

TECHNISCHE  
UNIVERSITÄT  
DARMSTADT



# Representation of Causal Knowledge and Causal Discovery

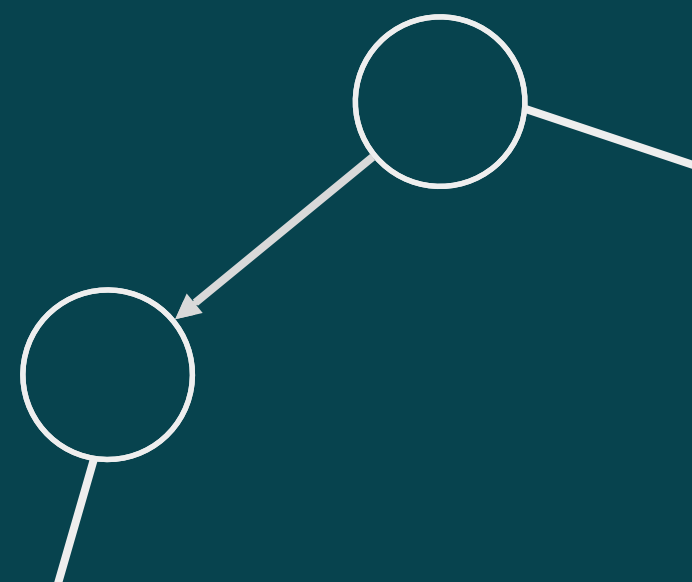
**Adèle Helena Ribeiro**

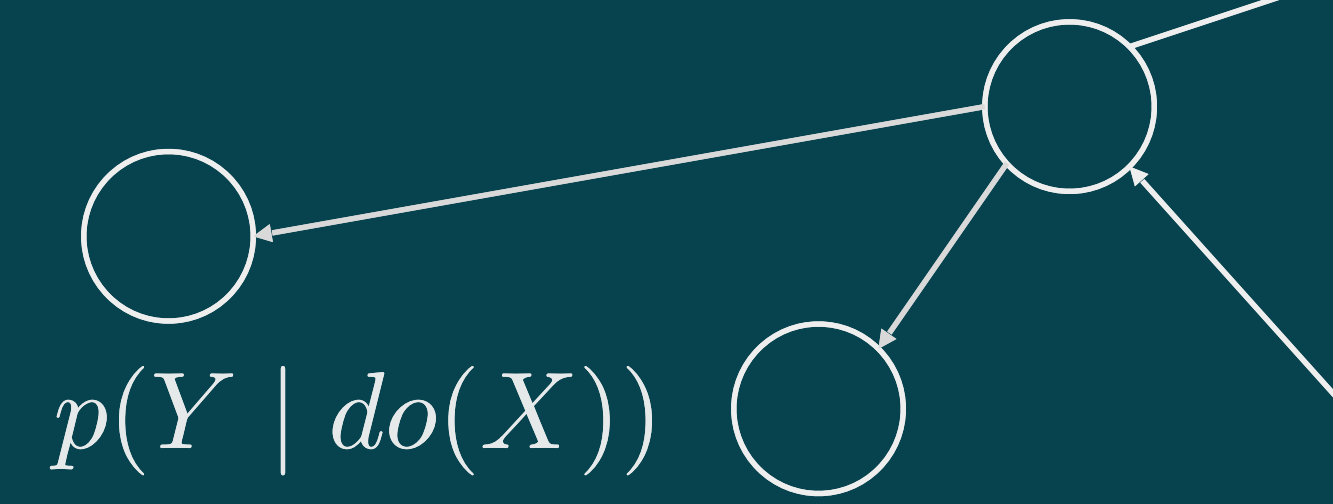
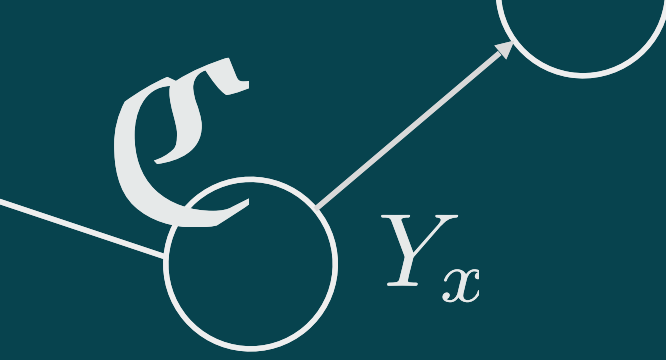
25<sup>th</sup> July 2023



ESSAI & ACAI 2023  
LJUBLJANA, SLOVENIA

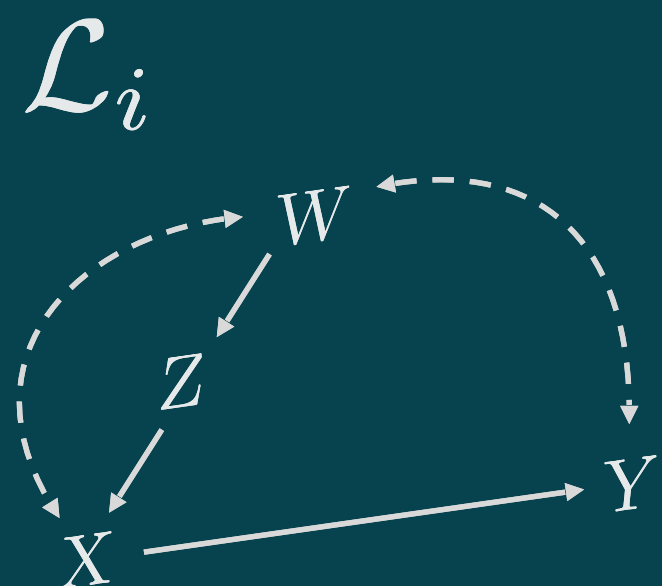
**Machines Climbing Pearl's Ladder of Causation**





# 1 Encoding Causal Structural Knowledge

## Causal Diagrams



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Machines Climbing Pearl's Ladder of Causation

# Causal Diagram: Encoder of *Structural* Knowledge

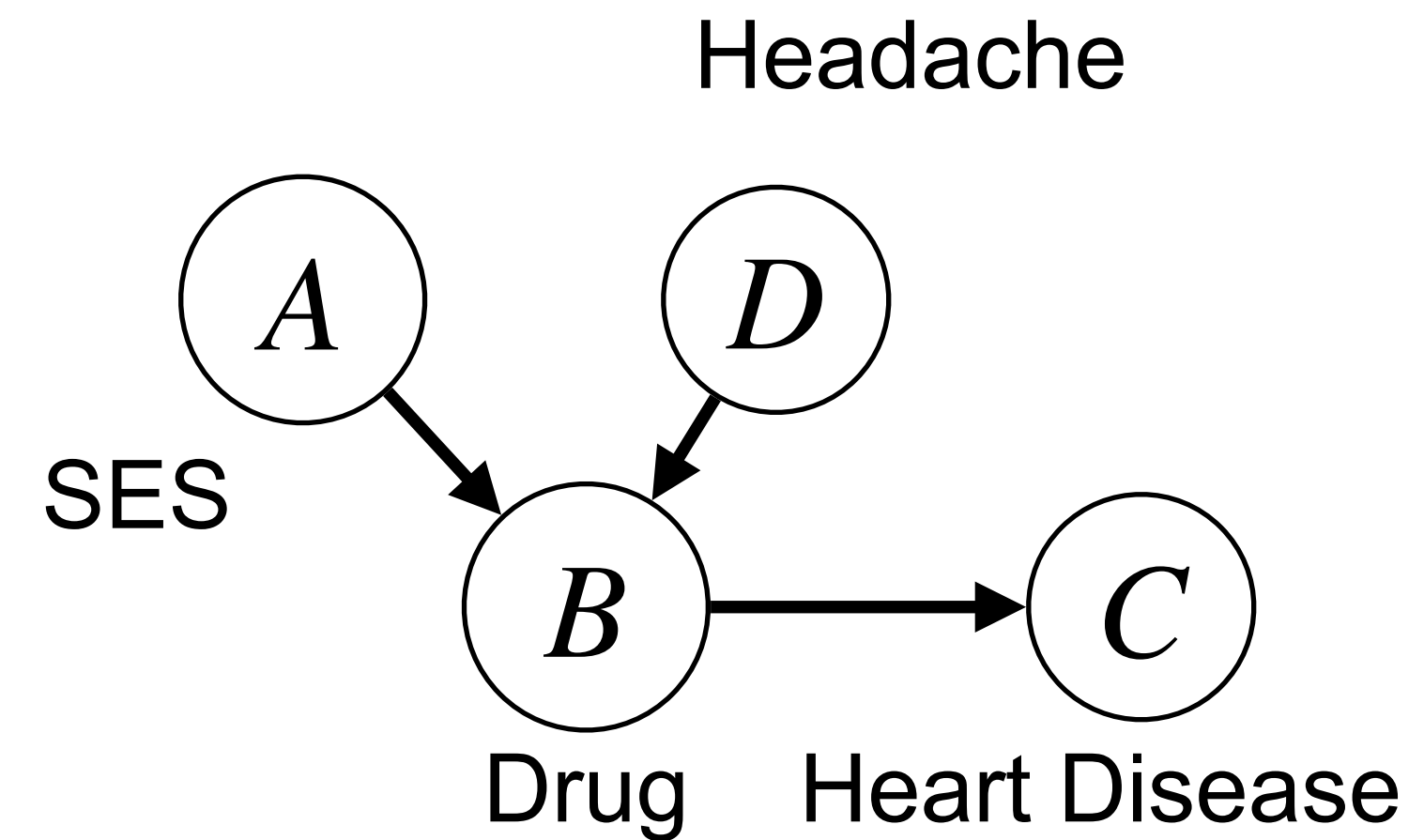
Structural Causal Model (SCM)

$$\mathcal{M} = \langle \mathbf{V}, \mathbf{U}, \mathcal{F}, P(\mathbf{u}) \rangle$$

$$\mathcal{M} = \left\{ \begin{array}{l} \mathbf{V} = \{A, B, C, D\} \\ \mathbf{U} = \{U_A, U_B, U_C, U_D, U_{CD}\} \\ \mathcal{F} = \left\{ \begin{array}{l} A \leftarrow f_A(U_A) \\ B \leftarrow f_B(A, D, U_B) \\ D \leftarrow f_Z(U_D, U_{CD}) \\ C \leftarrow f_X(B, U_C, U_{CD}) \end{array} \right. \\ P(\mathbf{U}) \end{array} \right.$$



Induced Causal Diagram



An SCM  $\mathcal{M} = \langle \mathbf{V}, \mathbf{U}, \mathcal{F}, P(\mathbf{u}) \rangle$  induces a causal diagram such that, **for every**  $V_i, V_j \in \mathbf{V}$ :

$V_i \rightarrow V_j$ , if  $V_i$  appears as argument of  $f_j \in \mathcal{F}$ .

# Causal Diagram: Encoder of *Structural* Knowledge

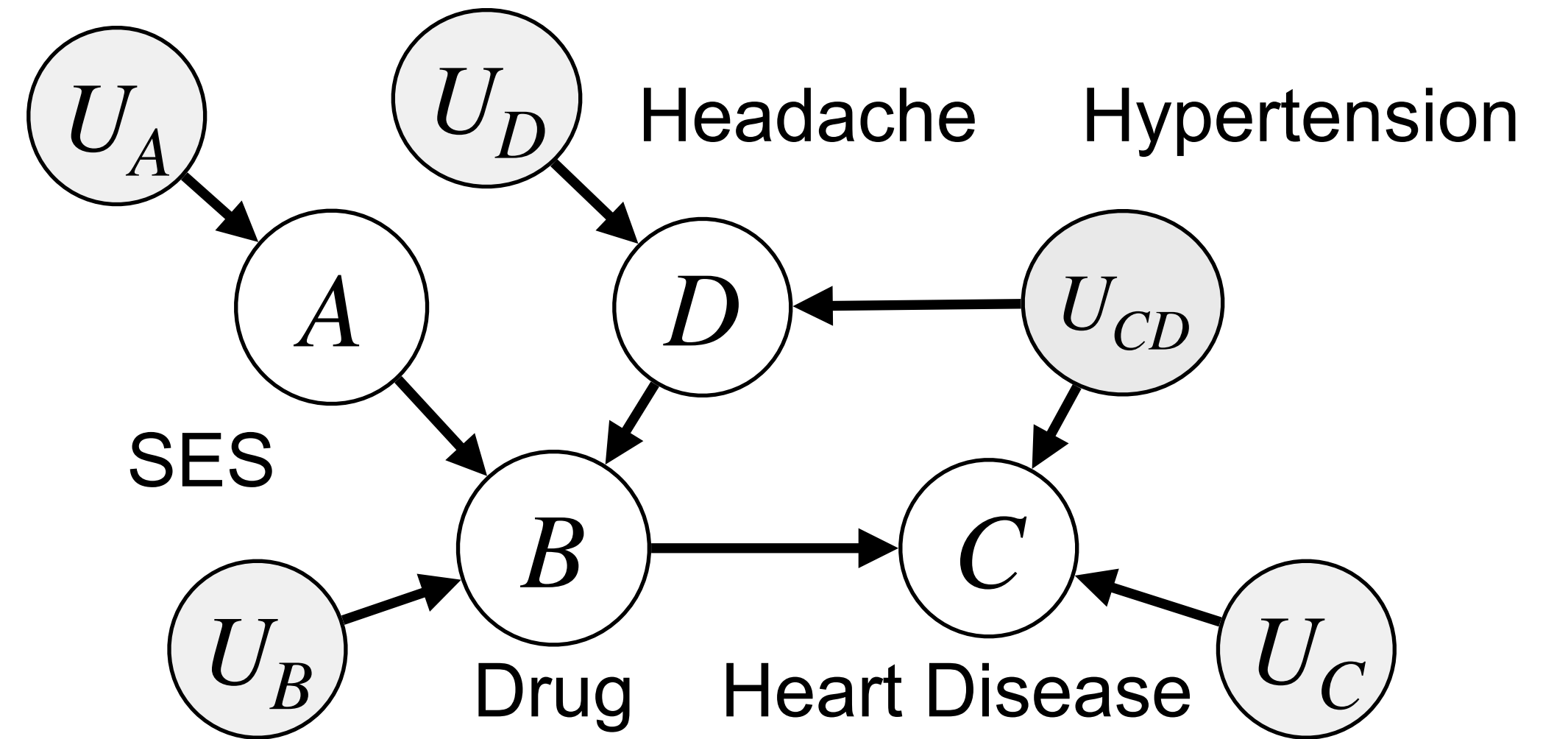
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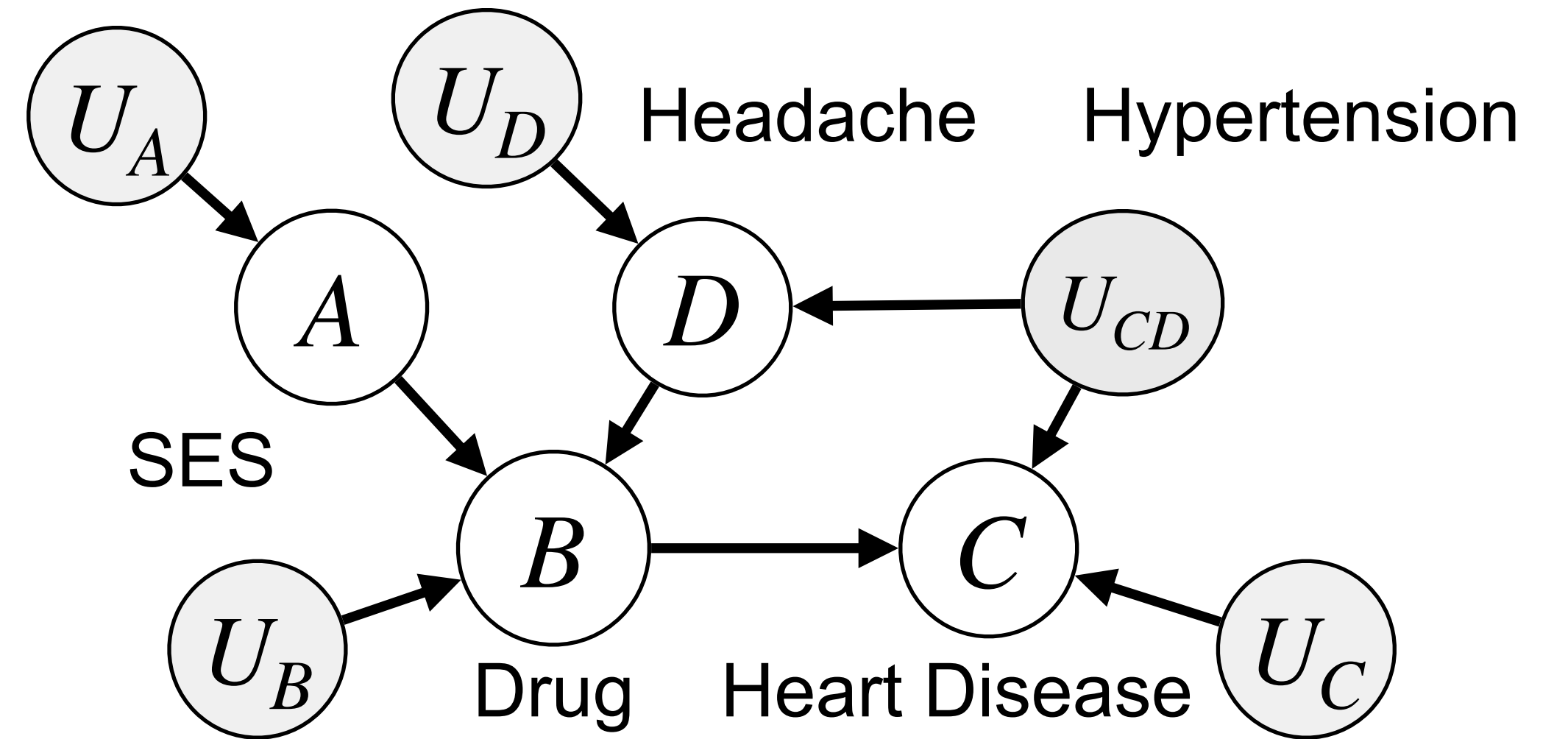
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$V_i \longleftrightarrow V_j$  if the corresponding  $U_i, U_j \in \mathbf{U}$  are correlated or  $f_i, f_j$  share some argument  $U \in \mathbf{U}$ .

