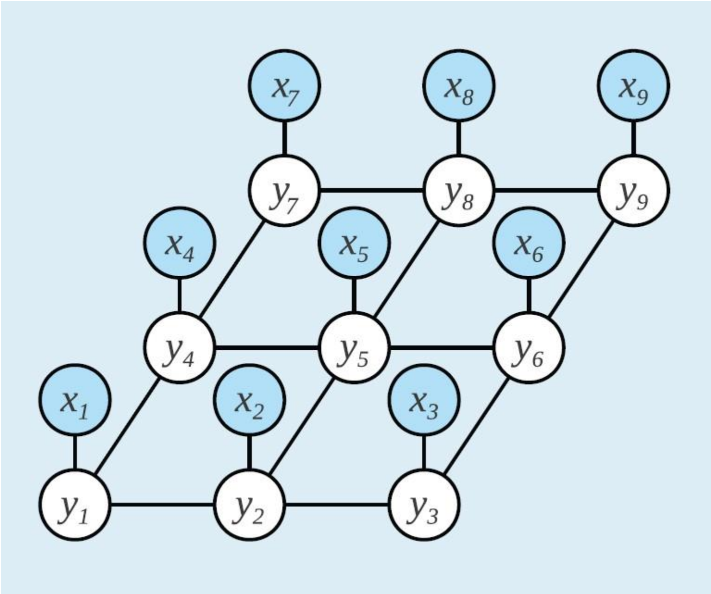
Probabilistic Graphical Models in Bioinformatics

Lecture 3: Bayesian network representation-2



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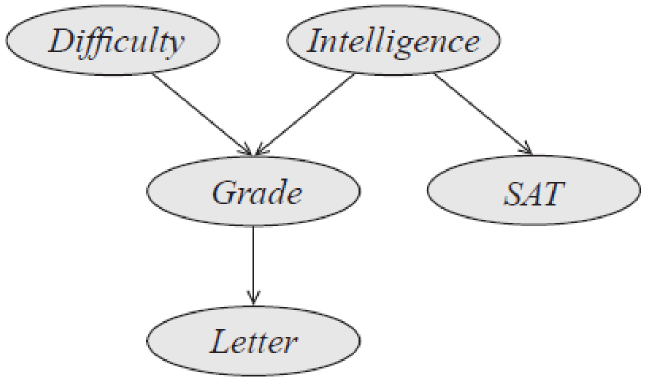
Independencies in Graphs

Review: local independencies in BNs

- Bayesian network G encodes the following set of local independencies for each variable X_i

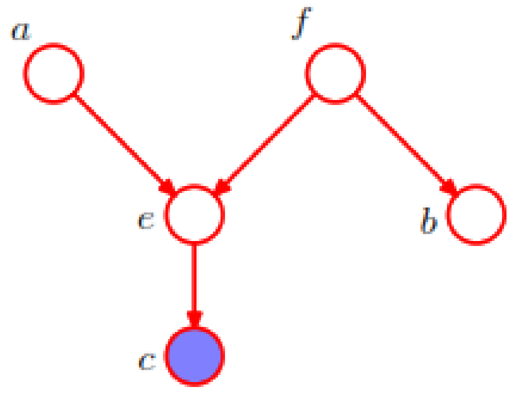
$$X_i \perp \mathrm{NonDescendants}_{X_i} \mid \mathrm{Pa_G(X_i)}$$

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



Independencies in Graphs

- Question: In a general DAG, is *X* dependence of Y given Z?
  - In the following DAG, are *a* and *b* independent given *c*?



- D-separation
  - to check whether an independence assertion $X \perp Y \mid Z$ is implied by a given DAG.

Independencies in Graphs- simple examples

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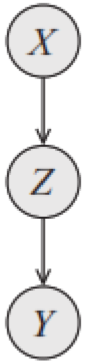
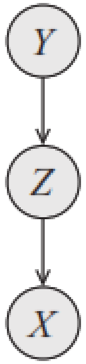
- Direct connection
  - $X \rightarrow Y$ or $Y \rightarrow X$

