimination:**  
("Only") exponential in tree-width

# Example: Large tree-width with small number of parents

Compact representation  $\nRightarrow$  Easy inference 😞

# Choosing an elimination order

- Choosing best order is NP-complete
  - Reduction from MAX-Clique
- Many good heuristics (some with guarantees)
- Ultimately, can't beat NP-hardness of inference
  - Even optimal order can lead to exponential variable elimination computation
- In practice
  - Variable elimination often very effective
  - Many (many many) approximate inference approaches available when variable elimination too expensive