# Causal Diagram: Encoder of *Structural* Knowledge

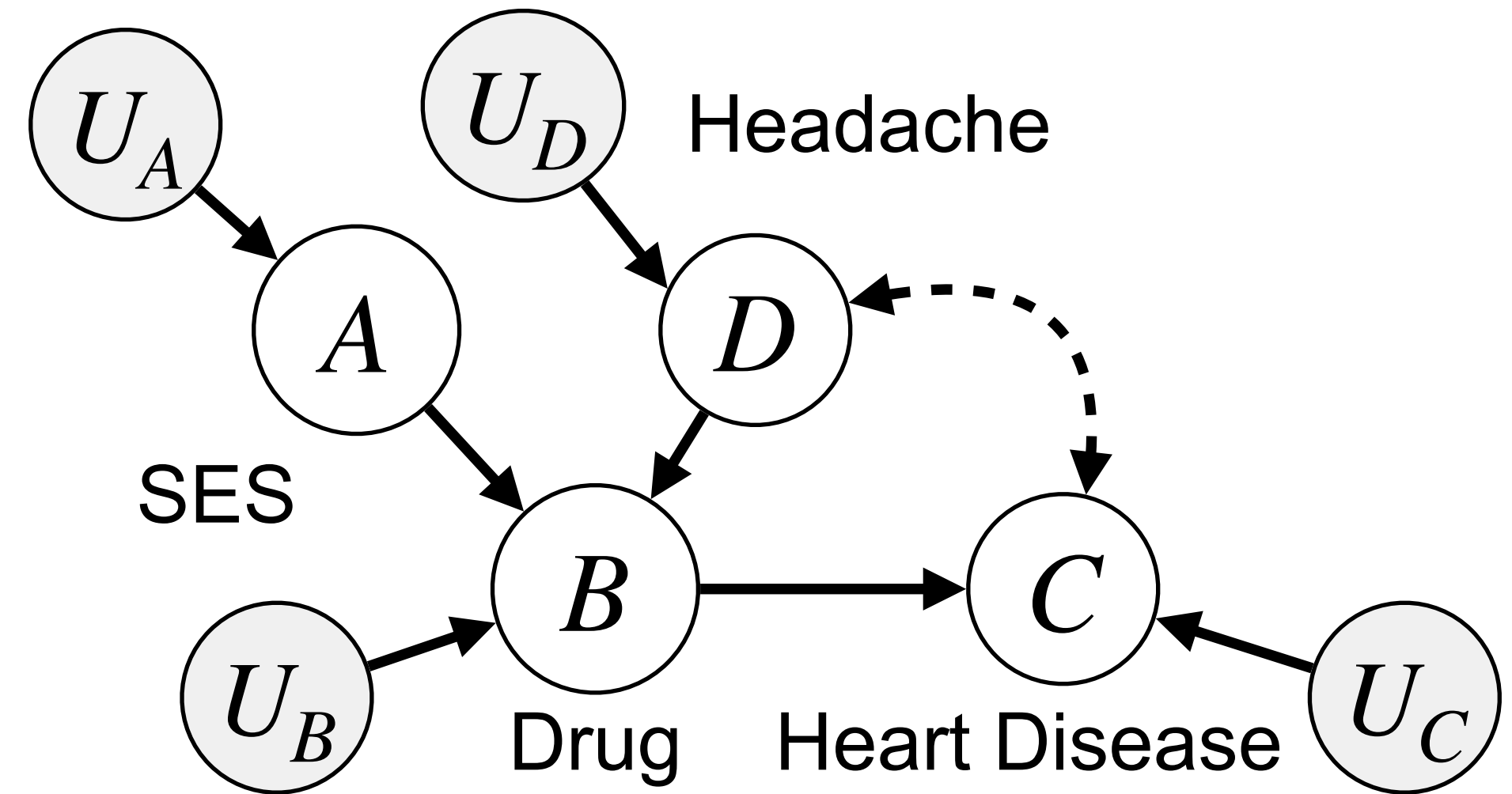
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# Causal Diagram: Encoder of *Structural* Knowledge

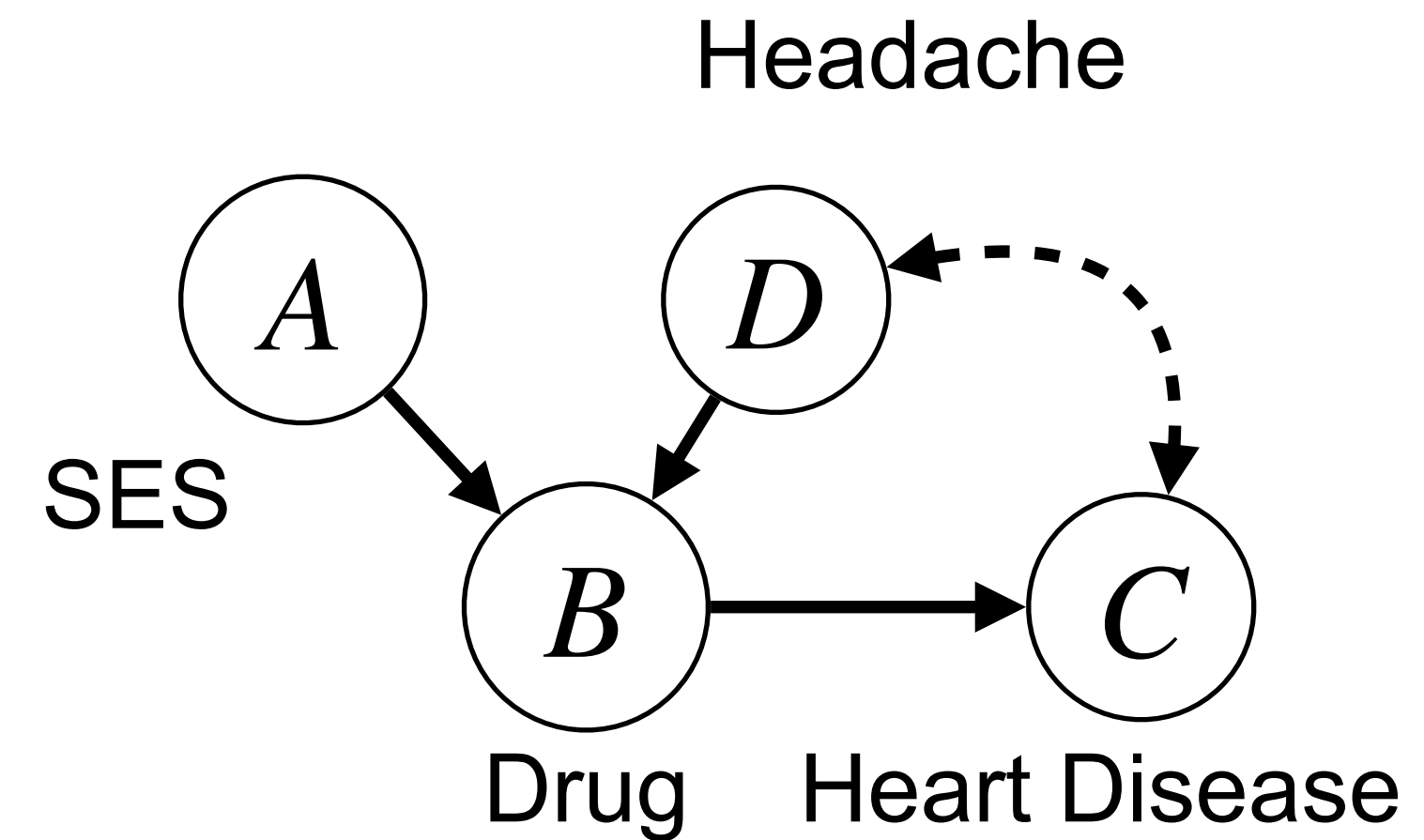
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Induced Causal Diagram



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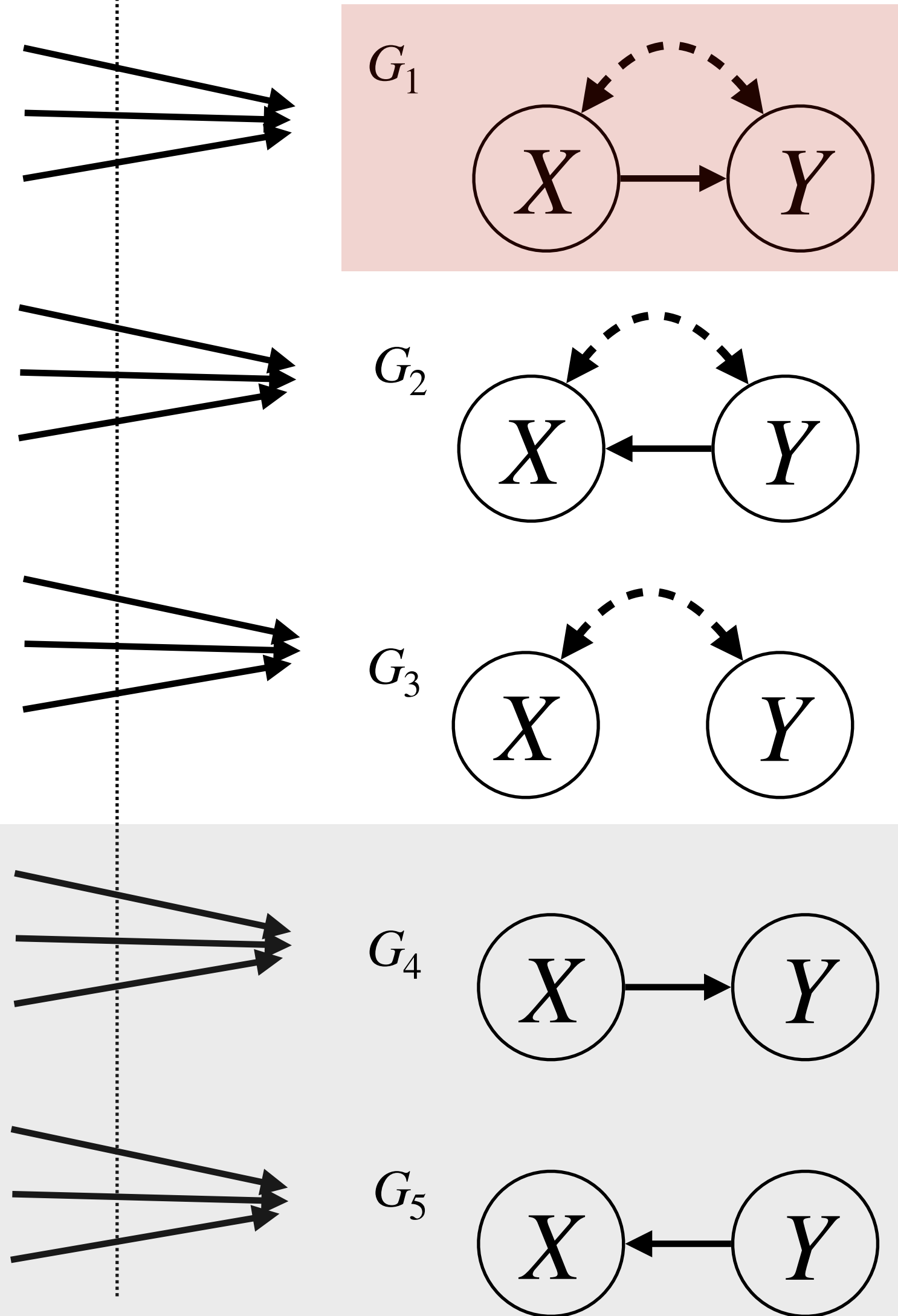
$V_i \longleftrightarrow V_j$  if the corresponding  $U_i, U_j \in \mathbf{U}$  are correlated or  $f_i, f_j$  share some argument  $U \in \mathbf{U}$ .

True  
Model

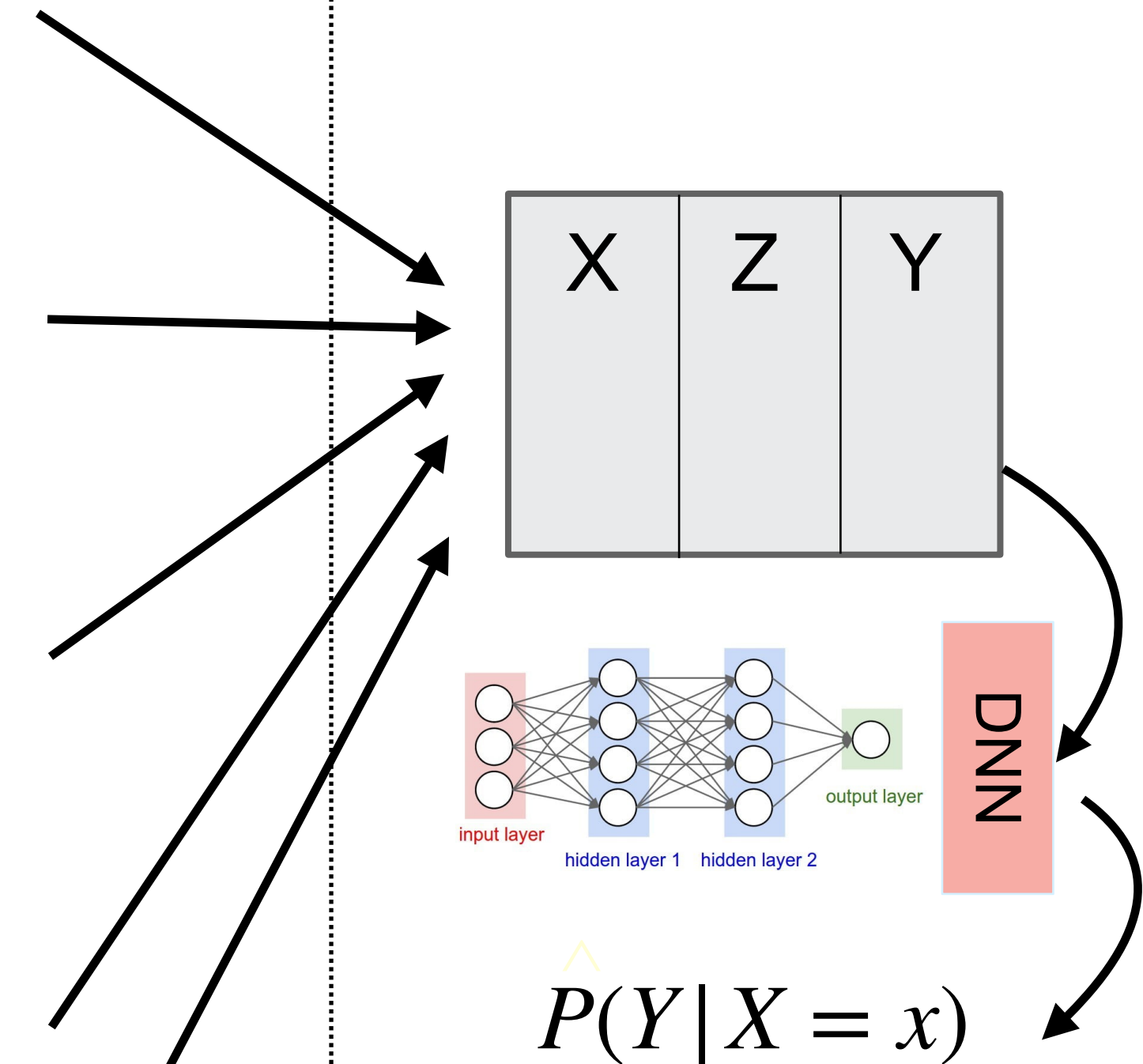
## Potential SCMs

$$\begin{aligned} \mathcal{M}_{11} &= \langle \mathbf{V}, \mathbf{U}_1, \mathcal{F}_{11}, P_{11}(\mathbf{u}_1) \rangle \\ &\vdots \\ \mathcal{M}_{1k_1} &= \langle \mathbf{V}, \mathbf{U}_1, \mathcal{F}_{1k_1}, P_{1k_1}(\mathbf{u}_1) \rangle \\ \mathcal{M}_{21} &= \langle \mathbf{V}, \mathbf{U}_2, \mathcal{F}_{21}, P_{21}(\mathbf{u}_2) \rangle \\ &\vdots \\ \mathcal{M}_{2k_2} &= \langle \mathbf{V}, \mathbf{U}_2, \mathcal{F}_{2k_2}, P_{2k_2}(\mathbf{u}_2) \rangle \\ \mathcal{M}_{31} &= \langle \mathbf{V}, \mathbf{U}_3, \mathcal{F}_{31}, P_{31}(\mathbf{u}_3) \rangle \\ &\vdots \\ \mathcal{M}_{3k_3} &= \langle \mathbf{V}, \mathbf{U}_3, \mathcal{F}_{3k_3}, P_{3k_3}(\mathbf{u}_3) \rangle \end{aligned}$$

## Potential Causal Diagrams



## Observational Data



Markovian  
Parametrization

$$\begin{aligned} \mathcal{M}_{41} &= \langle \mathbf{V}, \mathbf{U}_4, \mathcal{F}_{41}, P_{41}(\mathbf{u}_4) \rangle \\ &\vdots \\ \mathcal{M}_{4k_4} &= \langle \mathbf{V}, \mathbf{U}_4, \mathcal{F}_{4k_4}, P_{4k_4}(\mathbf{u}_4) \rangle \\ \mathcal{M}_{51} &= \langle \mathbf{V}, \mathbf{U}_5, \mathcal{F}_{51}, P_{51}(\mathbf{u}_5) \rangle \\ &\vdots \\ \mathcal{M}_{5k_5} &= \langle \mathbf{V}, \mathbf{U}_5, \mathcal{F}_{5k_5}, P_{5k_5}(\mathbf{u}_5) \rangle \end{aligned}$$