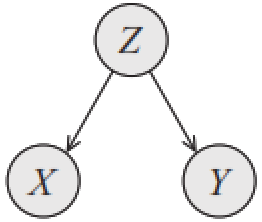
- Three-node networks



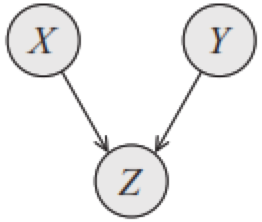
Indirect causal effect



Indirect evidential effect



common cause



common effect or v-structure

$$X \perp Y \mid Z$$

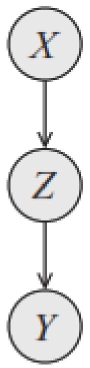
$$X \not\perp Y$$

$$X \not\perp Y \mid Z$$

$$X \perp Y$$

The joint distribution corresponding to the following graph is

$$P(X,Y,Z) = P(X)P(Z|X)P(Y \mid Z)$$



Case 1: first we show X and Y are independent given Z

$$P(X,Y \mid Z) = \frac{P(X,Y,Z)}{P(Z)} = \frac{P(X)P(Z|X)P(Y \mid Z)}{P(Z)} = \frac{P(X,Z)}{P(Z)}P(Y \mid Z)$$
$$= P(X \mid Z)P(Y \mid Z)$$

Hence $X \perp Y \mid Z$

Case 2: then we first show X and Y are marginally dependent

$$P(X,Y) = \sum_{Z} P(X)P(Z|X)P(Y \mid Z) = P(X)\sum_{Z} P(Z|X)P(Y \mid Z)$$
$$= P(X)\sum_{Z} P(Z|X)P(Y \mid Z,X) = P(X)\sum_{Z} P(Y,Z \mid X) = P(X)P(Y \mid X)$$

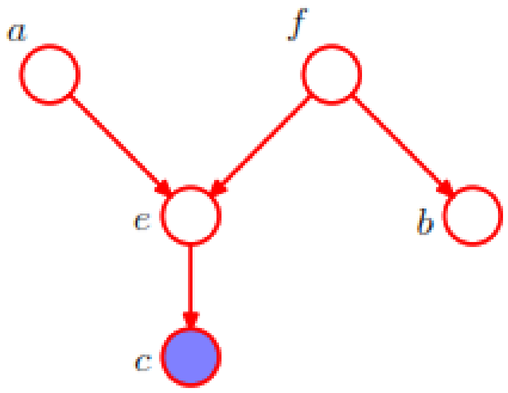
which in general does not factorize to $P(X)P(Y)$ hence $X \not\perp Y$

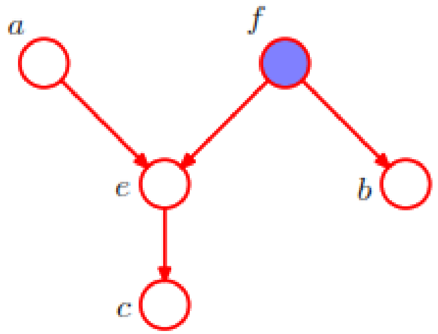
Homework: redo the above derivations for common cause and v-structure cases.

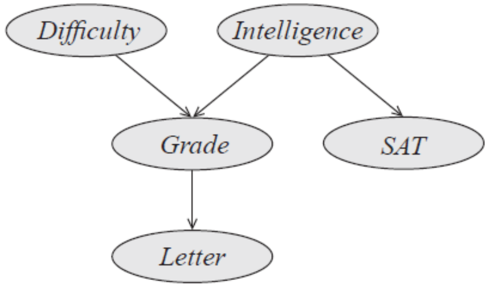
D-separation

- **Active trail**: A trail $X_1 - X_2 - \cdots - X_n$ is active given *Z* if
  - For any v-structure $X_{i-1} \rightarrow X_i \leftarrow X_{i+1}$, then X_i or one of its descendants are in *Z*;
  - No other node along the trail is in *Z*.

