Readings: K&F 3.1, 3.2, 3.3, 3.4.1

# Bayesian Network Representation

Lecture 2 – Mar 30, 2011
CSE 515, Statistical Methods, Spring 2011

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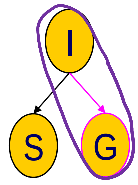
## Last time & today

- Last time
  - Probability theory
  - Conditional independence
  - Conditional parameterization
- Today
  - Naïve Bayes model
  - Definition of the Bayesian network (BN)
  - Independence properties encoded in BN graphs
  - From distributions to BN graphs

# Conditional parameterization

- S = SAT score, Val(S) = $\{s^0, s^1\}$
- I = Intelligence, Val(I) = $\{i^0, i^1\}$
- G = Grade, Val(G) = $\{g^0, g^1, g^2\}$
- Assume that G and S are independent given I




- P(I,S,G) = $p(I)p(S|I)p(G|I,S) = p(I)p(S|I)p(G|I)$

**Joint parameterization**

**P(I,S)**

| I | S | P(I,S) |
|---|---|---|
| $i^0$ | $s^0$ | 0.665 |
| $i^0$ | $s^1$ | 0.035 |
| $i^1$ | $s^0$ | 0.06 |
| $i^1$ | $s^1$ | 0.24 |

P(I,S,G)

| I | S | G | P(I,S,G) |
|---|---|---|---|
| $i^0$ | $s^0$ | $g^0$ | 0.425 |
| $i^0$ | $s^0$ | $g^1$ | 0.125 |
| $i^1$ | $s^1$ | $g^2$ | 0.01 |
| : | : | : | : |

3 parameters
11 parameters

**Conditional parameterization**

P(I)

| I | |
|---|---|
| $i^0$ | $i^1$ |
| 0.7 | 0.3 |

P(S|I)

| I | S | |
|---|---|---|
| | $s^0$ | $s^1$ |
| $i^0$ | 0.95 | 0.05 |
| $i^1$ | 0.2 | 0.8 |

P(G|I)

| I | G | | |
|---|---|---|---|
| | $g^0$ | $g^1$ | $g^2$ |
| $i^0$ | 0.75 | 0.05 | 0.2 |
| $i^1$ | 0.2 | 0.3 | 0.5 |

modularity

3 parameters
7 parameters



# Naïve Bayes model

- Class variable C, Val(C) = $\{c_1,\dots,c_k\}$
- Evidence variables $X_1,\dots,X_n$
- Naïve Bayes assumption: evidence variables are conditionally independent given C $(X_i \perp X_j \mid C)$ $i \neq j$

$$P(C, X_1,\dots, X_n) = p(C)p(X_1|C)p(X_2|C,X_1) \cdots p(X_n|C,X_1 \cdots X_{n-1}) = p(C)\prod_i p(X_i|C)$$

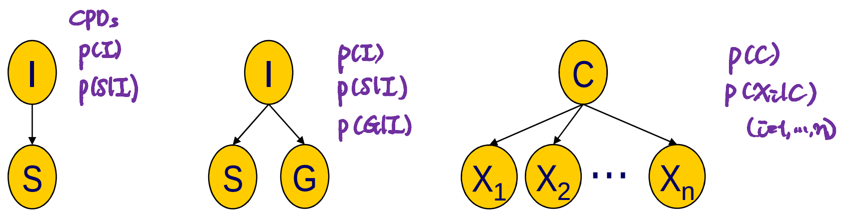
- Applications in medical diagnosis, text classification
- Used as a classifier:
  - Given $\{x_1,\dots,x_n\}$ on evidence variables $X_1,\dots,X_n$, predict the value on C :

$$\frac{P(C=c_1 \mid x_1,\dots,x_n)}{P(C=c_2 \mid x_1,\dots,x_n)} = \frac{p(C_1,x_1,\dots,x_n)}{p(C_2,x_1,\dots,x_n)} = \frac{p(C=C_1)}{p(C=C_2)} \prod_i \left\{\frac{p(x_i|C=C_1)}{p(x_i|C=C_2)}\right\}$$

- Problem: Double counting correlated evidence $(X_i \perp X_j \mid C) \rightarrow$ strong assumption $i \neq j$

# Bayesian network (informal)

- Directed acyclic graph (DAG) G
  - Nodes represent random variables
  - Edges represent direct influences between random variables
- Local probability models (conditional parameterization)
  - Conditional probability distributions (CPDs)
- Here are the networks we have been discussing so far…