Loss of Information / Knowledge

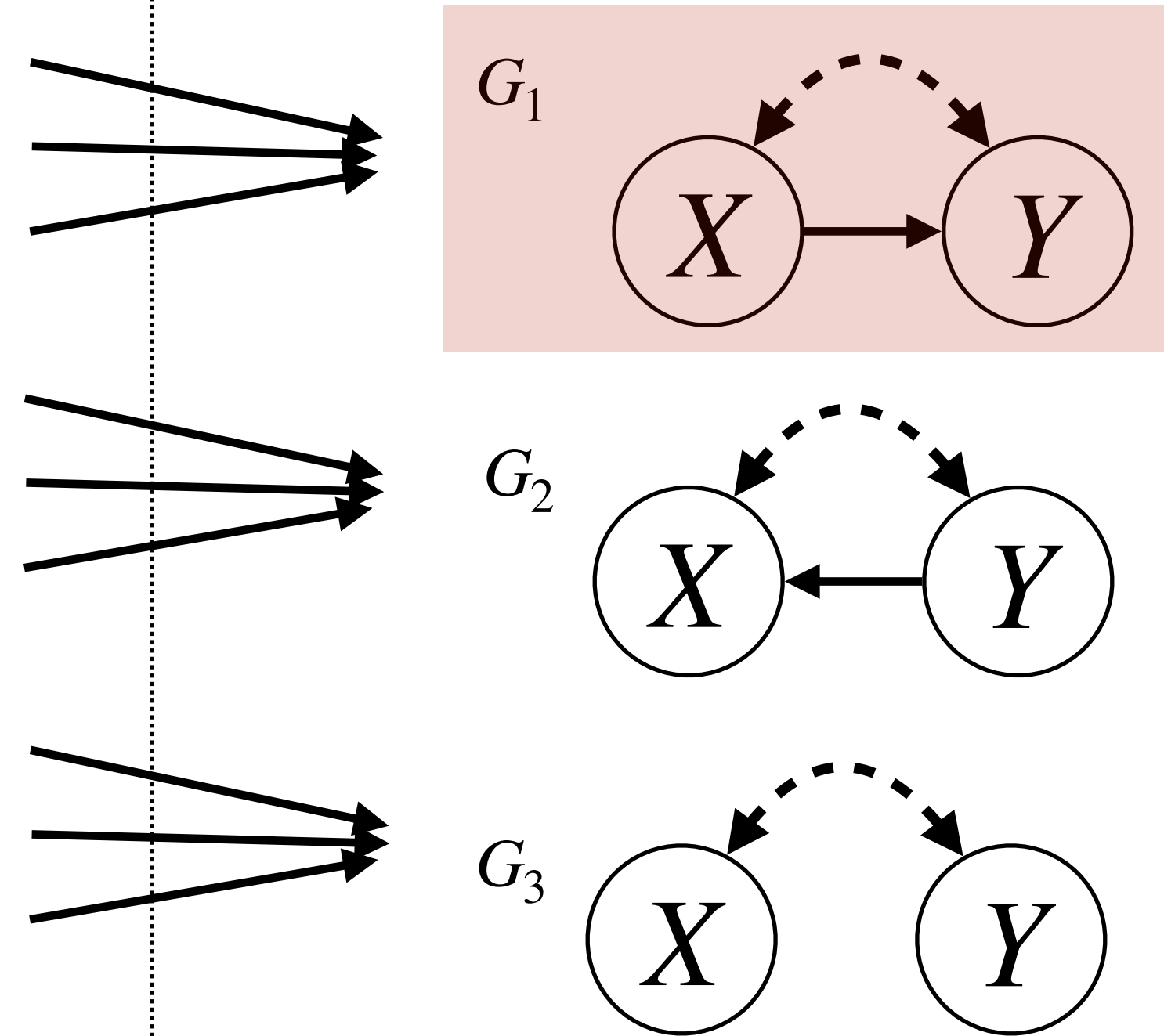


True  
Model

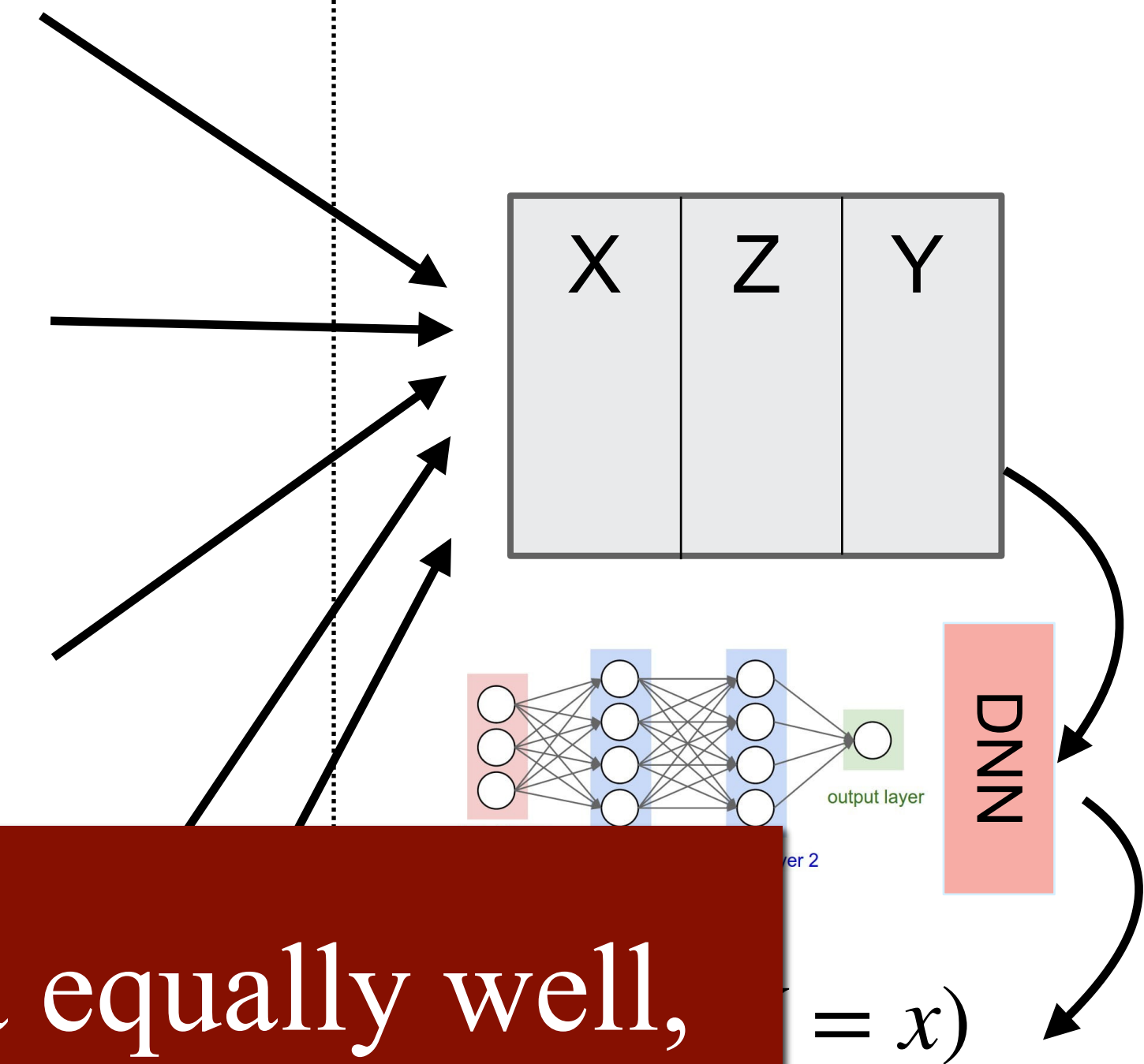
## Potential SCMs

$$\begin{aligned}\mathcal{M}_{11} &= \langle \mathbf{V}, \mathbf{U}_1, \mathcal{F}_{11}, P_{11}(\mathbf{u}_1) \rangle \\ &\vdots \\ \mathcal{M}_{1k_1} &= \langle \mathbf{V}, \mathbf{U}_1, \mathcal{F}_{1k_1}, P_{1k_1}(\mathbf{u}_1) \rangle \\ \mathcal{M}_{21} &= \langle \mathbf{V}, \mathbf{U}_2, \mathcal{F}_{21}, P_{21}(\mathbf{u}_2) \rangle \\ &\vdots \\ \mathcal{M}_{2k_2} &= \langle \mathbf{V}, \mathbf{U}_2, \mathcal{F}_{2k_2}, P_{2k_2}(\mathbf{u}_2) \rangle \\ \mathcal{M}_{31} &= \langle \mathbf{V}, \mathbf{U}_3, \mathcal{F}_{31}, P_{31}(\mathbf{u}_3) \rangle \\ &\vdots \\ \mathcal{M}_{3k_3} &= \langle \mathbf{V}, \mathbf{U}_3, \mathcal{F}_{3k_3}, P_{3k_3}(\mathbf{u}_3) \rangle\end{aligned}$$

## Potential Causal Diagrams



## Observational Data



Multiple neural nets fit the data equally well,  
leading to different causal explanations!

Loss of Information / Knowledge

# Super-Exponential Growth

The space of **Markovian Causal Diagrams** (a.k.a. Directed Acyclic Graphs, or DAGs for short) grows super-exponentially with the number  $n$  of variables, as shown by the following recurrence relation (Robinson, 1973):

$$|DAG(n)| = \sum_{i=1}^n \binom{n}{i} 2^{i(n-i)} |DAG(n-i)|$$

Inference through enumeration is  
not a good idea. :)

$n$	$ DAG(n) $
2	3
3	27
4	729
5	59.049
6	$1.4349 \times 10^7$
7	$1.0460 \times 10^{10}$
8	$2.2877 \times 10^{13}$

$$|ADMG(n)| \gg |DAG(n)|$$

The space of **Markovian Causal Diagrams** (a.k.a. Acyclic Directed Mixed Graphs, or ADMGs for short) also grows super-exponentially with the number  $n$  of variables, and it is much bigger than the space of DAGs:

$$|ADMG(n)| = |DAG(n)| \times 2^{n(n-1)/2}$$

Now, inference seems impossible...

Surprisingly, that is not the case!

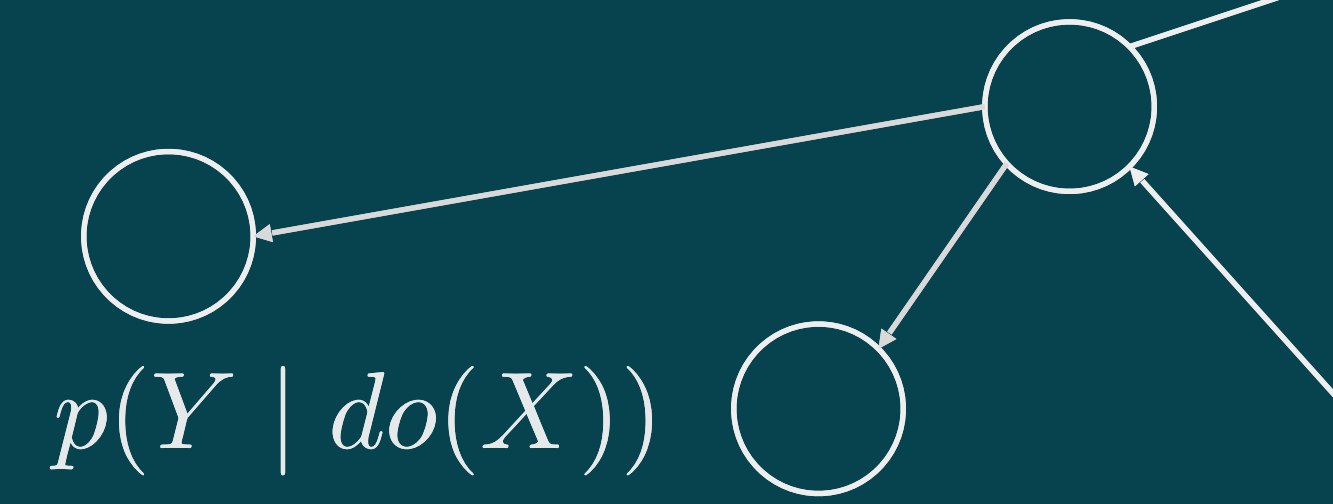
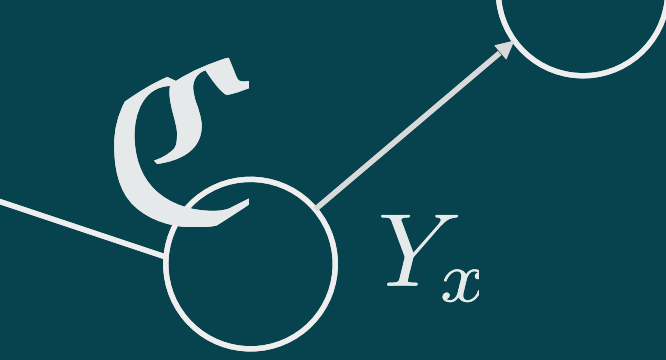
$n$	$ DAG(n) $	$ ADMG(n) $
2	3	6
3	27	216
4	729	46.656
5	59.049	$6.0457 \times 10^7$
6	$1.4349 \times 10^7$	$4.7019 \times 10^{11}$
7	$1.0460 \times 10^{10}$	$2.1936 \times 10^{16}$
8	$2.2877 \times 10^{13}$	$6.1410 \times 10^{21}$

# Causal Discovery



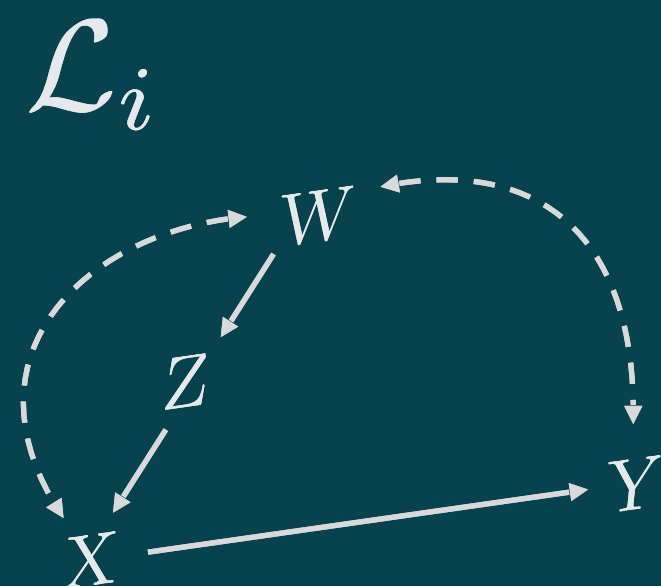
Can we learn a causal diagram  $\mathcal{G}$  from observational data?

In non-parametric settings, we can't learn the true causal diagram, but **Causal Discovery** algorithms such as the **Fast Causal Inference (FCI)** can learn a graphical representation of its ***Markov Equivalence Class (MEC)***!



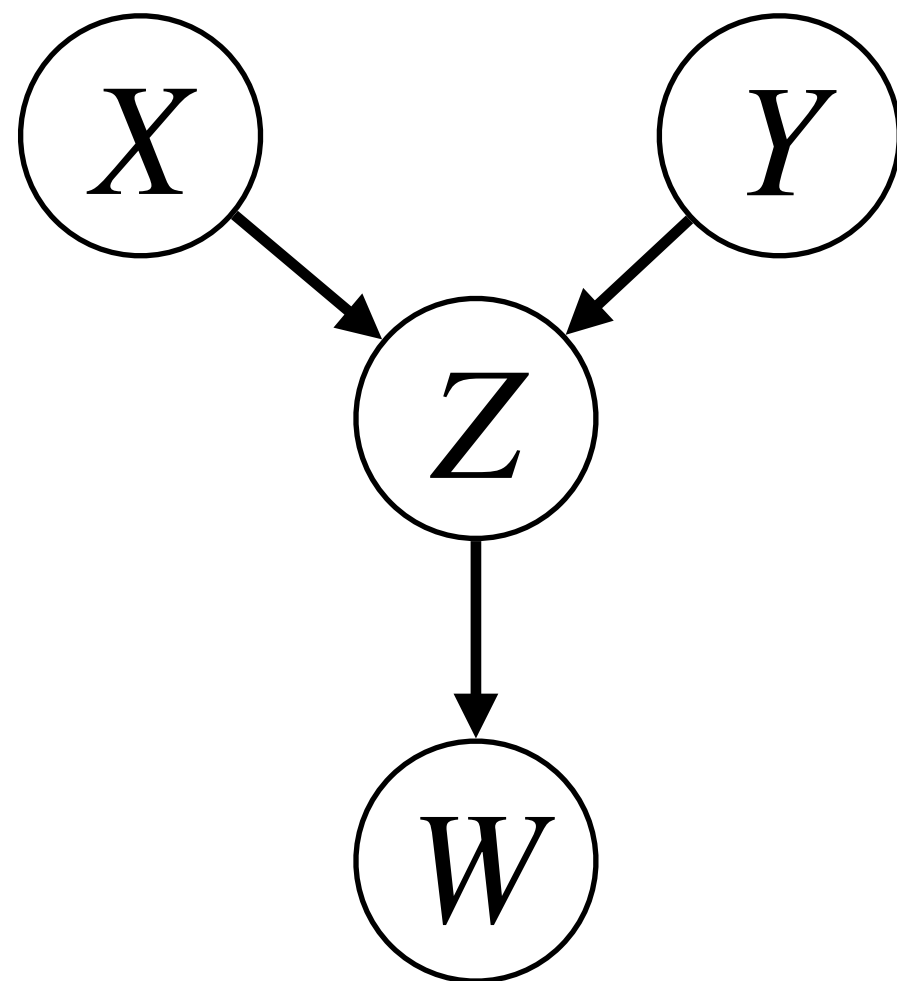
# 2 Encoding Conditional Independencies

## D-Separation and I-Maps





# Graphical Notation



$X$  and  $Y$  are *parents* of  $Z$ , i.e.,  $X, Y \in Pa(Z)$

$Z$  is a *child* of  $Y$ , i.e.,  $Z \in Ch(Y)$

$W$  is a *descendent* of  $X$ , i.e.,  $W \in De(X)$

$Y$  is *ancestor* of  $W$ , i.e.,  $Y \in An(W)$

$Y$  is *non-descendant* of  $X$ , i.e.,  $Y \in NDesc(X)$

$\langle X, Z, Y \rangle$  is a *collider triplet*

$\langle X, Z, W \rangle$  and  $\langle Y, Z, W \rangle$  is a *non-collider triplets*

**Note:** In many settings, the variable itself is included in their own set of parents, ancestors, children, and descendants.