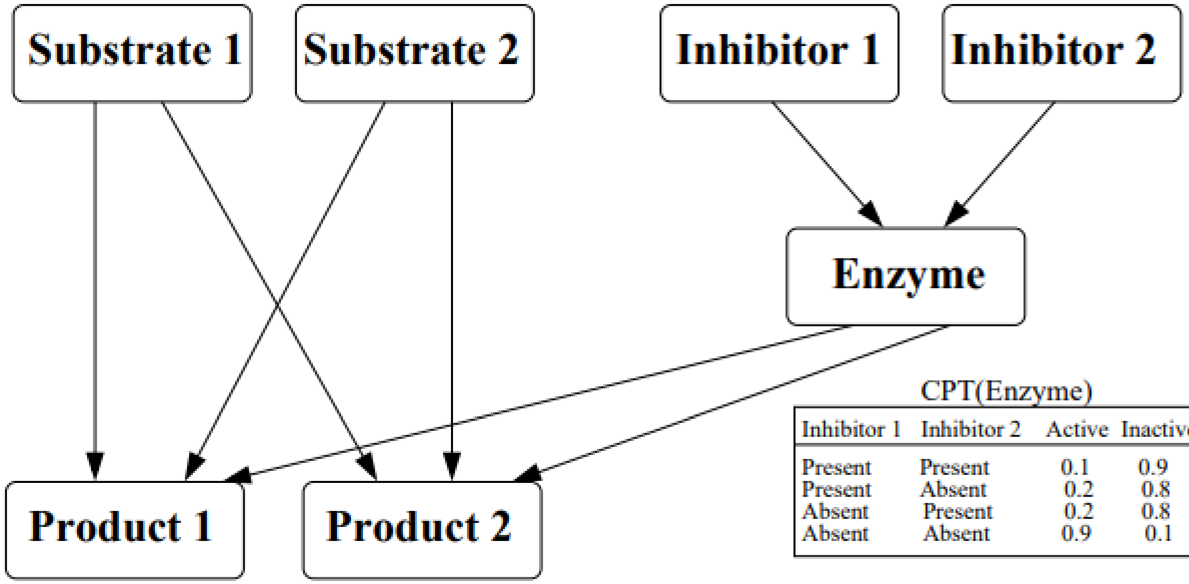
- **D-separation:** Let X, Y, Z be three sets of node in the input graph. ***X*** and ***Y*** are d-separated given ***Z*** if there is no active trail between any node $X \in \boldsymbol{X}$ and $Y \in \boldsymbol{Y}$ given ***Z***.







Example: a Bayesian network for a single reaction metabolic pathway

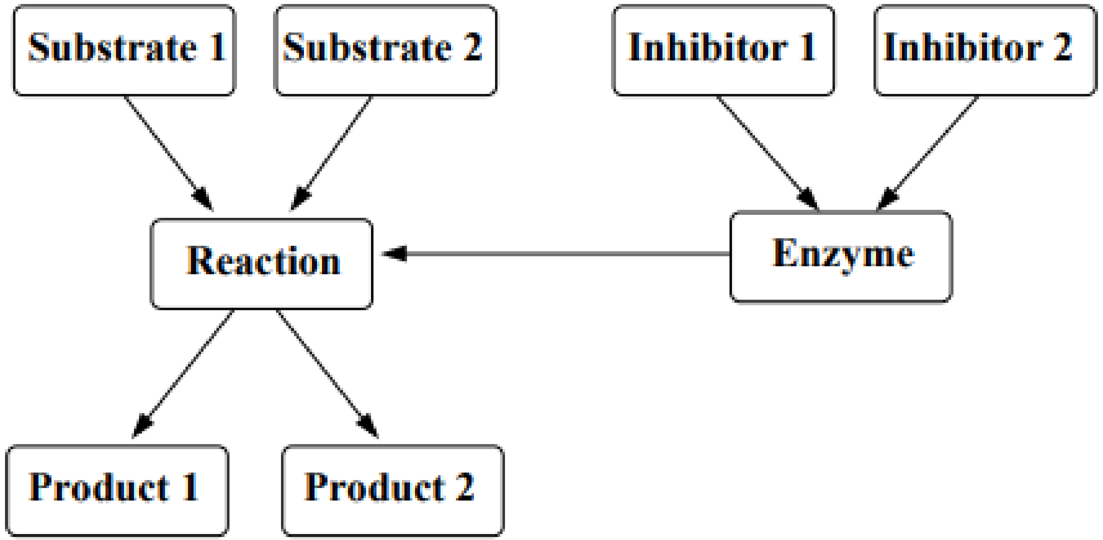


CPT(Enzyme)

Inhibitor 1	Inhibitor 2	Active	Inactive
Present	Present	0.1	0.9
Present	Absent	0.2	0.8
Absent	Present	0.2	0.8
Absent	Absent	0.9	0.1

CPT(Product2)

Substrate 1	Substrate 2	Enzyme	Present	Absent
Present	Present	Active	0.9	0.1
Present	Present	Inactive	0.2	0.8
Present	Absent	Active	0.2	0.8
Present	Absent	Inactive	0.15	0.85
Absent	Present	Active	0.2	0.8
Absent	Present	Inactive	0.15	0.85
Absent	Absent	Active	0.15	0.85
Absent	Absent	Inactive	0.10	0.9