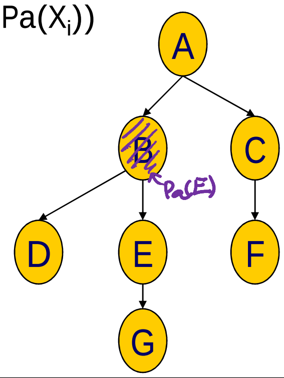

Example 1 Example 2 Naïve Bayes



# Bayesian network structure

- Directed acyclic graph (DAG) G
  - Nodes $X_1,\ldots,X_n$ represent random variables
- G encodes the following set of independence assumptions (called, local independencies)
  - $X_i$ is independent of its non-descendants given its parents
  - Formally: $(X_i \perp \mathrm{NonDesc}(X_i) \mid \mathrm{Pa}(X_i))$
  - Denoted by $I_L(G)$

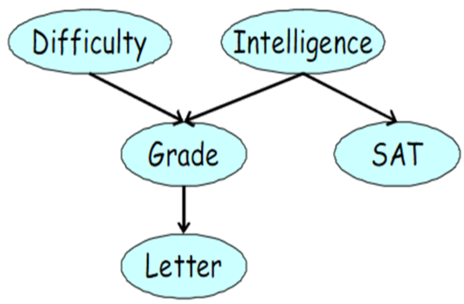
$E \perp \{A,C,D,F\} \mid B$ ⬅



# The *Student* example

- Course difficulty (**D**), Val(D) = {easy, hard}
- Intelligence (**I**) , Val (I) = {high, low}
- Grade (**G**), Val (G) = {A, B, C}
- Quality of the rec. letter (**L**), Val(L) = {strong, weak}
- SAT (**S**), Val (S) = {high, low}

**Graph $G_{student}$**




Local independencies $I_L(G_{student})$

$\{X_i \perp ND(X_i) \mid Pa(X_i)\}$

$D \perp I$, $D \perp S$,

$G \perp S \mid I, D$,

$L \perp I, D, S \mid G$,

$S \perp D, G, L \mid I$



# The *Student* Bayesian network

- Joint distribution
  - P(I,D,G,S,L) = $P(I)\underbrace{P(D|I)}_{P(D)}\, P(G|I,D)\, \underbrace{P(S|I,\cancel{D},\cancel{G})}_{P(S|I)}\, \underbrace{P(L|\cancel{I},\cancel{D},G,\cancel{S})}_{P(L|G)}$

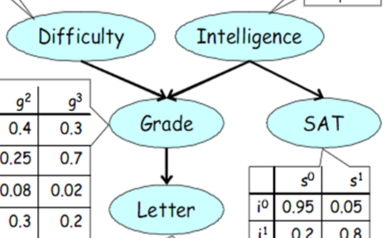
$S \perp D,G,L \mid I$ $\qquad$ $L \perp I,D,S \mid G$

$= \prod_{X \in \{I,D,S,G,L\}} P(X \mid Pa(X))$

↳ chain rule of B.N.

| $d^0$ | $d^1$ |
|---|---|
| 0.6 | 0.4 |

| $i^0$ | $i^1$ |
|---|---|
| 0.7 | 0.3 |




| | $g^1$ | $g^2$ | $g^3$ |
|---|---|---|---|
| $i^0,d^0$ | 0.3 | 0.4 | 0.3 |
| $i^0,d^1$ | 0.05 | 0.25 | 0.7 |
| $i^1,d^0$ | 0.9 | 0.08 | 0.02 |
| $i^1,d^1$ | 0.5 | 0.3 | 0.2 |

| | $s^0$ | $s^1$ |
|---|---|---|
| $i^0$ | 0.95 | 0.05 |
| $i^1$ | 0.2 | 0.8 |

| | $l^0$ | $l^1$ |
|---|---|---|
| $g^1$ | 0.1 | 0.9 |
| $g^2$ | 0.4 | 0.6 |
| $g^2$ | 0.99 | 0.01 |