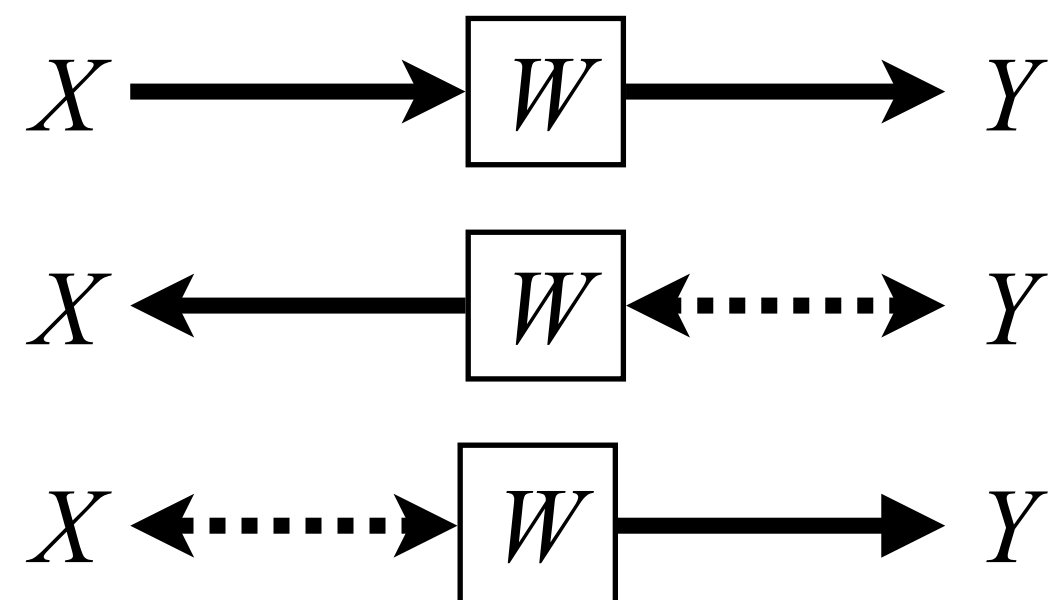
For example,  $X \in Ch(X)$ ,  $An(W) = \{X, Y, Z, W\}$ ,  $Pa(Z, W) = \{X, Y, Z, W\}$

# D-Separation and Implied Conditional Independencies

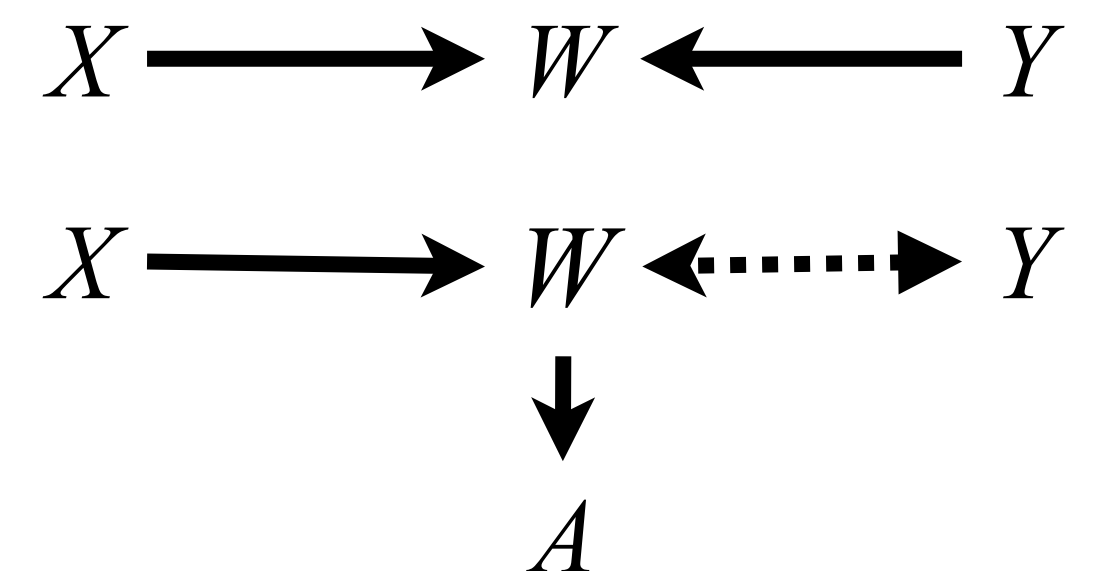
**Definition (active triplet):** A triplet in a subpath  $\langle V_i, V_m, V_j \rangle$  is said to be **active** relative to a set  $\mathbf{Z}$  if  $V_m$ :

1. Is a non-collider and not a member of  $\mathbf{Z}$ ; or
2. Is a collider and an ancestor of some member of  $\mathbf{Z}$ .

$W$  is non-collider  
(active if  $W \notin \mathbf{Z}$ )



$W$  is a collider  
(active if  $W \in \mathbf{Z}$  or any of  
its descendants is in  $\mathbf{Z}$ ,  
e.g.,  $A \in \mathbf{Z}$ )



# D-Separation and Implied Conditional Independencies

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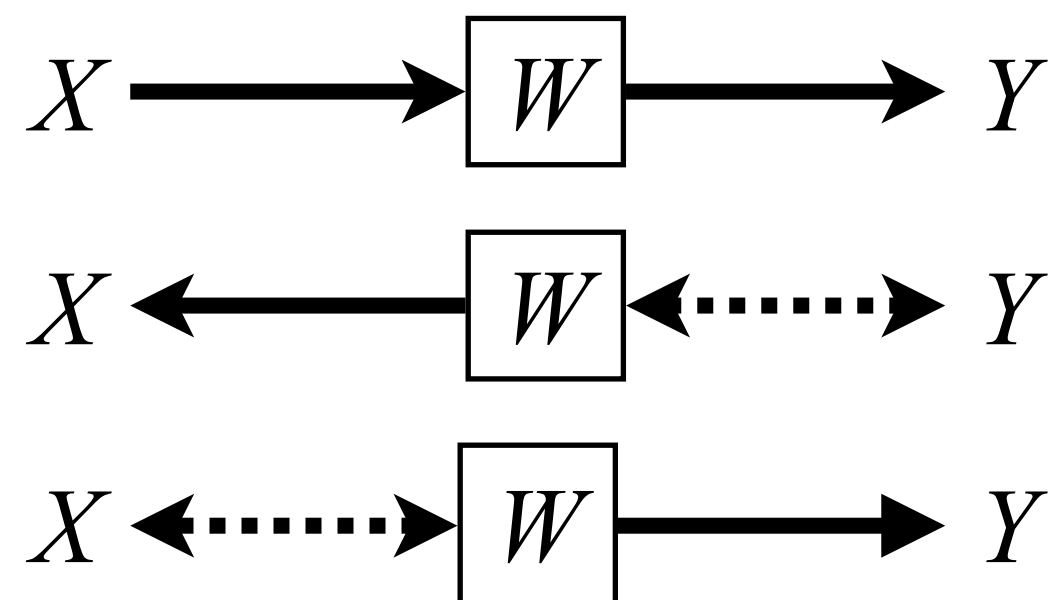
**Definition (d-connecting path):** A path  $p$  between  $X$  and  $Y$  in a causal diagram  $G$  is said to be **d-connecting** (or open/active) relative to a (possibly empty) set  $\mathbf{Z}$  ( $X, Y \notin \mathbf{Z}$ ) if and only if all triplets in it are active.

**Definition (d-separation):** A set  $\mathbf{Z}$  d-separates  $\mathbf{X}$  and  $\mathbf{Y}$  if and only if there is no d-connecting path between them relative to  $\mathbf{Z}$ . This is denoted by  $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G$ .

**Global Markov property:**  $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G \Rightarrow (\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_P$

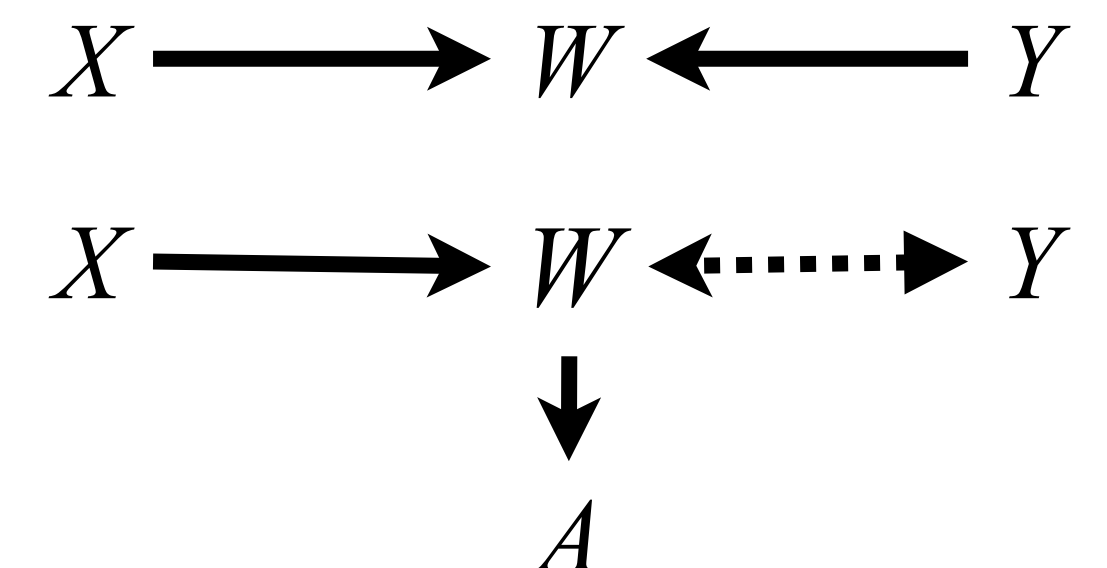
D-separations in  $G$  imply  
conditional independencies in  $P$

$W$  is non-collider  
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# D-Separation and Implied Conditional Independencies

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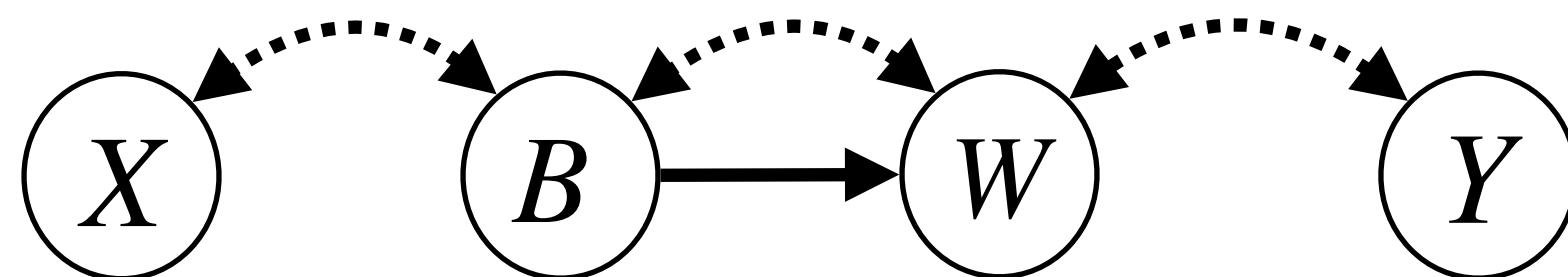
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D-separations in  $G$  imply  
conditional independencies in  $P$



Does  $\mathbf{Z}$  d-separates  $X$  and  $Y$ ?

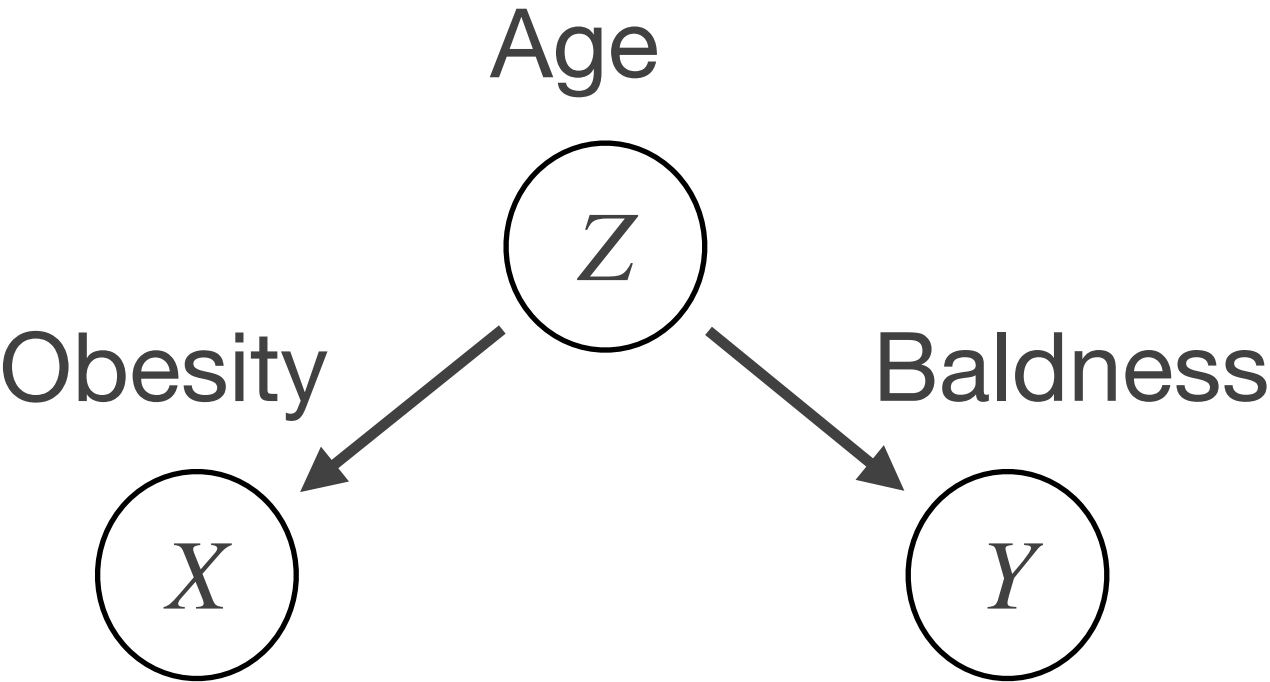
$\mathbf{Z}$ : ☒  $\{\}$  ☒  $\{B\}$  ☒  $\{W\}$  ☒  $\{B, W\}$

We have that  $(X \perp\!\!\!\perp Y)$  and  $(X \perp\!\!\!\perp Y \mid B)$ , but  $(X \not\perp\!\!\!\perp Y \mid W)$  and  $(X \not\perp\!\!\!\perp Y \mid B, W)$

# Special Triplets and Formations

## Fork

*Z* as a common cause

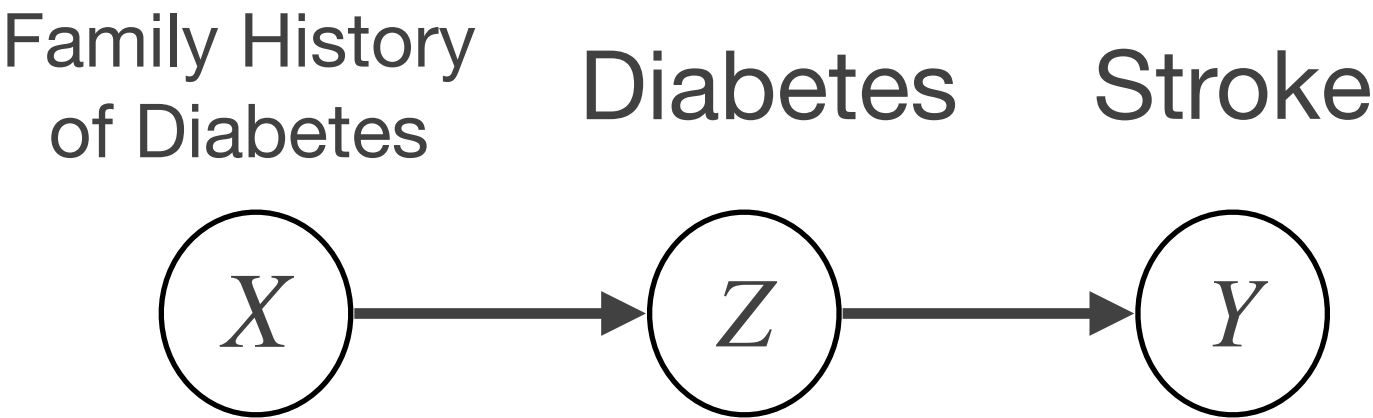


$$\cancel{X \perp\!\!\!\perp Y}$$

$$X \perp\!\!\!\perp Y|Z$$

## Chain

*Z* as a mediator

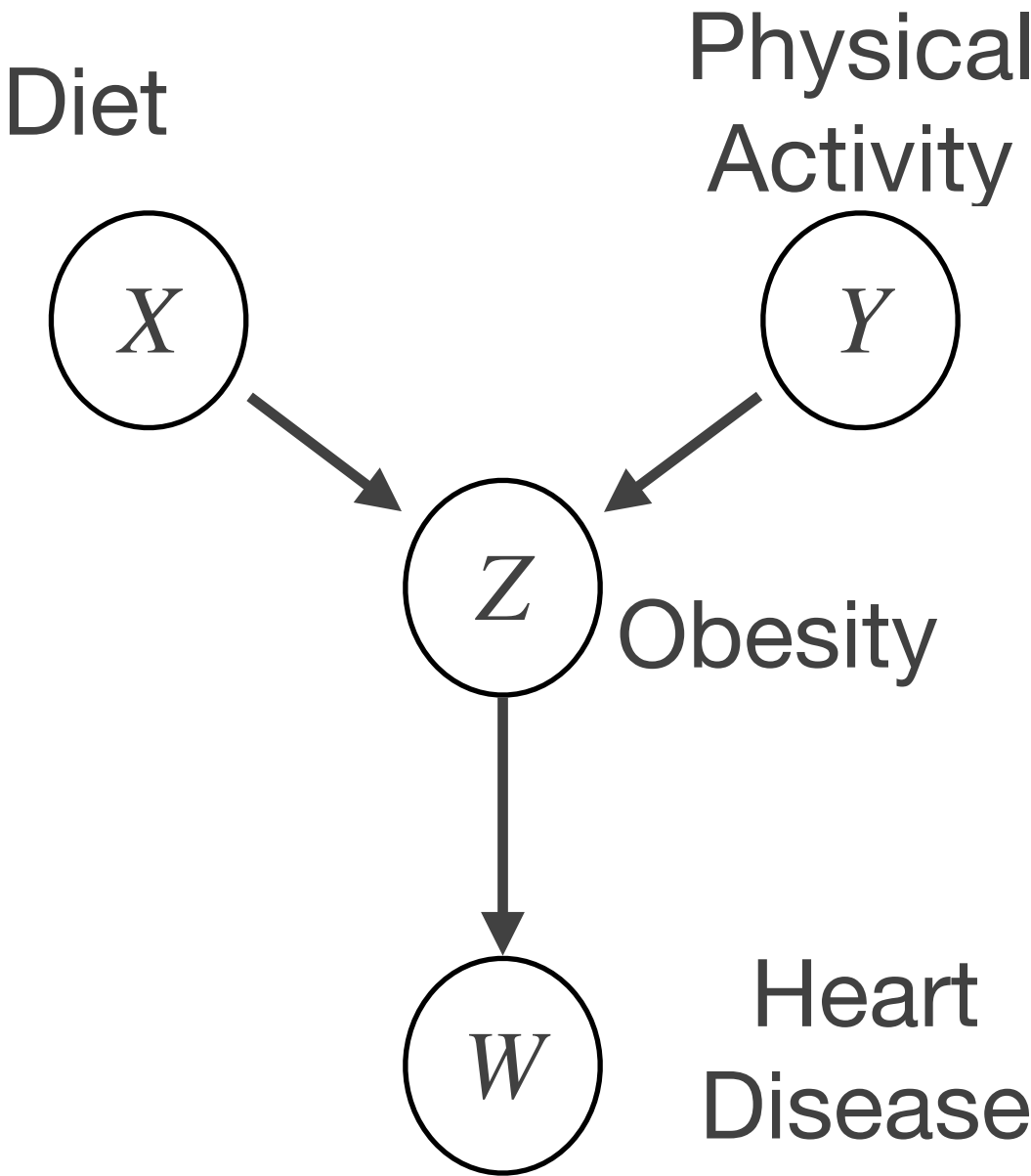


$$\cancel{X \perp\!\!\!\perp Y}$$

$$X \perp\!\!\!\perp Y|Z$$

## V-Structure

*Z* as a collider or common effect



$$X \perp\!\!\!\perp Y$$

$$\cancel{X \perp\!\!\!\perp Y|Z}$$

$$\cancel{X \perp\!\!\!\perp Y|W}$$

In both cases, *Z* is a non-collider!