Another possibility

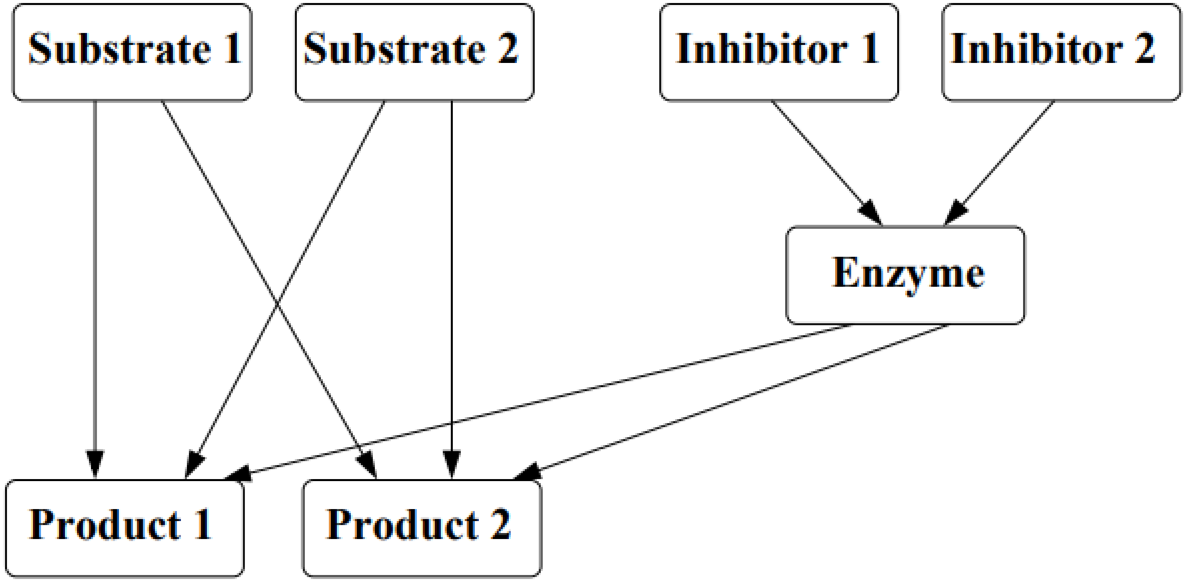
[Tamaddoni-Nezhad, 2003]

Example: a Bayesian network for a single reaction metabolic pathway

Check the following Independence statements:

- $P_1 \perp P_2$
- $P_1 \perp P_2 \mid E$
- $P_1 \perp P_2 \mid E, S_1$
- $P_1 \perp P_2 \mid E, S_1, S2$

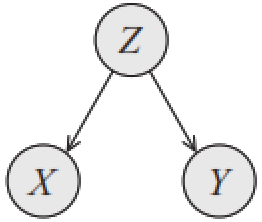
- $S_1 \perp I_1$
- $S_1 \perp I_1 \mid P_1$
- $S_1 \perp I_1 \mid E$
- $S_1 \perp I_1 \mid P_1, P_2, E$



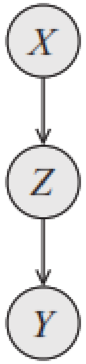
I-Equivalence

- Same set of conditional independence assertions for different BN structures

G1:

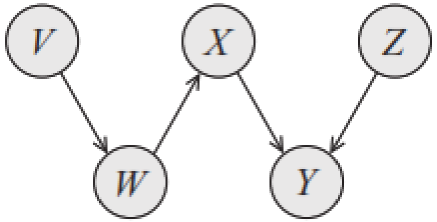


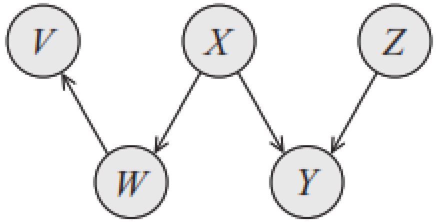
G2:



$$I(G_1) = I(G_2) = \{X \perp Y \mid Z\}$$

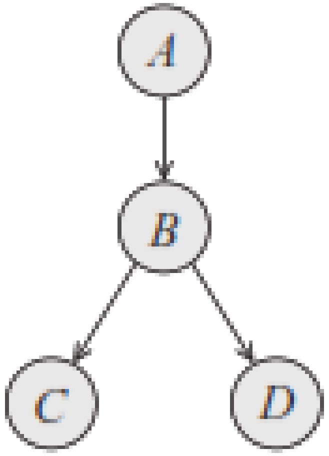
- **Theorem:** If two BN graphs have the **same skeleton** and the **same set of v-structures** then they are I-equivalent