**$I_L(G_{student})$**

**D $\perp$ I**

**D $\perp$ S**

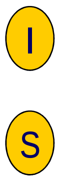
**G $\perp$ S | D, I**

**L $\perp$ I,D,S | G**

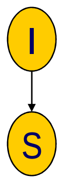
**S $\perp$ D,G,L | I**

# Independency mappings (I-Maps)

- Let P be a distribution over X
- Let I(P) be the independencies $(X \perp Y \mid Z)$ in P
- A Bayesian network structure G is an I-map (independency mapping) for P, if $I_L(G) \subseteq I(P)$




| I | S | P(I,S) |
|---|---|---|
| $i^0$ | $s^0$ | 0.25 |
| $i^0$ | $s^1$ | 0.25 |
| $i^1$ | $s^0$ | 0.25 |
| $i^1$ | $s^1$ | 0.25 |




| I | S | P(I,S) |
|---|---|---|
| $i^0$ | $s^0$ | 0.4 |
| $i^0$ | $s^1$ | 0.3 |
| $i^1$ | $s^0$ | 0.2 |
| $i^1$ | $s^1$ | 0.1 |

$I_L(G)=\{I \perp S\}$ $I(P)=\{I \perp S\}$

$I_L(G) \subseteq I(P)$

$I_L(G)=\emptyset$ $I(P)=\emptyset$

$I_L(G) \subseteq I(P)$ holds



# Factorization theorem

***"P factorizes over G"***

- G is an I-Map of P → $P(X_1,\ldots,X_n)=\prod_{i=1}^{n} P(X_i \mid Pa(X_i))$
  - The conditional independencies encoded in G imply factorization according to G.
- $P(X_1,\ldots,X_n)=\prod_{i=1}^{n} P(X_i \mid Pa(X_i))$ → G is an I-Map of P
  - Factorization according to G implies the associated conditional independencies.

## Factorization theorem

- If G is an I-Map of P, then $P(X_1,\ldots,X_n)=\prod_{i=1}^{n} P(X_i \mid Pa(X_i))$

Proof:

- wlog. $X_1,\ldots,X_n$ is an ordering consistent with *G*
- By chain rule: $P(X_1,\ldots,X_n)=\prod_{i=1}^{n} P(X_i \mid X_1,\ldots,X_{i-1})$
- From assumption: $Pa(X_i) \subseteq \{X_1,\ldots,X_{i-1}\}$

$$U = \{X_1,\ldots,X_{i-1}\} - Pa(X_i) \subseteq NonDesc(X_i)$$

- Since G is an I-Map → ($X_i$; NonDesc($X_i$)| Pa($X_i$))$\in$I(P)

$\{X_i \perp U \mid Pa(X_i)\}$

$= P(X_i \mid U, Pa(X_i)) = P(X_i \mid Pa(X_i))$

$$P(X_i \mid X_1,\ldots,X_{i-1}) = P(X_i \mid Pa(X_i))$$



## Factorization implies I-Map

- $P(X_1,\ldots,X_n)=\prod_{i=1}^{n} P(X_i \mid Pa(X_i))$ → G is an I-Map of P

Proof:

- Need to show ($X_i$; NonDesc($X_i$)| Pa($X_i$))$\in$I(P) or
  that P($X_i$ | NonDesc($X_i$)) = P($X_i$ | Pa($X_i$))
- wlog. $X_1,\ldots,X_n$ is an ordering consistent with G

$$P(X_i \mid NonDesc(X_i)) = \frac{P(X_i, NonDesc(X_i))}{P(NonDesc(X_i))} = \frac{\prod_{k=1}^{i} P(X_k \mid Pa(X_k))}{\prod_{k=1}^{i-1} P(X_k \mid Pa(X_k))} = P(X_i \mid Pa(X_i))$$

# Bayesian network definition

- A Bayesian network is a pair (G,P)
  - P factorizes over G
  - P is specified as set of CPDs associated with G's nodes
- Parameters
  - Joint distribution: $2^n$
  - Bayesian network (bounded in-degree k): $n2^k$



# Bayesian network design

- Variable considerations
  - Clarity test: can an omniscient being determine its value?
  - Hidden variables?
  - Irrelevant variables
- Structure considerations
  - Causal order of variables
  - Which independencies (approximately) hold?
- Probability considerations
  - Zero probabilities
  - Orders of magnitude
  - Relative values

# Independencies in a BN

- G encodes local independencies
  - $X_i$ is independent of its non-descendants given its parents
  - Formally: $(X_i \perp NonDesc(X_i) \mid Pa(X_i))$

Does G encode other independence assumptions that hold in every distribution P that factorizes over G?