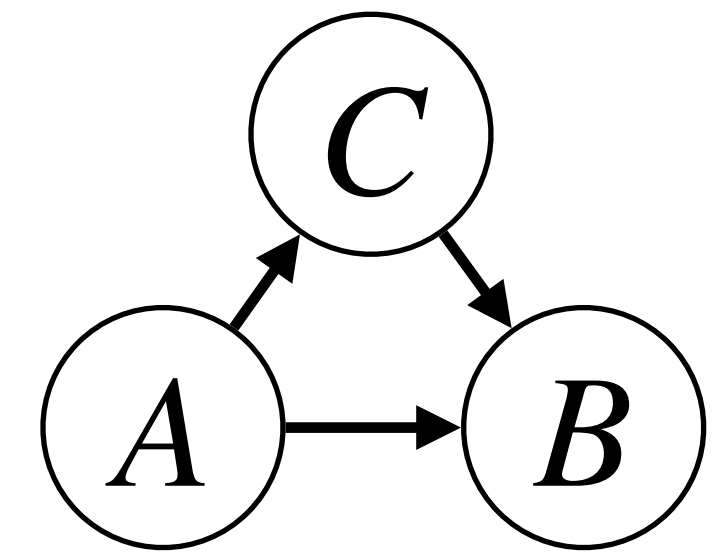
# Independence Maps (I-Maps)

**Definition (I-Map):** If, for a distribution  $P(\mathbf{V})$ , and any sets  $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathbf{V}$ , it holds that

$$(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G \Rightarrow (\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_P,$$

then  $G$  is an *I-Map of  $P$* .

And,  $P$  is Markov Relative to  $G$



$G$  is I-Map of any  
 $P(A, B, C)$

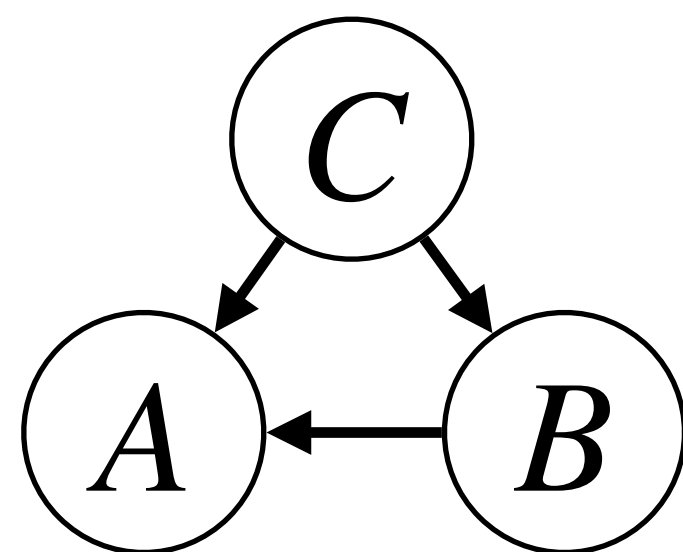
A complete graph trivially  
satisfies any distribution

# Minimal I-Maps and Bayesian Networks

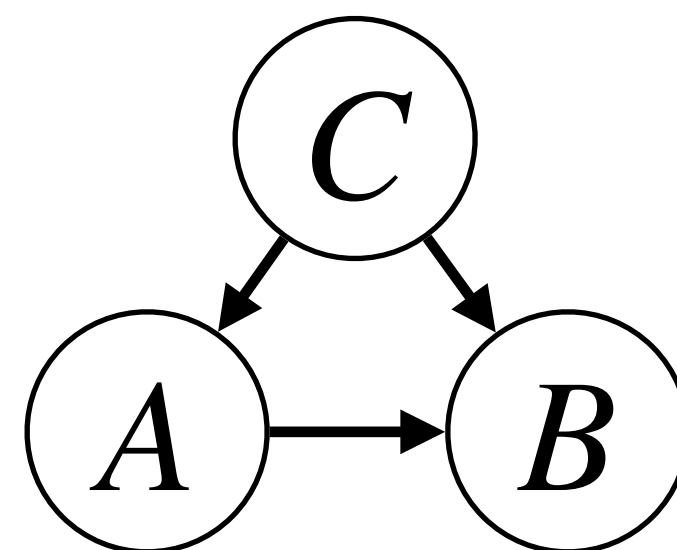
**Definition (Minimal I-Map):** If  $G$  is an I-Map of  $P$  and none of its edges can be removed without ceasing its I-Map property of  $P$ , then  $G$  is a **minimal I-Map of  $P$** .

**Definition (Bayesian Network, BN for short):** A Bayesian Network is a directed acyclic graph (DAG) or acyclic directed mixed graph (ADMG)  $G$  over  $\mathbf{V}$  that is a minimal I-map of  $P(\mathbf{V})$ .

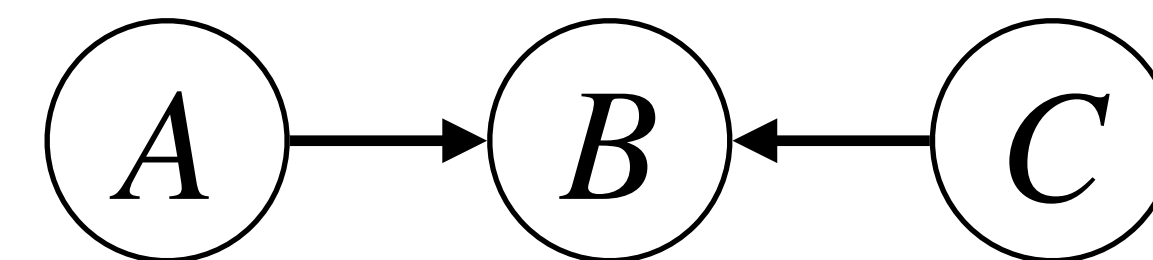
Consider  $P(A, B, C)$  with  $A \perp\!\!\!\perp C$  being the **only** independence relation.



$G_1$  is I-Map of  
 $P(A, B, C)$



$G_2$  is I-Map of  
 $P(A, B, C)$

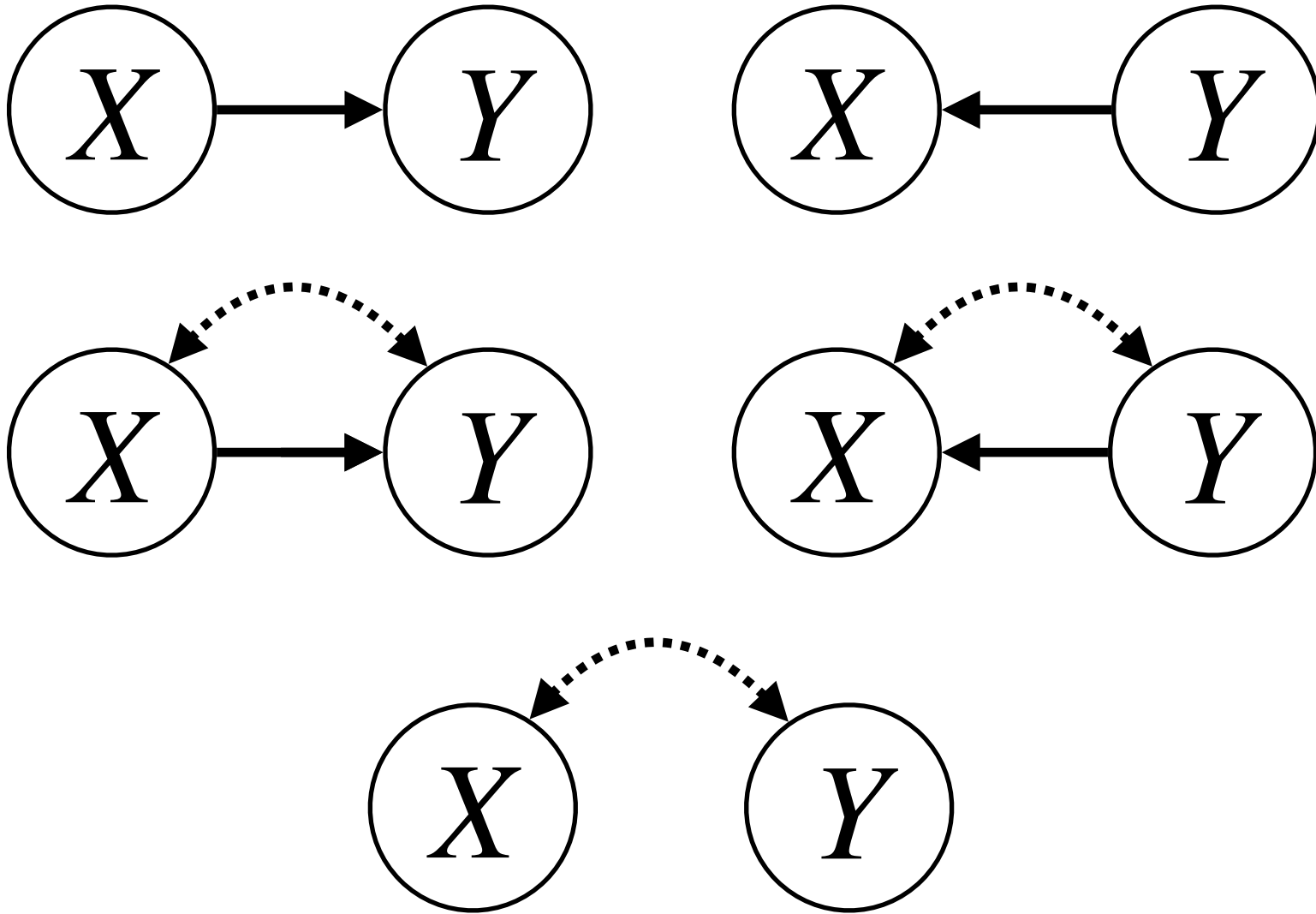


$G_3$  is minimal I-Map of  
 $P(A, B, C)$

$A \perp\!\!\!\perp C$   
 ~~$A \perp\!\!\!\perp C \mid B$~~   
 ~~$A \perp\!\!\!\perp B$~~   
 ~~$A \perp\!\!\!\perp B \mid C$~~   
 ~~$B \perp\!\!\!\perp C$~~   
 ~~$B \perp\!\!\!\perp C \mid A$~~

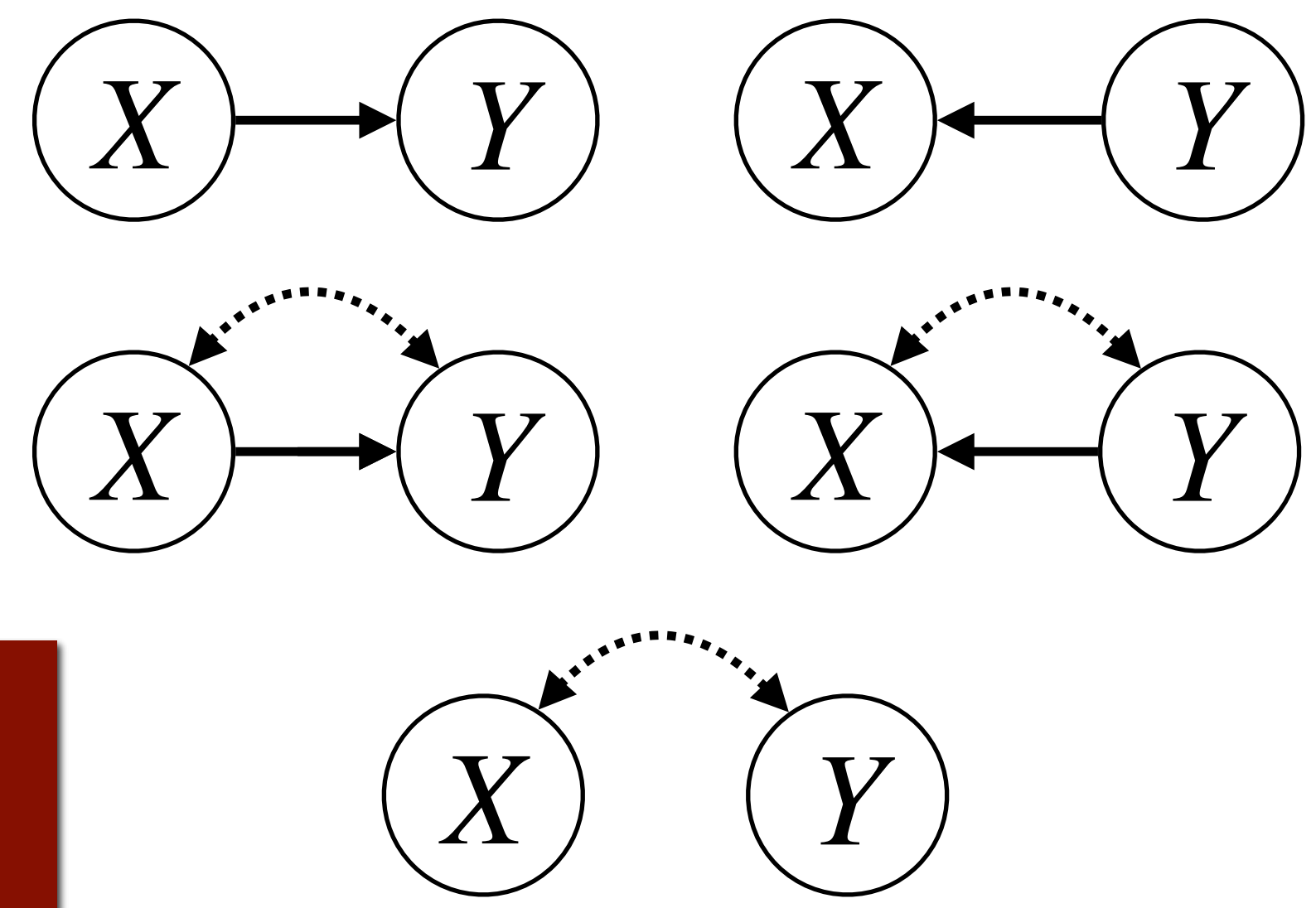
# Markov Equivalence Class

**Definition (Markov Equivalence Class, MEC for short):** A Markov Equivalence Class is a set of models that encode the same set of conditional independencies.

Distribution	Factorization	Bayesian Networks
$P(X, Y)$ with $P(Y X) \neq P(Y)$ i.e., $X \not\perp\!\!\!\perp Y$	$P(x, y) = P(y x)P(x)$ $P(x, y) = P(x y)P(y)$	<div data-bbox="2902 647 3312 789">Markov Equivalent BNs</div> 

# Markov Equivalence Class

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All models imply no independence and no other invariance

# Markov Equivalence Class

Distribution	Factorization	Bayesian Networks
$P(X, Y, Z)$ with $P(Y X, Z) = P(Y X)$ i.e., $X \perp\!\!\!\perp Y Z$	$P(x, y, z) = P(y x, z)P(z x)P(x)$ $= P(y z)P(z x)P(x)$ $P(x, y, z) = P(x y, z)P(y z)P(z)$ $= P(x z)P(z y)P(y)$ $P(x, y, z) = P(y x, z)P(x z)P(z)$ $= P(y z)P(x z)P(z)$	<p>Markov Equivalent</p>



# Markov Equivalence Class

## Distribution

$$P(X, Y, Z)$$

$$\text{with } P(Y|X, Z) = P(Y|X)$$

$$\text{i.e., } X \perp\!\!\!\perp Y|Z$$

## Factorization

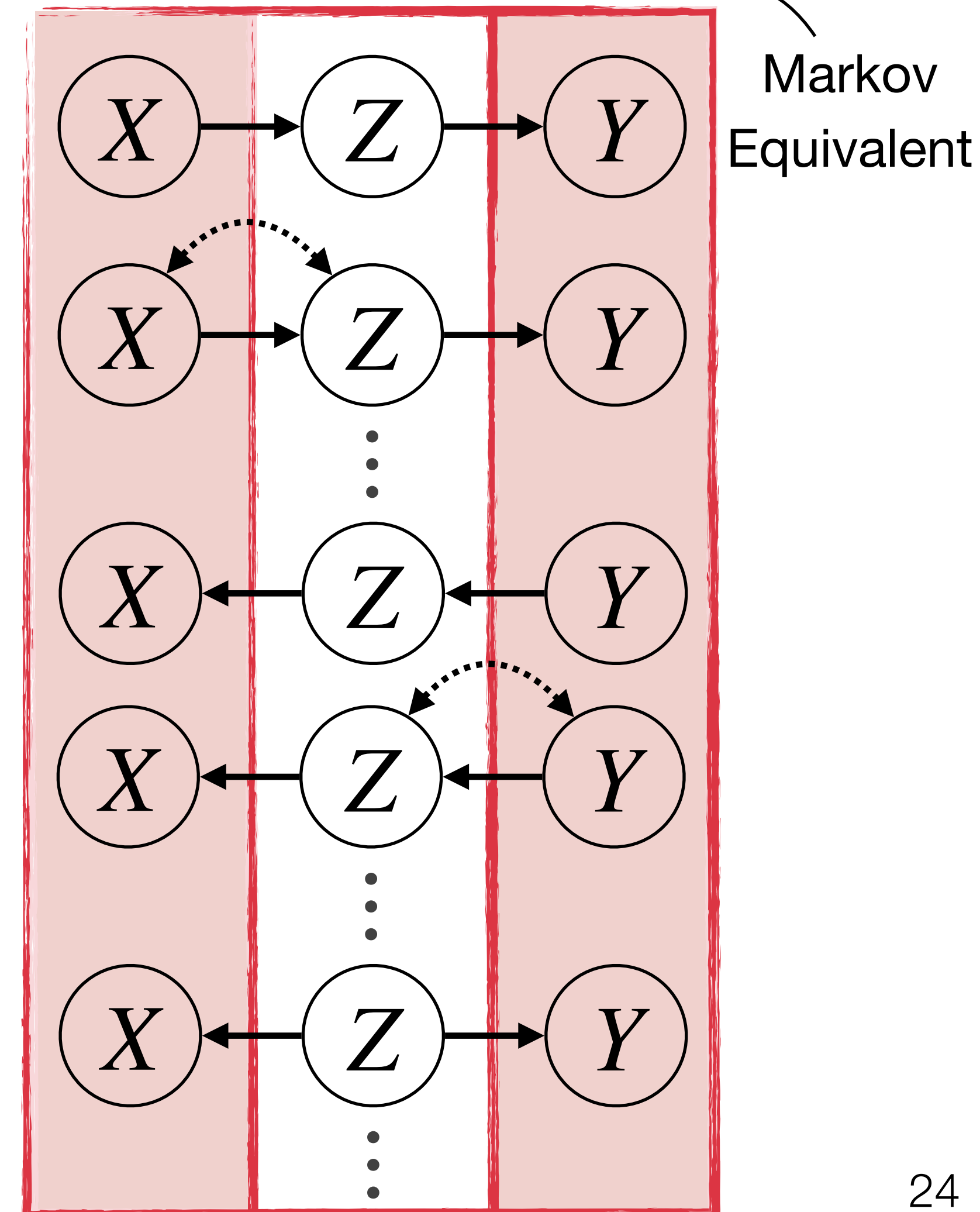
$$\begin{aligned} P(x, y, z) &= P(y|x, z)P(z|x)P(x) \\ &= P(y|z)P(z|x)P(x) \end{aligned}$$

$$\begin{aligned} P(x, y, z) &= P(x|y, z)P(y|z)P(z) \\ &= P(x|z)P(z|y)P(y) \end{aligned}$$