I-Equivalence

- **Question**: Find I-equivalent BNs of the following BN



I-Equivalence

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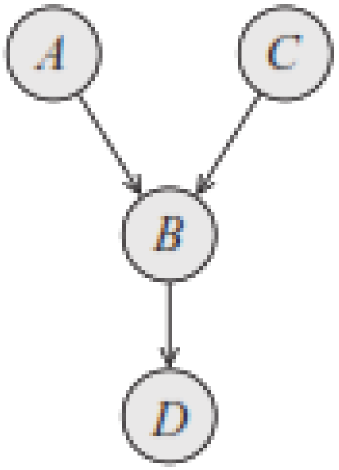
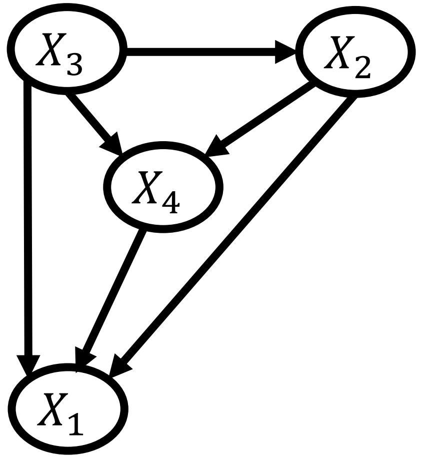
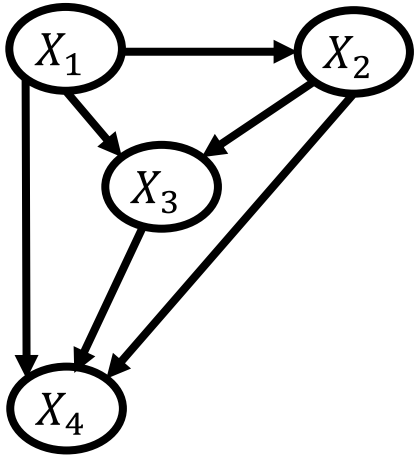


I-Equivalence

- **Question**: Are the following BNs I-equivalent?





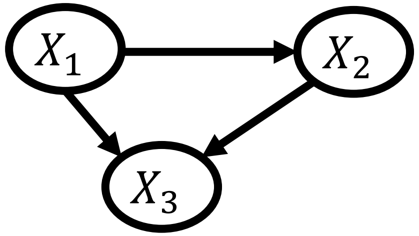
- Factorize the joint distribution according to each of the BNs.

Any two complete graphs are I-equivalent but is not detected by the criterion of previous theorem!

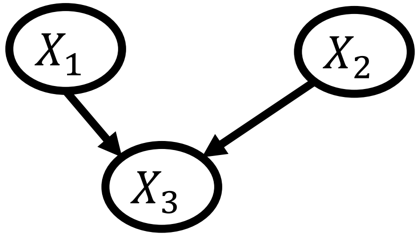
I-Equivalence

- **Definition:** A v-structure $X \rightarrow Z \leftarrow Y$ is an immorality if there is no direct edge between X and Y. If there is such an edge, it is called a covering edge for the v-structure.

V-structure



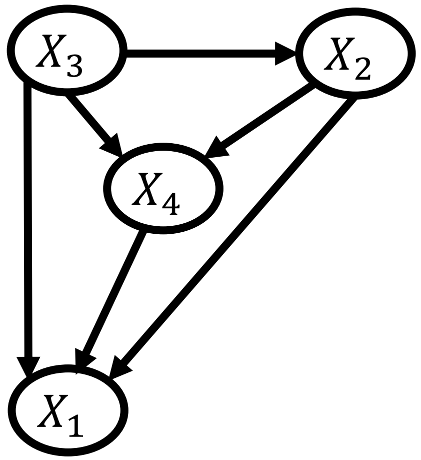
v-structure and immorality

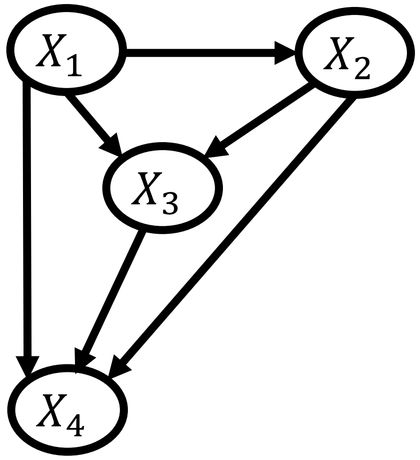


- **Theorem:** Two BN graphs have the **same skeleton** and the **same set of immoralities** if and only if they are I-equivalent.

I-Equivalence

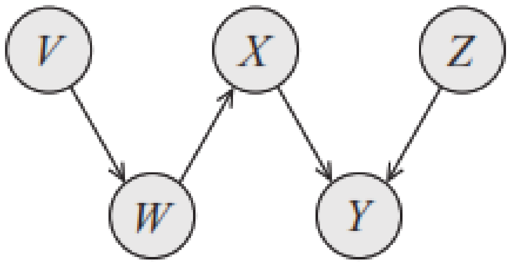
- **Question**: Are the following BNs I-equivalent?