⬇

Devise a procedure to find all independencies in G

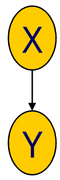


# d-Separation (directed separation)

- Goal: procedure that d-sep(**X**;**Y** | **Z**, G)
  - Return "true" iff Ind(**X**;**Y** | **Z**) follows from the local independencies in G, $I_L(G)$.
- Strategy: since influence must "flow" along paths in G, consider reasoning patterns between **X**, **Y**, and **Z,** in various structures in G
- Active path: creates dependencies between nodes
- Inactive path: cannot create dependencies

# Direct connection

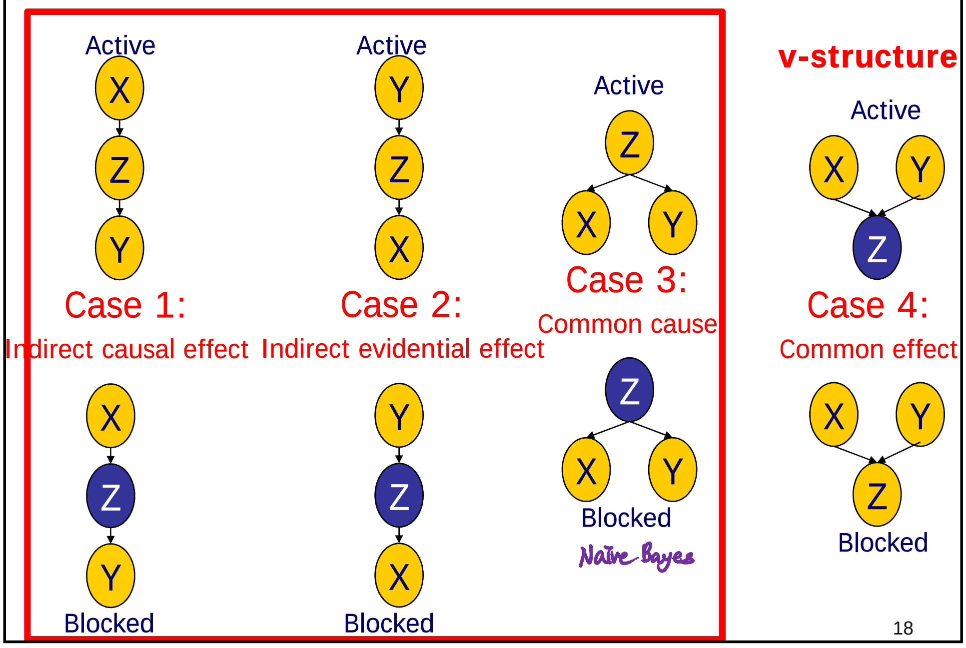
- **X** and **Y** directly connected in G → no Z exists for which Ind(X;Y | Z)
  - Example: deterministic function






# Indirect connection

**X can influence Y via Z iff Z is not observed.**



## The general case

- Let G be a Bayesian network structure
- Let $X_1 \leftrightarrow \ldots \leftrightarrow X_n$ be a trail in G
- Let **E** be a subset of evidence nodes in G

⬇

The trail $X_1 \leftrightarrow \ldots \leftrightarrow X_n$ is active given evidence E if:

- ALL the three-node networks along the trail is active.
  - For every V-structure $X_{i-1} \rightarrow X_i \leftarrow X_{i+1}$, $X_i$ or one of its descendants is observed
  - No other nodes along the trail is in **E**



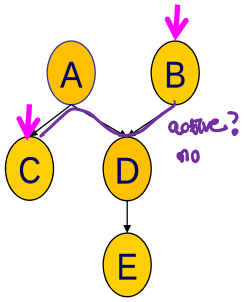
## d-Separation

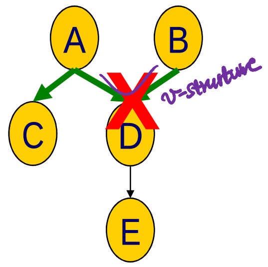
- **X** and **Y** are d-separated in G given **Z**, denoted $\text{d-sep}_G(\mathbf{X};\mathbf{Y} \mid \mathbf{Z})$ if there is no active trail between any node $X \in \mathbf{X}$ and any node $Y \in \mathbf{Y}$ in G

- $I(G) = \{(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) : \text{d-sep}_G(\mathbf{X};\mathbf{Y} \mid \mathbf{Z})\}$

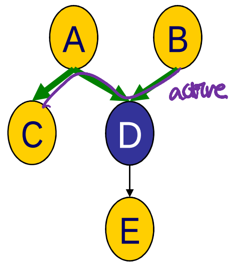
# Examples

Are B and C d-separated?