All models imply *only*  $X \perp\!\!\!\perp Y|Z$  and  $Z$  is always a *non-collider* in such models.

$$= P(y|z)P(x|z)P(z)$$

## Bayesian Networks



# Markov Equivalence Class

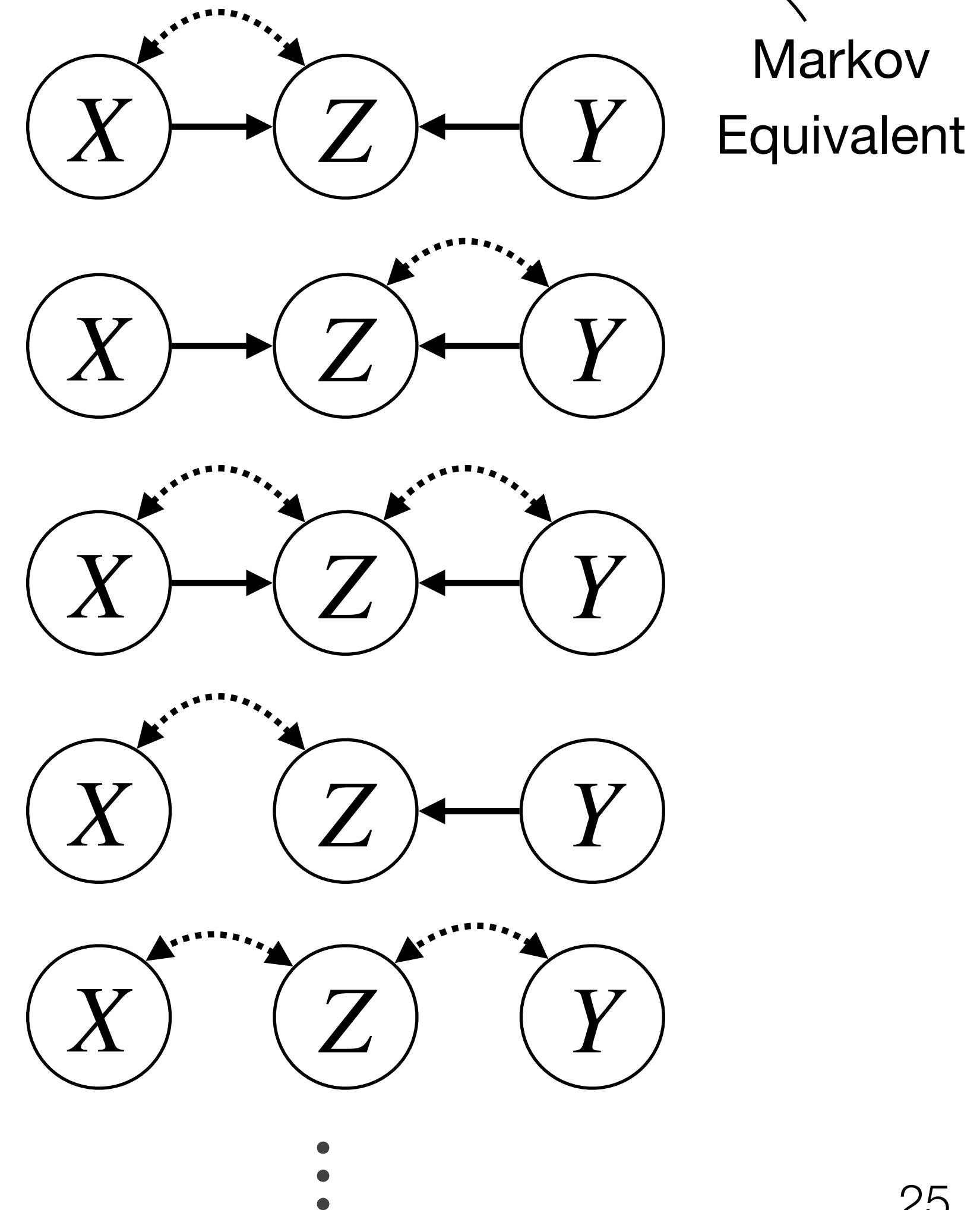
## Distribution

$P(X, Y, Z)$   
 with  $P(Y|X) = P(Y)$   
 i.e.,  $X \perp\!\!\!\perp Y$

## Factorization

$$\begin{aligned} P(x, y, z) &= P(z|x, y)P(x|y)P(y) \\ &= P(z|x, y)P(x)P(y) \end{aligned}$$

## Bayesian Networks



# Markov Equivalence Class

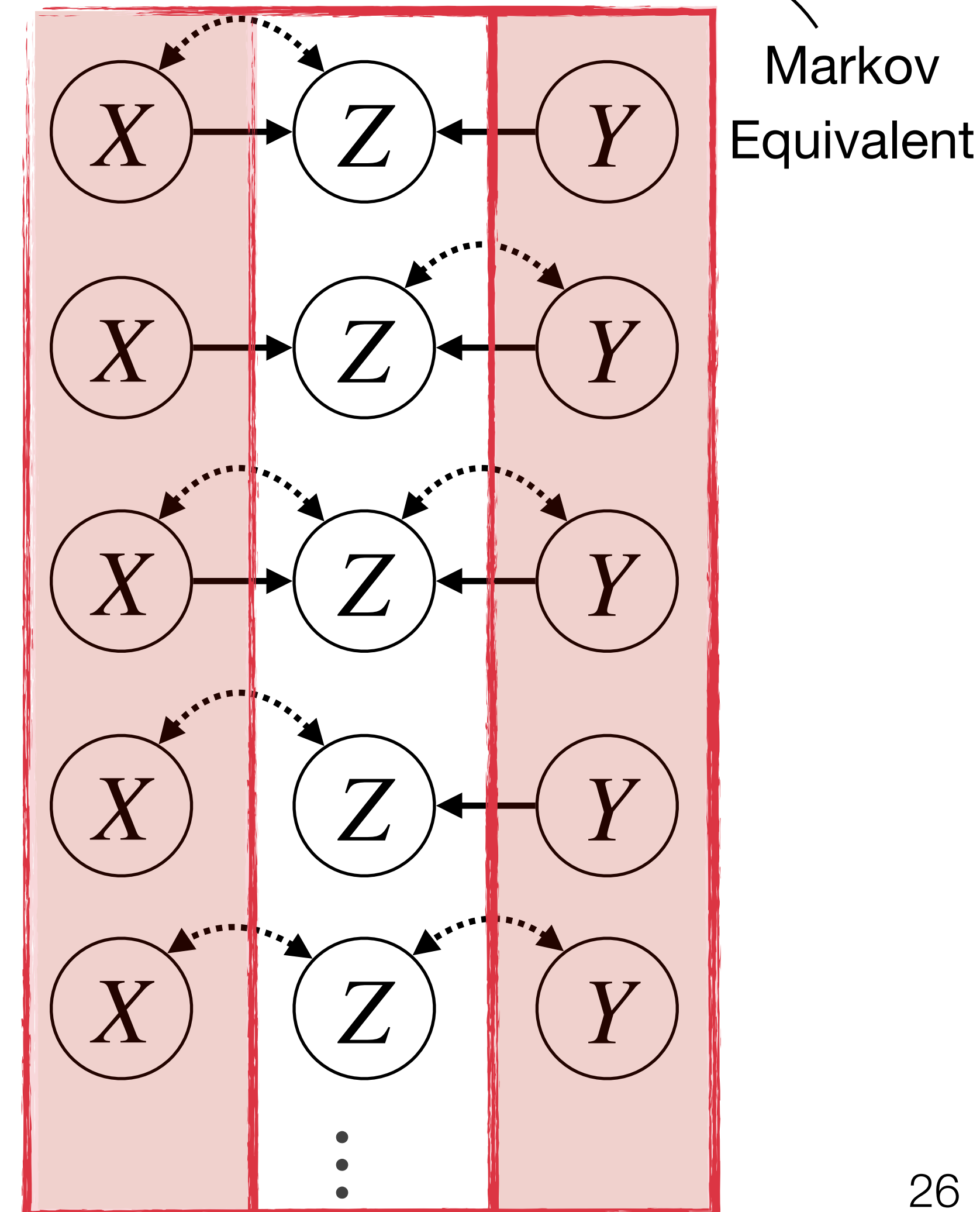
## Distribution

$P(X, Y, Z)$   
 with  $P(Y|X) = P(Y)$   
 i.e.,  $X \perp\!\!\!\perp Y$

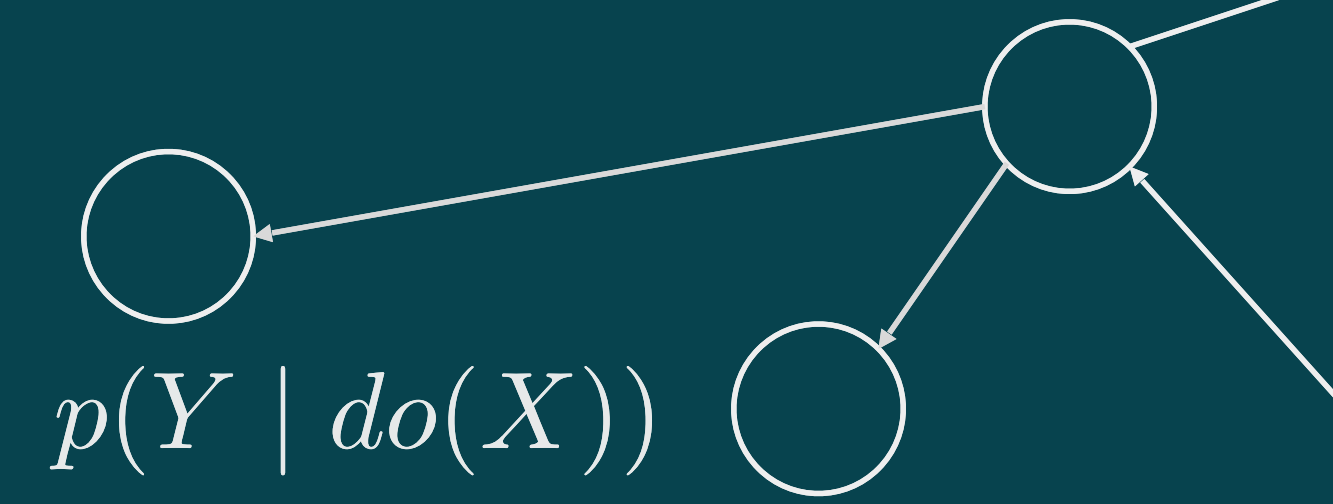
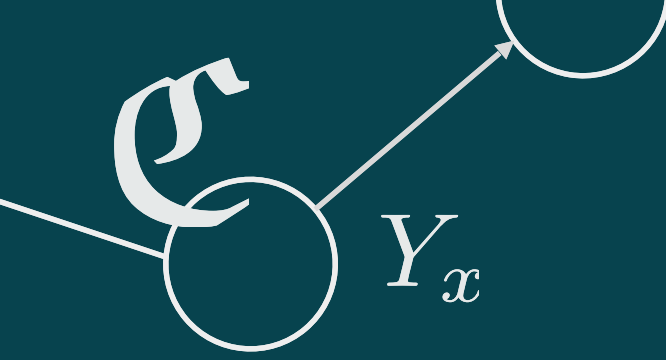
## Factorization

$$P(x, y, z) = P(z|x, y)P(x|y)P(y) \\ = P(z|x, y)P(x)P(y)$$

## Bayesian Networks

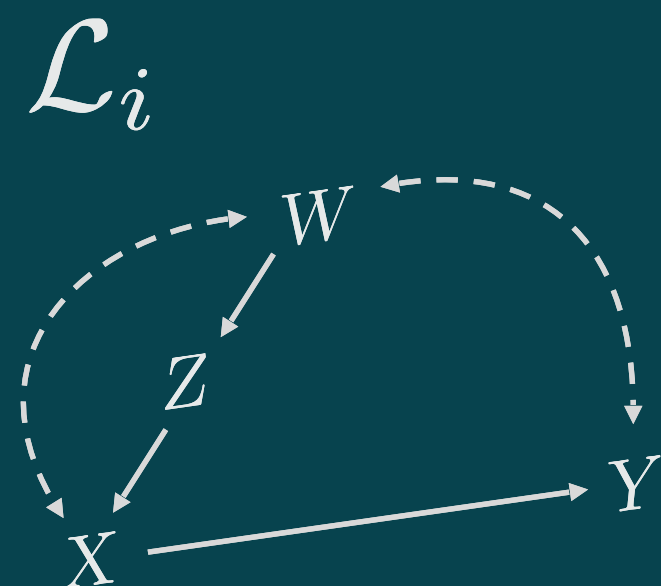


All models imply *only*  $X \perp\!\!\!\perp Y$  and  
 $Z$  is always a *collider* in such models,  
 Note:  $Z$  is never an ancestor of  $X$  or  $Y$



# 3 Representing Markov Equivalence Classes

## Partial Ancestral Graphs



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Machines Climbing Pearl's Ladder of Causation

# Inducing Paths

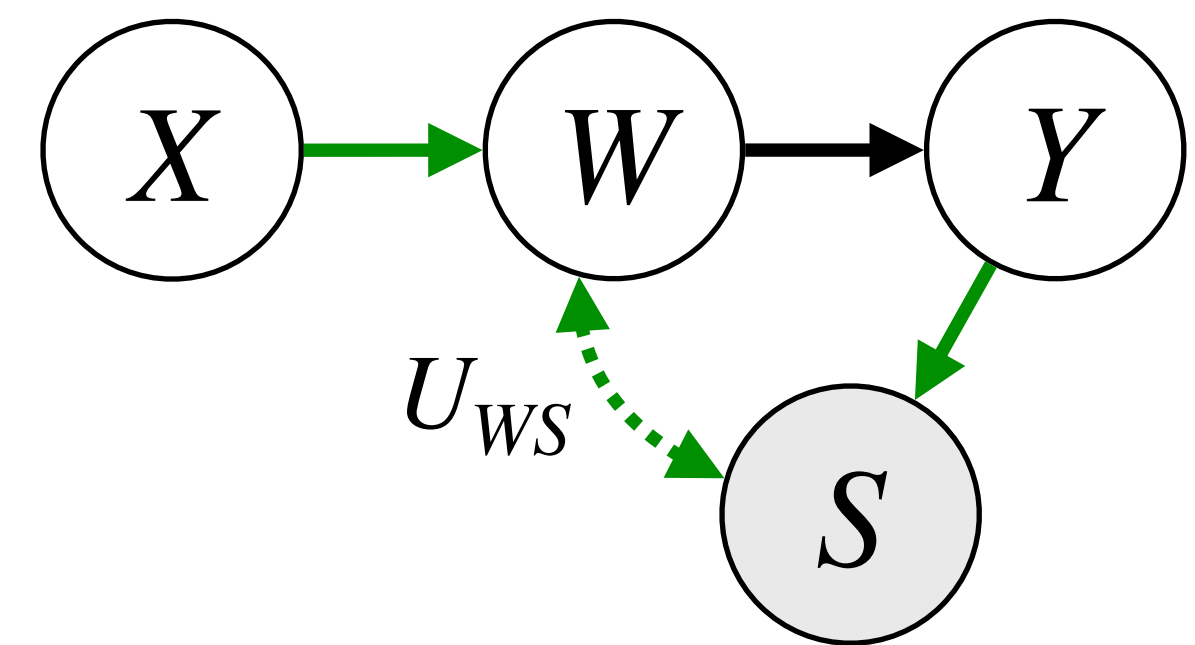
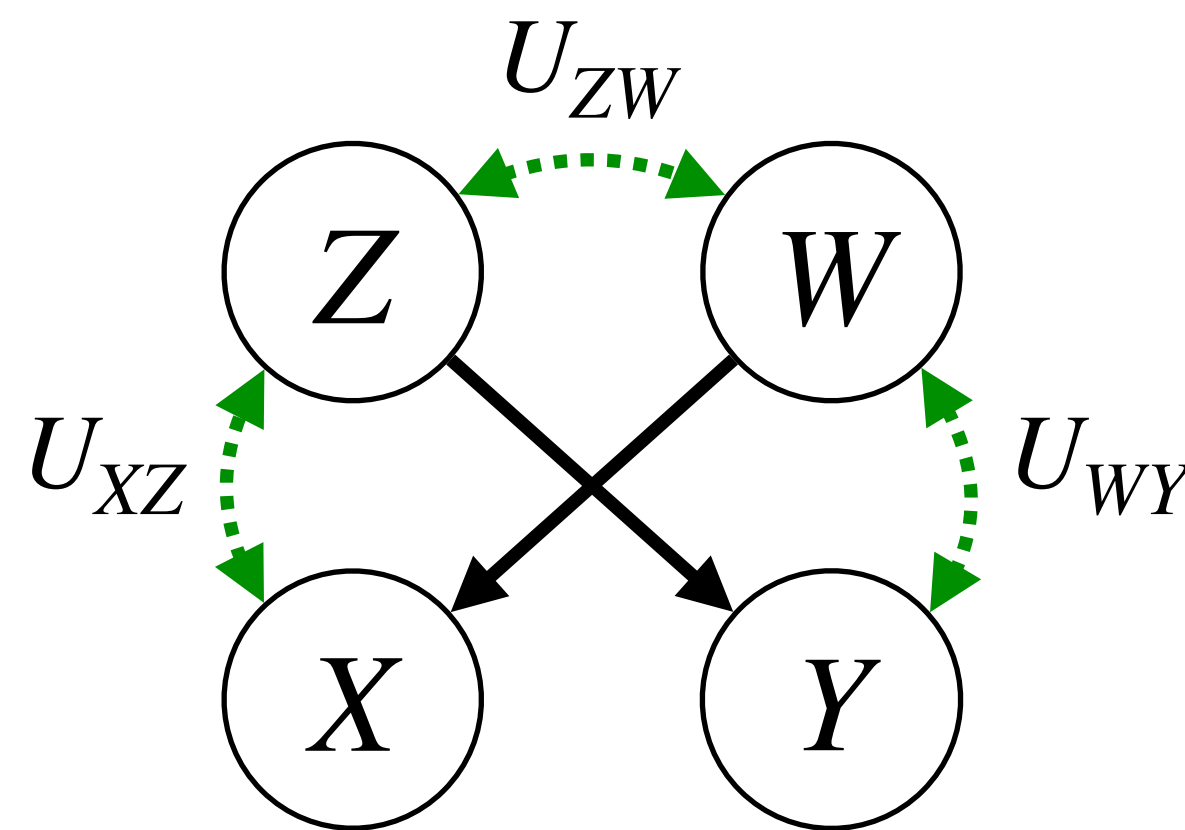
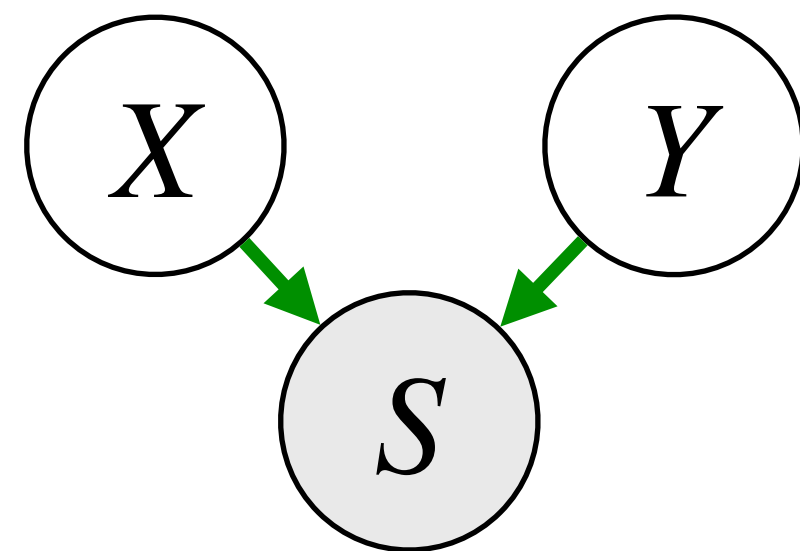
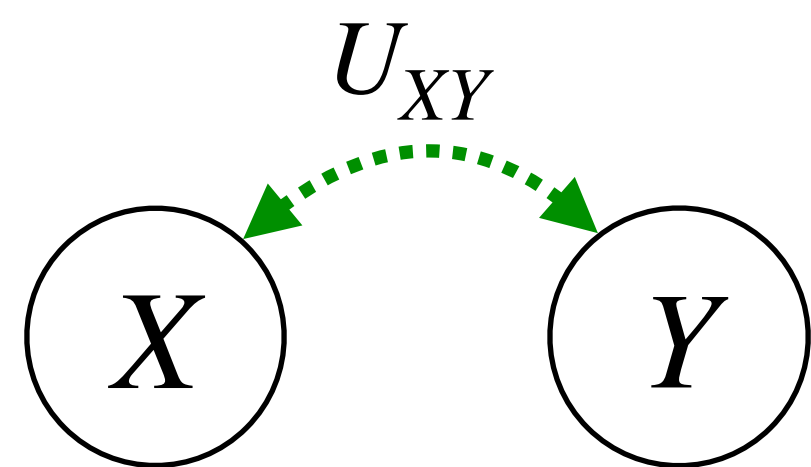
For an Bayesian Network over  $\mathbf{V} \cup \mathbf{U} \cup \mathbf{S}$ , where