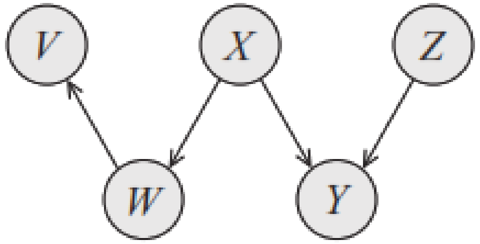




I-Equivalence

- **Question**: Are the following BNs I-equivalent?





Markov blanket

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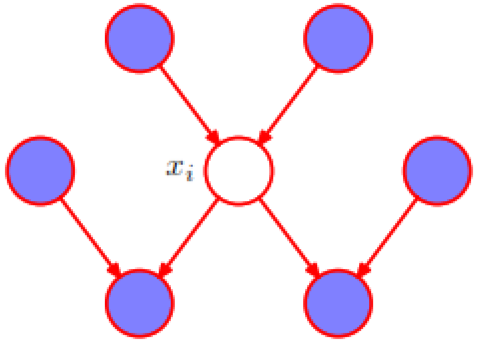
- Markov blanket of a node is the set of its parents, co-parents, and children.

$$P(X_i|X_{k\neq i}) = P(X_i \mid X_{\mathrm{MB(i)}})$$



Sketch of the proof:

$$P(X_i|X_{n\neq i}) = \frac{P(X_1, \ldots, X_n)}{\sum_{X_i} P(X_1, \ldots, X_n)}$$

$$= \frac{\prod_k P(X_k \mid \mathrm{Par}(X_k))}{\sum_{X_i} \prod_k P(X_k \mid \mathrm{Par}(X_k))}$$

Factors not depending on X_i can be taken outside summation and are canceled between numerator and denominator

From Distributions to Graphs

From Distributions to Graphs

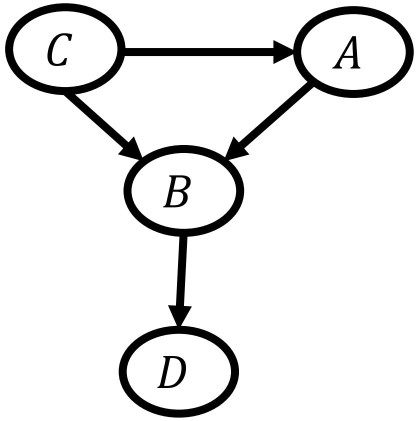
- **Question:** Given a distribution P (e.g. in terms of independence assertions), to what extent can we construct a graph G whose independencies reasonably represent independencies in P?

- Two approaches
  - Minimal I-maps
  - Perfect maps

Minimal I-maps

- A graph $\mathcal{K}$ is a minimal I-map for a set of independencies I if
  A. it is an I-map for I, *i.e.* $\mathrm{I}(\mathcal{K}) \subseteq I$.
  B. and removal a single edge from graph $\mathcal{K}$ makes it not an I-map.

- **Example:** given the set of independencies $I = \{A \perp B,\ D \perp A, C \mid B\}$



$\mathcal{K}$: a minimal I-map for I

Question: what is $\mathrm{I}(\mathcal{K})$?

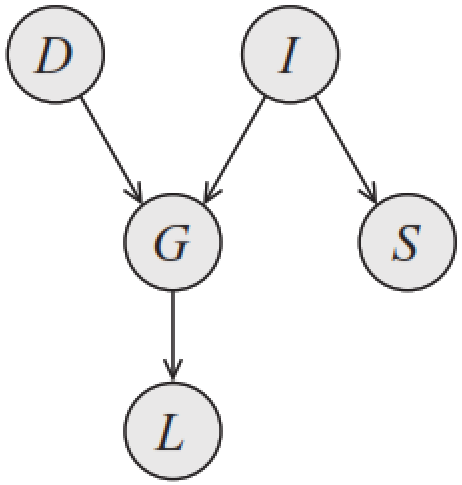
Minimal I-maps

- Algorithm to obtain minimal I-map
  - It depends on a given ordering of the variables
  - Obtained minimal I-maps are not unique.