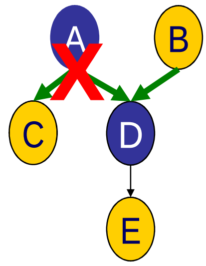



d-sep(B,C)=yes




d-sep(B,C|D)=no




d-sep(B,C|A,D)=yes

# d-Separation: soundness

- Theorem:

| | | |
|---|---|---|
| ▪ G is an I-map of P<br>▪ d-sep$_G$(**X**;**Y** \| **Z**) = yes | ➡ | ▪ P satisfies Ind(**X**;**Y** \| **Z**) |

- Defer proof

# d-Separation: completeness

- Theorem:

| | | |
|---|---|---|
| ▪ d-sep$_G$(**X**;**Y** \| **Z**) = no | ➡ | There exists P such that<br>▪ G is an I-map of P<br>▪ P does not satisfy Ind(**X**;**Y** \| **Z**) |

- Proof outline:
  - Construct distribution P where independence does not hold
  - Since there is no d-sep, there is an active path
  - For each interaction in the path, correlate the variables through the distribution in the CPDs
  - Set all other CPDs to uniform, ensuring that influence flows only in a single path and cannot be cancelled out
  - Detailed distribution construction quite involved



# Algorithm for d-separation

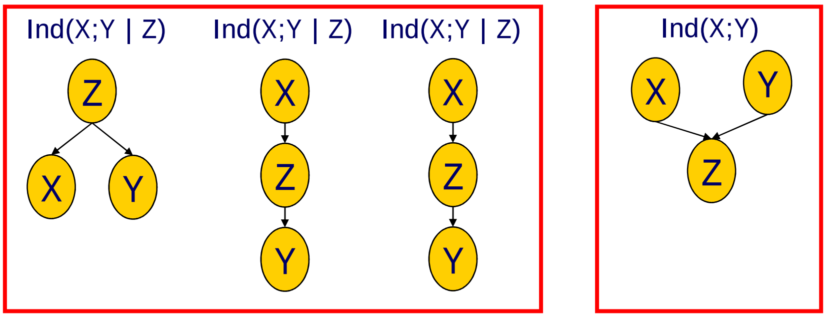
- Goal: answer whether d-sep(**X**;**Y** | **Z**, G)
  - Enumerate all possible trails between X and Y? NO

- Algorithm:
  - Mark all nodes in **Z** or that have descendants in **Z**
  - BFS traverse G from **X** breadth first search
  - Stop traversal at blocked nodes:
    - Node that is in the middle of a v-structure and not in marked set
    - Not such a node but is in **Z**
  - If we reach any node in **Y** then there is an active path and thus d-sep(**X**;**Y** | **Z**, G) does not hold

- Theorem: algorithm returns all nodes reachable from **X** via trails that are active in G

# I-equivalence between graphs

- I(G) describe all conditional independencies in G
- Different Bayesian networks can have same Ind.




Equivalence class I

Equivalence class II

Two BN graphs $G_1$ and $G_2$ are I-equivalent if $I(G_1) = I(G_2)$



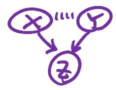
# I-equivalence between graphs

- If P factorizes over a graph in an I-equivalence class
  - P factorizes over all other graphs in the same class
  - P cannot distinguish one I-equivalent graph from another
- Implications for structure learning
  - We cannot find the "correct" structure from within the same equivalent class. -> will revisit later.
- Test for I-equivalence: d-separation

# Test for I-equivalence

- Necessary condition: same graph skeleton
  - Otherwise, can find active path in one graph but not other
  - But, not sufficient: v-structures

- Sufficient condition: same skeleton and v-structures
  - But, not necessary: complete graphs (no independence)




- Define X→Z←Y as immoral if X, Y are not directly connected
  - Necessary and Sufficient: same skeleton and immoral set of v-structures

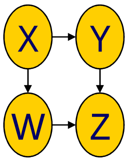


# Constructing graphs for P

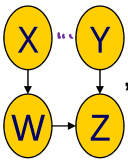
- Can we construct a graph for a distribution P?
  - Any graph which is an I-map for P
  - But, this is not so useful: complete graphs
    - A DAG is complete if adding an edge creates cycles
    - Complete graphs imply no independence assumptions
    - Thus, they are I-maps of any distribution

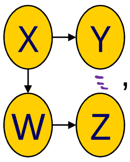
# Minimal I-Maps

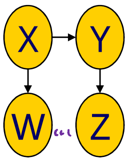
- A graph G is a minimal I-Map for P if:
  - G is an I-map for P
  - Removing any edge from G renders it not an I-map

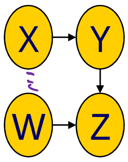
- Example: if 

is a minimal I-map for P,

Then: 

, 

, 

, 

is not I-maps.