$\mathbf{V}$ : set of observed variables

$\mathbf{U}$ : set of latent or unobserved variables, and

$\mathbf{S}$ : set of unobserved selection variables,

A path  $p$  between  $X$  and  $Y$  is called an **inducing path** if it every non-endpoint vertex on  $p$  is a collider that is either an ancestor of  $X$  or  $Y$ , or a member of  $\mathbf{S}$ .



$X, Y, Z, W \in \mathbf{V}$

$S \in \mathbf{S}$

$U_{XY}, U_{XZ}, U_{ZW}, U_{WY}, U_{WS} \in \mathbf{U}$

$X$  and  $Y$  are not separable when there is an inducing path connecting them!



# Partial Ancestral Graphs

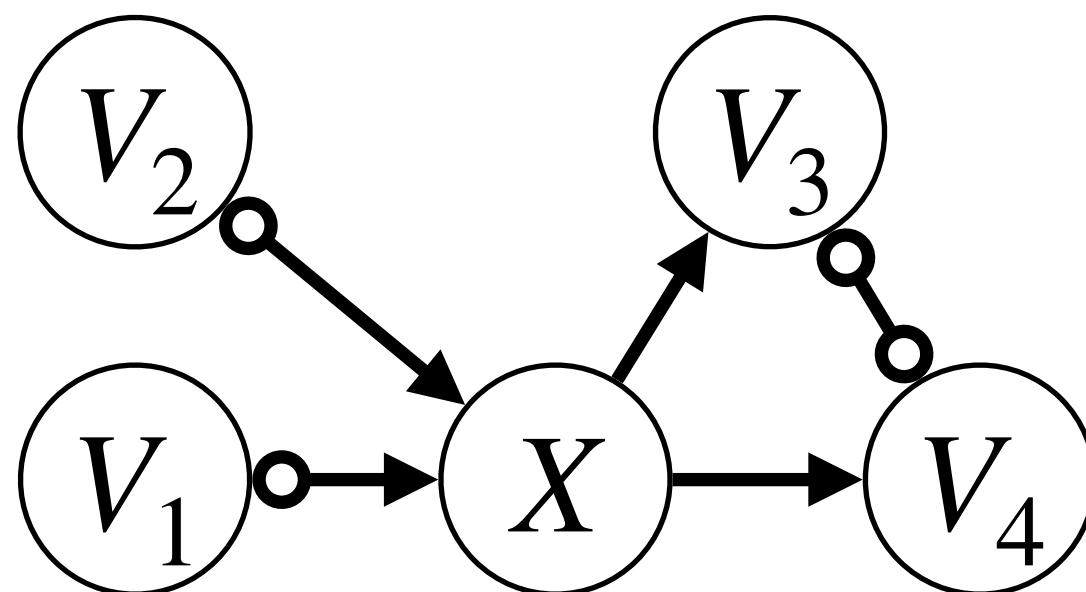
A **partial ancestral graph (PAG)** for a BN  $G$  is a graph  $\mathcal{P}$  with six kinds of edges ( $-$ ,  $\rightarrow$ ,  $\leftrightarrow$ ,  $\circ-$ ,  $\circ\rightarrow$ ,  $\circ\leftrightarrow$ ), such that

- (1) Every edge in  $\mathcal{P}$  corresponds to an inducing path in any member of the MEC of  $G$ ;
- (2) Every non-circle edge mark represents an **invariant ancestral or non-ancestral relationship** in the MEC of  $G$

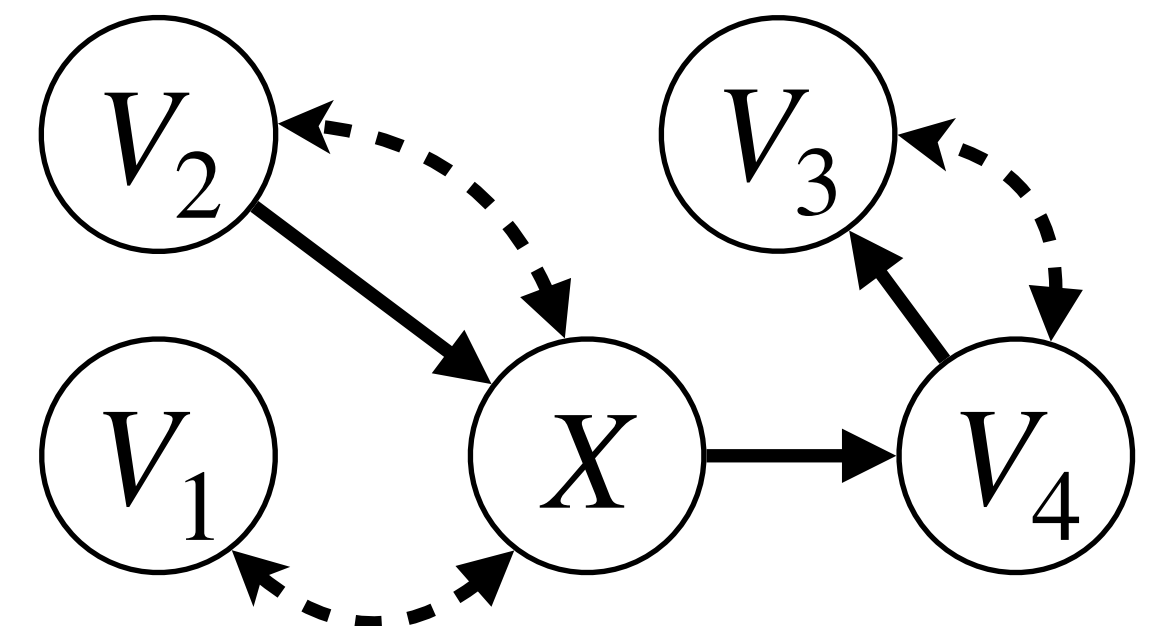
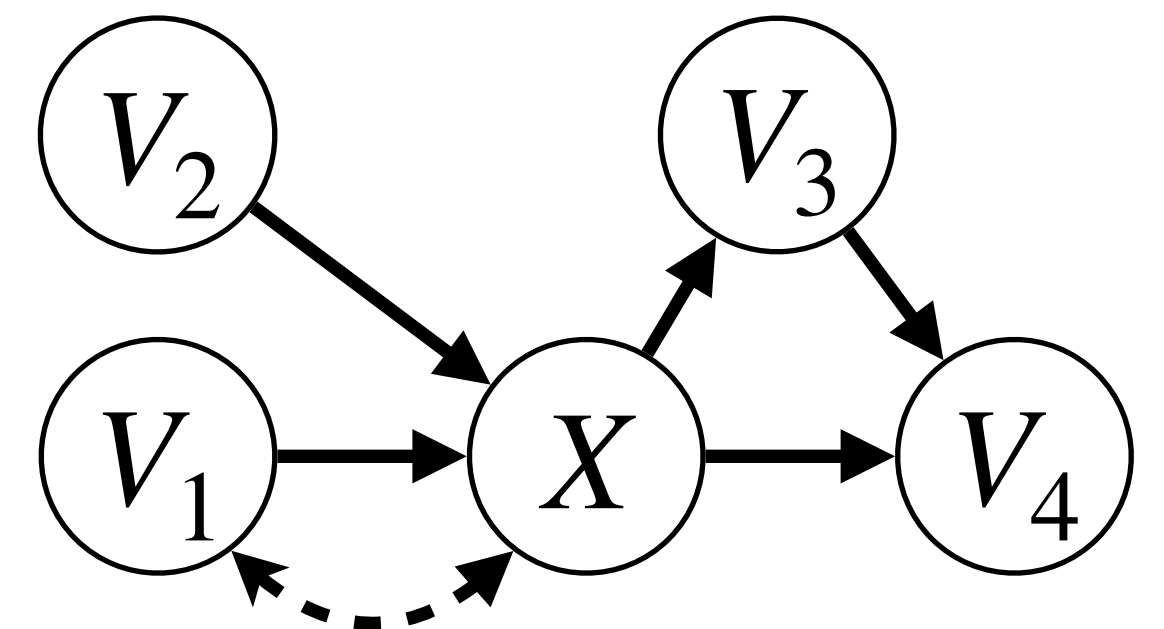
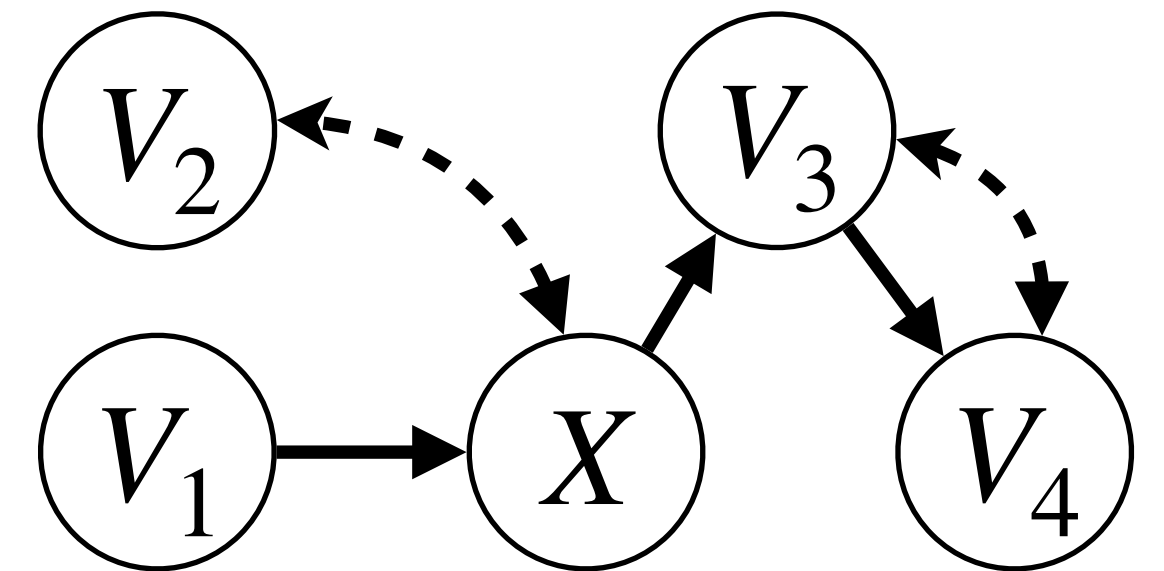
Arrowhead  $\Rightarrow$  non-ancestrality

Tail  $\Rightarrow$  ancestrally

PAG

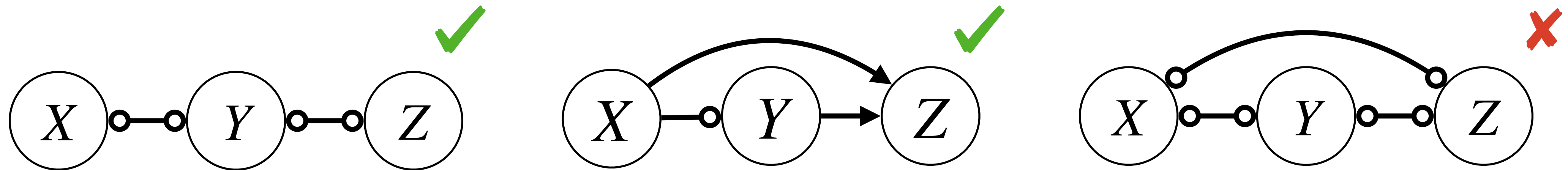


$X \rightarrow V_3$	$\Rightarrow$ $X$ ancestral of $V_3$
$X \rightarrow V_4$	$\Rightarrow$ $X$ ancestral of $V_4$
$V_1 \circ \rightarrow X$	$\Rightarrow$ $X$ non-ancestral of $V_1$
$V_2 \circ \rightarrow X$	$\Rightarrow$ $X$ non-ancestral of $V_2$

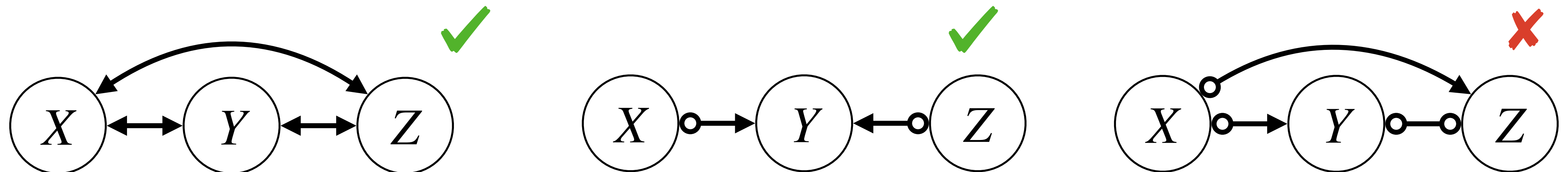


# Definite Triplets in PAGs

**Definition (definite non-collider):** A node  $Y$  of a triplet  $\langle X, Y, Z \rangle$  in a PAG is a definite non-collider if the edge between  $X$  and  $Y$  or the edge between  $Y$  and  $Z$  is out of  $Y$ , or both edges have a circle mark at  $Y$  and  $X$  and  $Z$  are not adjacent.



**Definition (collider):** As before, a node  $Y$  of a triplet  $\langle X, Y, Z \rangle$  in a PAG is a definite collider if both the between  $X$  and  $Y$  and the edge between  $Y$  and  $Z$  are into  $Y$ .

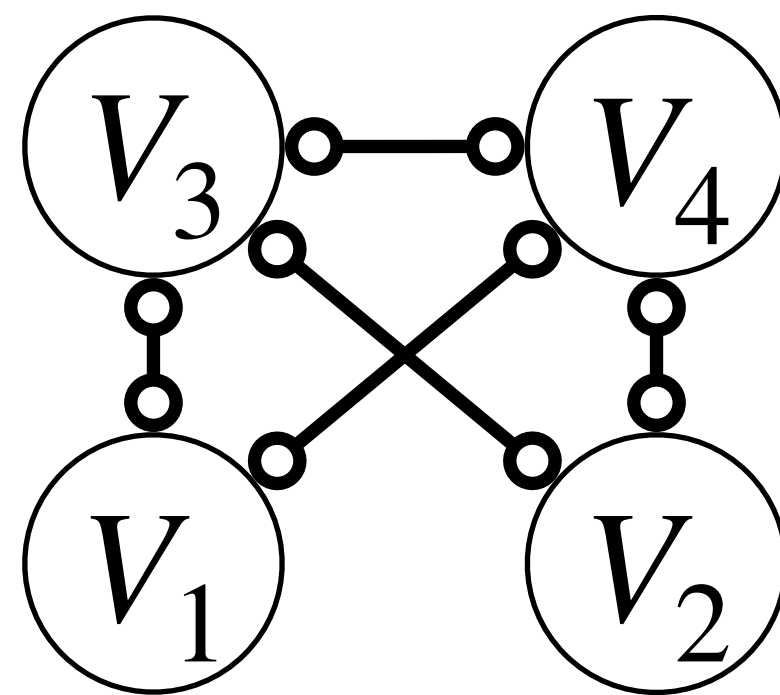


# M-Separation in PAGs

**Definition (definite m-connecting path):** In a PAG, a path  $p$  between  $X$  and  $Y$  is a *definite m-connecting path* relative to a (possibly empty) set  $\mathbf{Z}$  ( $X, Y \notin \mathbf{Z}$ ) if every non-endpoint vertex on  $p$  is either a definite non-collider or a collider and:

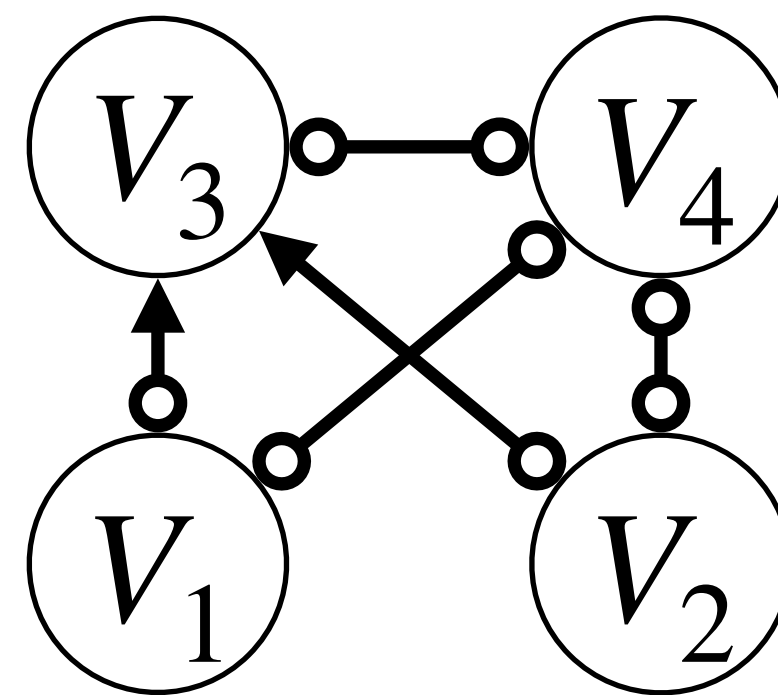
- i. Every definite non-collider on  $p$  is not a member of  $\mathbf{Z}$ ;
- ii. Every collider on  $p$  is an ancestor of some member of  $\mathbf{Z}$ .