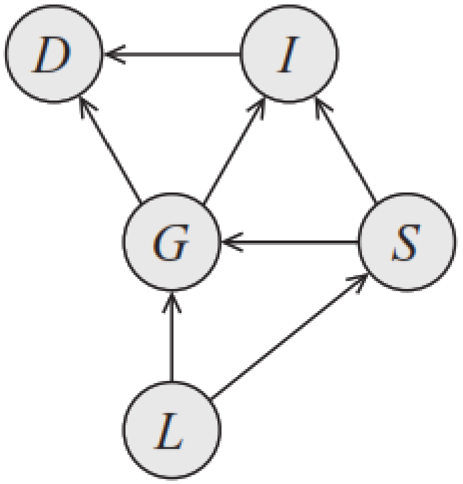
Algorithm 3.2 Procedure to build a minimal I-map given an ordering

Procedure Build-Minimal-I-Map (
  $X_1, \ldots, X_n$ // an ordering of random variables in $\mathcal{X}$
  $\mathcal{I}$ // Set of independencies
)
  Set $\mathcal{G}$ to an empty graph over $\mathcal{X}$
  for $i = 1, \ldots, n$
    $U \leftarrow \{X_1, \ldots, X_{i-1}\}$ // U is the current candidate for parents of X_i
    for $U' \subseteq \{X_1, \ldots, X_{i-1}\}$
      if $U' \subset U$ and $(X_i \perp \{X_1, \ldots, X_{i-1}\} - U' \mid U') \in \mathcal{I}$ **then**
        $U \leftarrow U'$
      // At this stage U is a minimal set satisfying $(X_i \perp \{X_1, \ldots, X_{i-1}\} - U \mid U)$
      // Now set U to be the parents of X_i
    for $X_j \in U$
      Add $X_j \rightarrow X_i$ to $\mathcal{G}$
  return $\mathcal{G}$

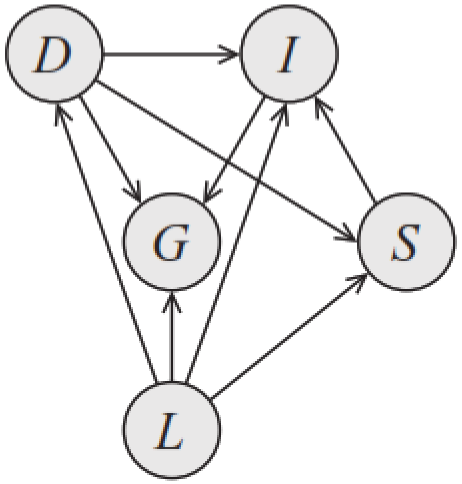
Examples of minimal I-maps



D, I , S, G, L



L, S, G, I, D



L, D, S, I, G

- **Minimal I-maps fail to capture some or all of independencies that hold in the distribution.**

Perfect maps

- A graph $\mathcal{K}$ is a perfect map for P if $\mathrm{I}(\mathcal{K}) = I(P)$.
- Existence of P-maps: not every distribution has a P-map.
- Example:

$$P(x,y,z) = \begin{cases} 1/12 & x \oplus y \oplus z = \mathit{false} \\ 1/6 & x \oplus y \oplus z = \mathit{true} \end{cases}$$

$$I(P) = \{\, X \perp Y, X \perp Z, Y \perp Z \,\}$$

Important: Note the pair X and Y are not independent given Z. The same is true for other pairs.

Question: find a Bayesian network G with I(G) = I(P). Is it possible?

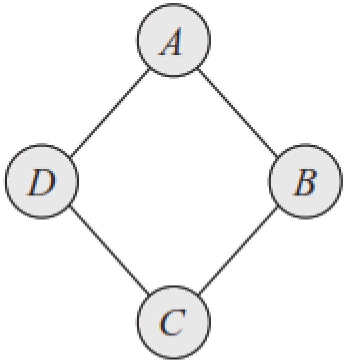
Existence of P-maps- misconception example

1. Four students study in pairs Alice and Bob; Bob and Charles; Charles and Debbie; Debbie and Alice.

2. Professor accidentally misspoke in the class, leading to a possible misconception

3. Students may have figured out the problem by reading the textbook

4. Students transmits their understanding to their partners

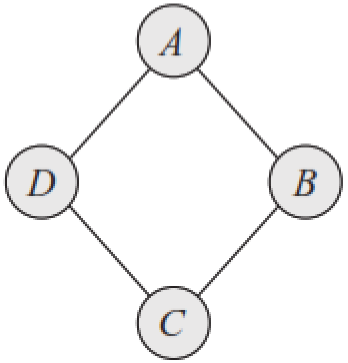


Study pairs for students

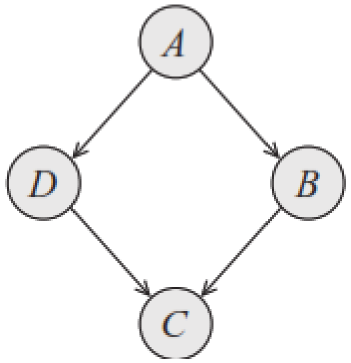
$A \perp C \mid D, B$

$B \perp D \mid A, C$

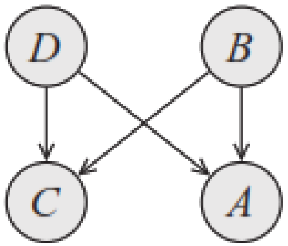
Failed attempts to identify a P-map for the misconception example