# BayesNet definition revisited

- A Bayesian network is a pair (G,P)
  - P factorizes over G
  - P is specified as set of CPDs associated with G's nodes
  - Additional requirement: G is a minimal I-map for P

## Constructing minimal I-Maps

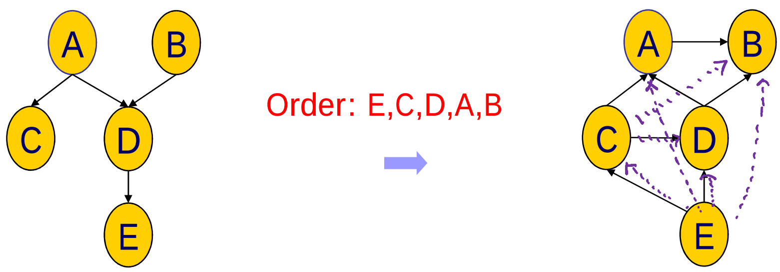
- Reverse factorization theorem
  - $P(X_1,...,X_n) = \prod_{i=1}^{n} P(X_i \mid Pa(X_i))$ → G is an I-Map of P
- Algorithm for constructing a minimal I-Map
  - Fix an ordering of nodes $X_1,\ldots,X_n$
  - Select parents of $X_i$ as minimal subset of $X_1,\ldots,X_{i-1}$, such that $Ind(X_i ; X_1,\ldots X_{i-1} - Pa(X_i) \mid Pa(X_i))$
- (Outline of) Proof of minimal I-map
  - I-map since the factorization above holds by construction
  - Minimal since by construction, removing one edge destroys the factorization



## Non-uniqueness of minimal I-Map

- Applying the same I-Map construction process with different orders can lead to different structures

Assume: I(G) = I(P)




Different independence assumptions (different skeletons, e.g., Ind(A;B) holds on left)

# Choosing order

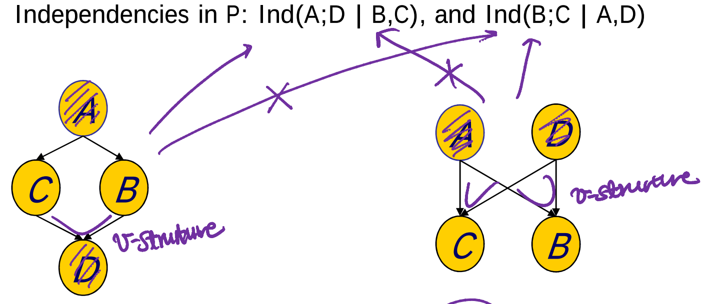
- Drastic effects on complexity of minimal I-Map graph
- Heuristic: use causal order



# Perfect maps

- G is a perfect map (P-Map) for P if I(P)=I(G)

- Does every distribution have a P-Map?
  - No: independencies may be encoded in CPD Ind(X;Y|Z=1)
  - No: some structures cannot be represented in a BN
    - Independencies in P: Ind(A;D | B,C), and Ind(B;C | A,D)




Ind(B;C | A,D) does not hold

Ind(A,D) also holds

# Finding a perfect map

- If P has a P-Map, can we find it?
  - Not uniquely, since I-equivalent graphs are indistinguishable
  - Thus, represent I-equivalent graphs and return it
- Recall I-Equivalence
  - Necessary and Sufficient: same skeleton and immoral set of v-structures
- Finding P-Maps
  - Step I: Find skeleton
  - Step II: Find immoral set of v-structures
  - Step III: Direct constrained edges