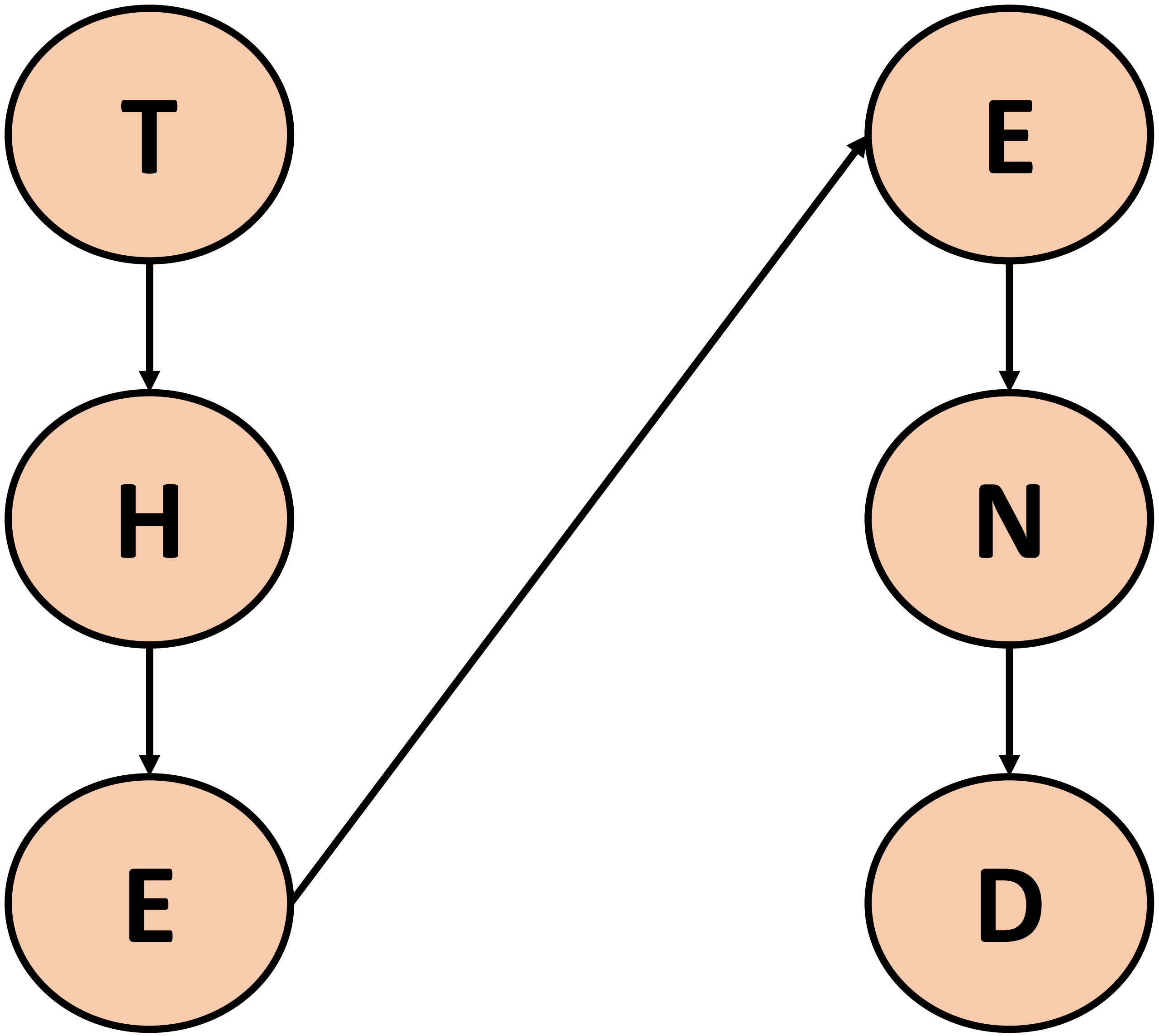
Study pairs
for students



First attempt



Second attempt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