# Step I: Identifying the skeleton

- Query P for Ind(X;Y | **Z**)
  - If there is no **Z** for which Ind(X;Y | **Z**) holds, then X→Y or Y→X in G*
    - Proof: Assume no **Z** exists, and G* does not have X→Y or Y→X
    - Then, can find a set **Z** such that the path from X to Y is blocked
    - Then, G* implies Ind(X;Y | **Z**) and since G* is a P-Map
    - Contradiction
- Algorithm: For each pair X,Y query all **Z**
  - X–Y is in skeleton if no **Z** is found
  - If graph in-degree bounded by d → running time $O(n^{2d+2})$
    - Since if no direct edge exists, Ind(X;Y | Pa(X), Pa(Y))

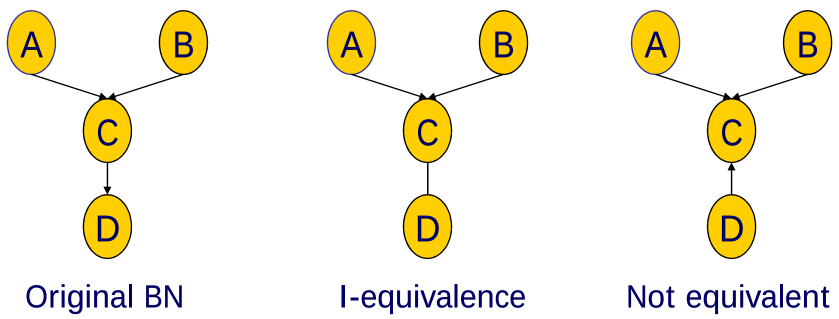
## Step II: Identifying immoralities

- Find all X–Z–Y triplets where X–Y is not in skeleton
  - X→Z←Y is a potential immorality
  - If there is no **W** such that Z is in **W** and Ind(X;Y | **W**), then X→Z←Y is an immorality
    - Proof: Assume no **W** exists but X–Z–Y is not an immorality
    - Then, either X→Z→Y or X←Z←Y or X←Z→Y exists
    - But then, we can block X–Z–Y by Z
    - Then, since X and Y are not connected, can find **W** that includes Z such that Ind(X;Y | **W**)
    - Contradiction
- Algorithm: For each pair X,Y query candidate triplets
  - X→Z←Y if no **W** is found that contains Z and Ind(X;Y | **W**)
  - If graph in-degree bounded by d → running time $O(n^{2d+3})$
    - If **W** exists, Ind(X;Y|**W**), and X→Z←Y not immoral, then Z∈**W**



## Step III: Direct constrained edges

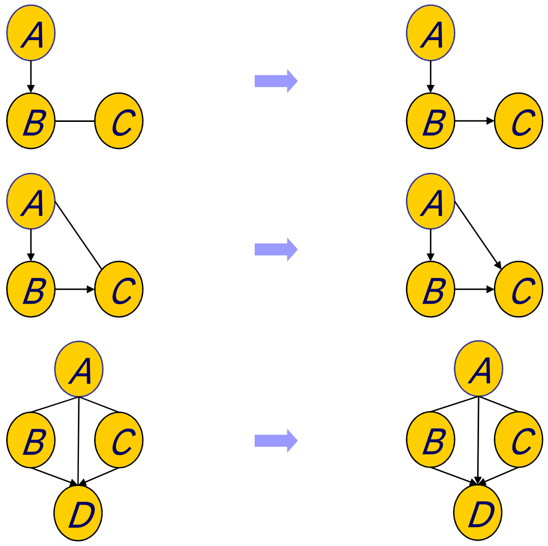
- If skeleton has k undirected edges, at most $2^k$ graphs
- Given skeleton and immoralities, are there additional constraints on the edges?




Equivalence class is a singleton

## Step III: Direct constrained edges

- Local constraints for directing edges






## Step III: Direct constrained edges

- Algorithm: iteratively direct edges by 3 local rules
  - Guaranteed to converge since each step directs an edge
- Algorithm is sound and complete
  - Proof strategy for completeness: show that for any single edge that is undirected, we can find two graphs, one for each possible direction

## Summary

- Local independencies $I_L(G)$– basic BN independencies
- d-separation – all independencies via graph structure
- G is an I-Map of P if and only if P factorizes over G
- I-equivalence – graphs with identical independencies
- Minimal I-Map
  - All distributions have I-Maps (sometimes more than one)
  - Minimal I-Map does not capture all independencies in P
- Perfect map – not every distribution P has one

- Reading assignment: K&F 3.1, 3.2, 3.3, 3.4
- HW1 will be handed out next Monday!

## Acknowledgement


- These lecture notes were generated based on the slides from Prof Eran Segal.