**Definition (m-separation):** In a PAG,  $X$  and  $Y$  are m-separated by  $\mathbf{Z}$  if there is no definite m-connecting path between them relative to  $\mathbf{Z}$ .



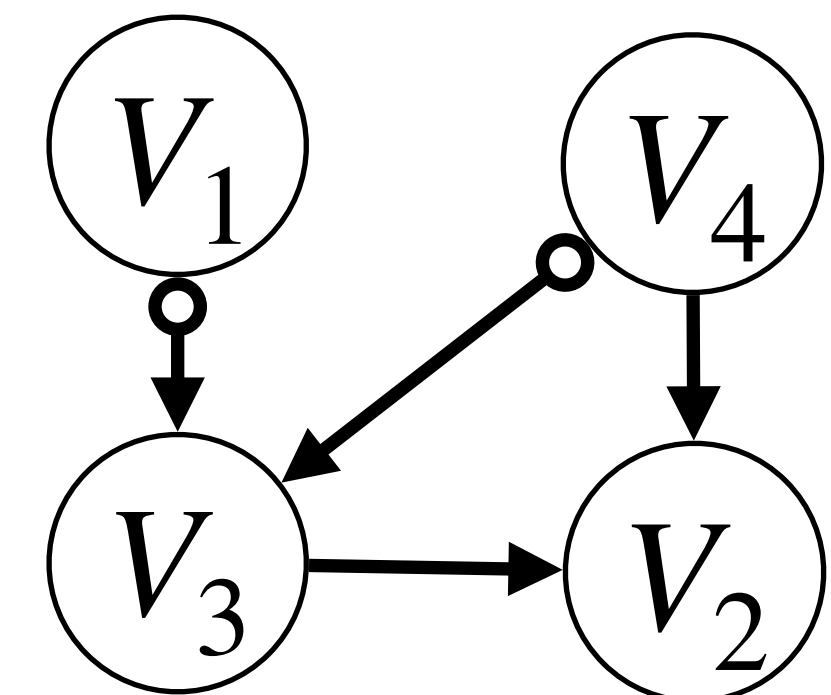
$$V_1 \perp\!\!\!\perp V_2 \mid V_3, V_4$$

$$\cancel{V_1 \perp\!\!\!\perp V_2 \mid V_3} \quad \cancel{V_1 \perp\!\!\!\perp V_2 \mid V_4}$$



$$V_1 \perp\!\!\!\perp V_2 \mid V_4$$

$$\cancel{V_1 \perp\!\!\!\perp V_2 \mid V_3, V_4} \quad \cancel{V_1 \perp\!\!\!\perp V_2 \mid V_3}$$



$$V_1 \perp\!\!\!\perp V_2 \mid V_3, V_4 \quad V_1 \perp\!\!\!\perp V_4$$

$$\cancel{V_1 \perp\!\!\!\perp V_4 \mid V_3}$$

# M-Separation in PAGs

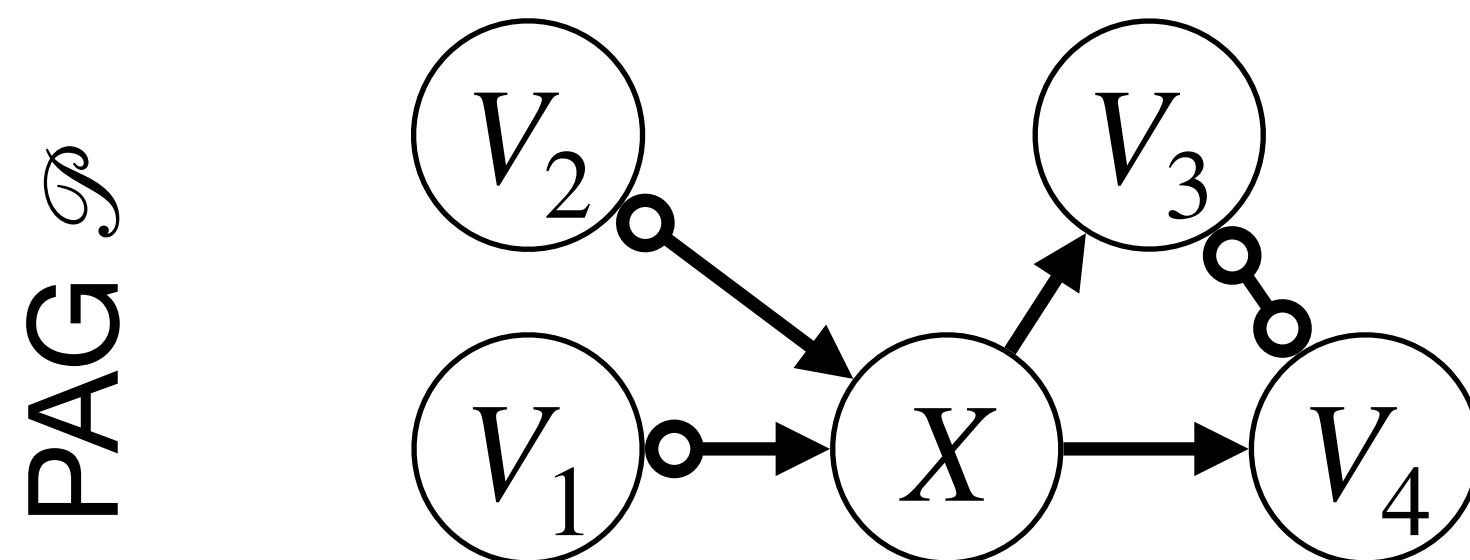
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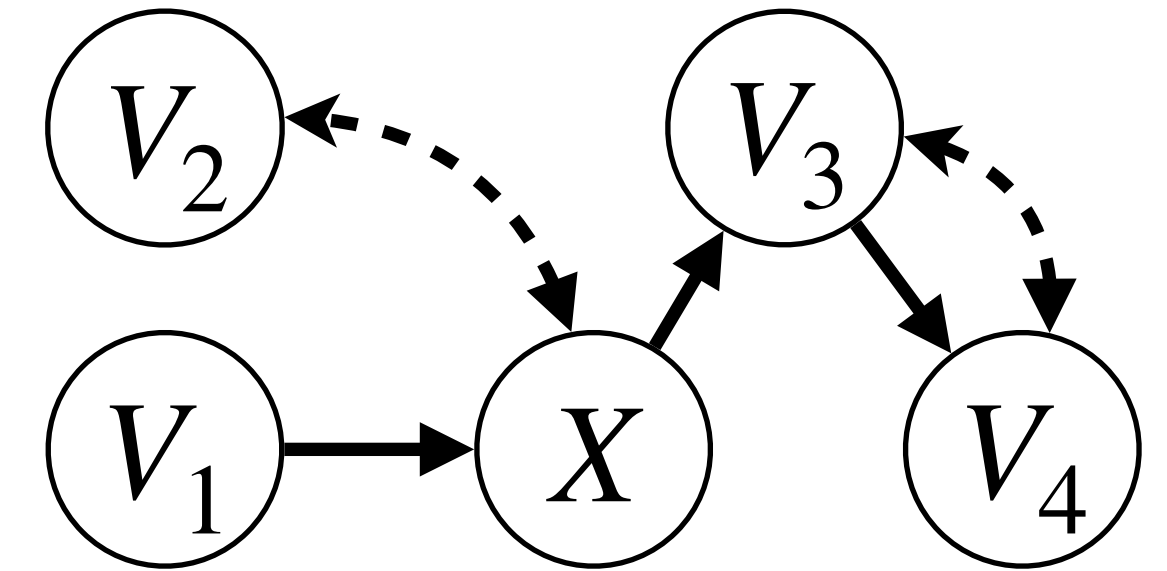
**Definition (m-separation):** In a PAG,  $X$  and  $Y$  are m-separated by  $\mathbf{Z}$  if there is no definite m-connecting path between them relative to  $\mathbf{Z}$ .

A PAG  $\mathcal{P}$  represents all BNs the **Markov Equivalence Class (MEC)**, i.e.:

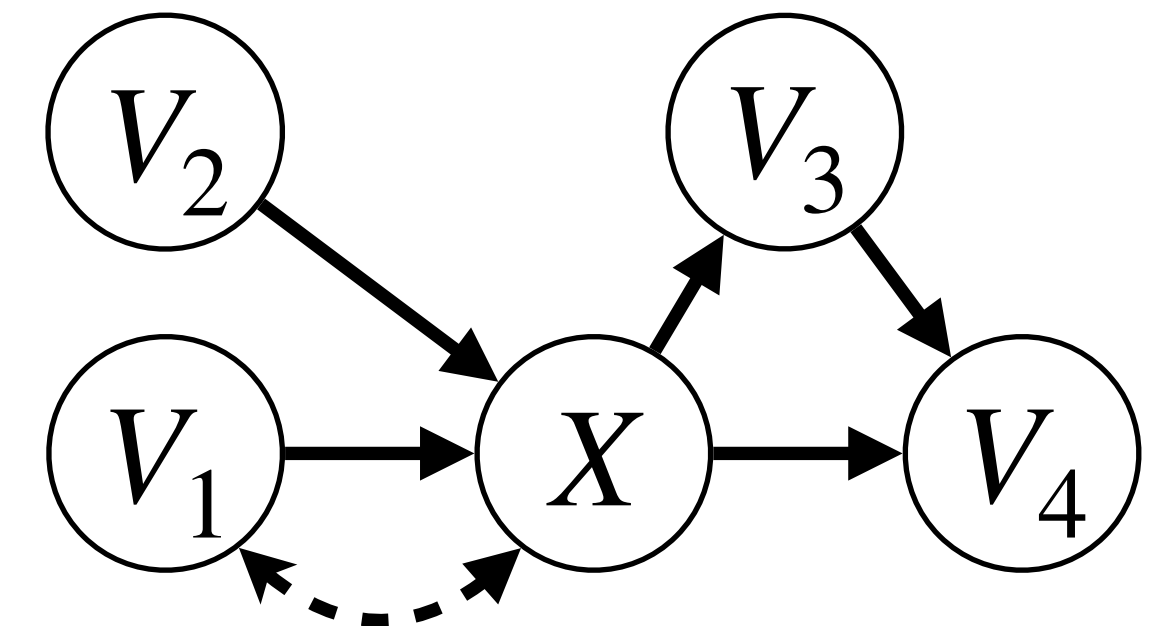
$$(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_{\mathcal{P}} \Leftrightarrow (\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G$$



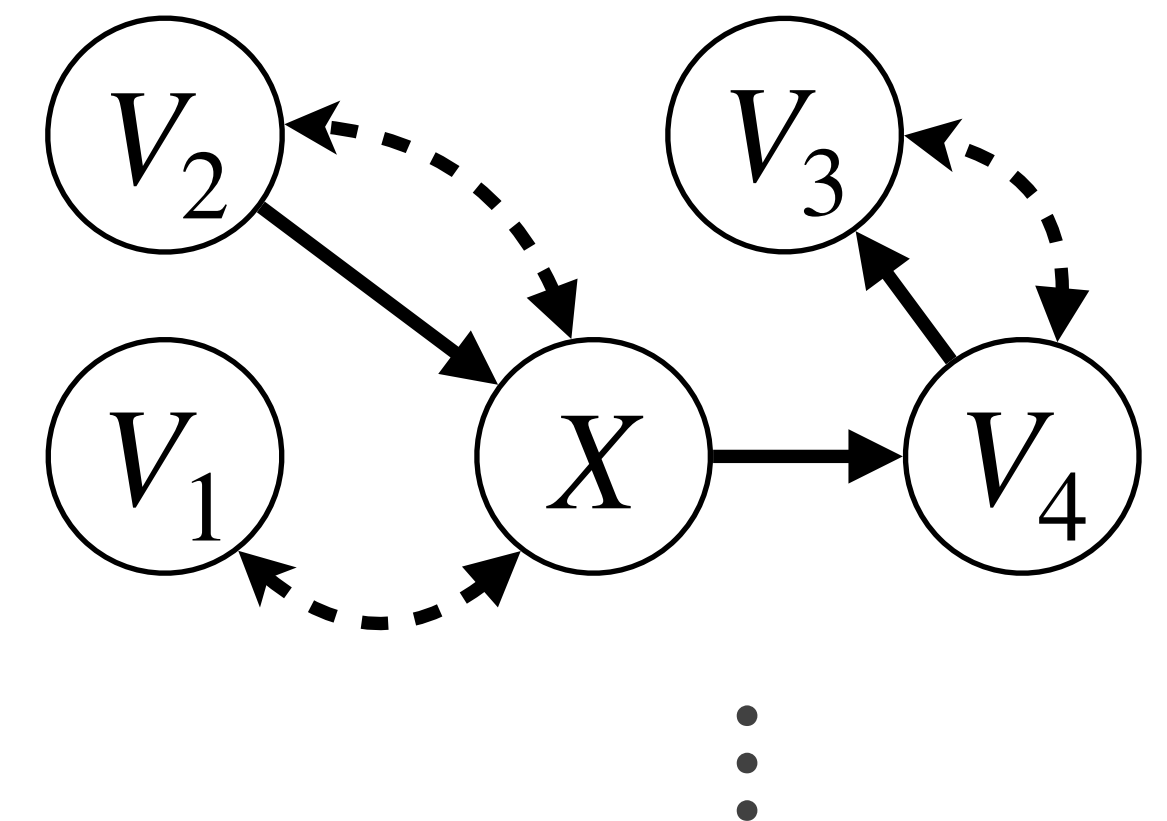
$$\begin{aligned} V_1 &\perp\!\!\!\perp V_2 \\ V_1 &\perp\!\!\!\perp V_3 \mid X \\ V_1 &\perp\!\!\!\perp V_4 \mid X \\ V_2 &\perp\!\!\!\perp V_3 \mid X \\ V_2 &\perp\!\!\!\perp V_4 \mid X \end{aligned}$$



BN  $G_1$



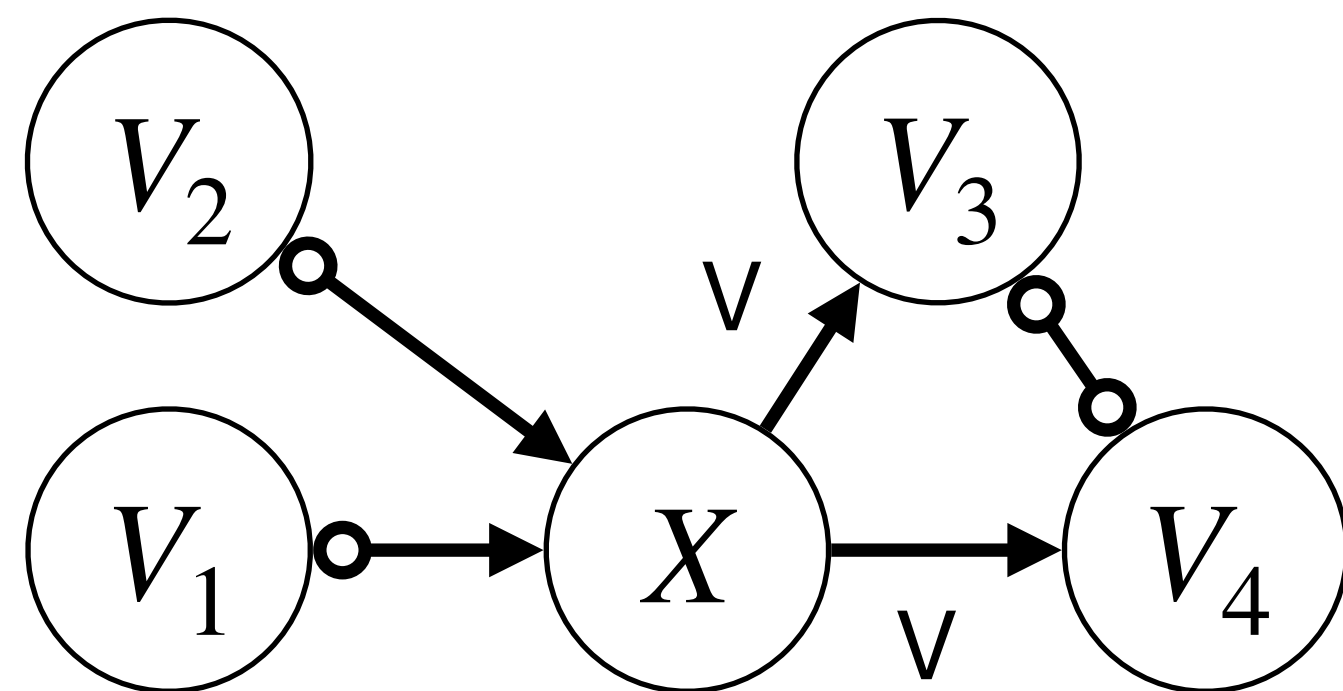
BN  $G_2$



BN  $G_3$

# Edge Visibility

- Definition (Visibility of an Edge):** Given a PAG  $\mathcal{P}$ , a directed edge  $X \rightarrow Y$  is visible if:
1. there is a node  $V$  not adjacent to  $Y$  such that there is an edge between  $V$  and  $X$  that is into  $X$ , or
  2. if there is a collider path from  $V$  to  $X$  that is into  $X$  and every non-endpoint node on the path is a parent of  $Y$ . Otherwise,  $X \rightarrow Y$  is said to be invisible.



Edges labeled with 'v' are referred to as visible edges

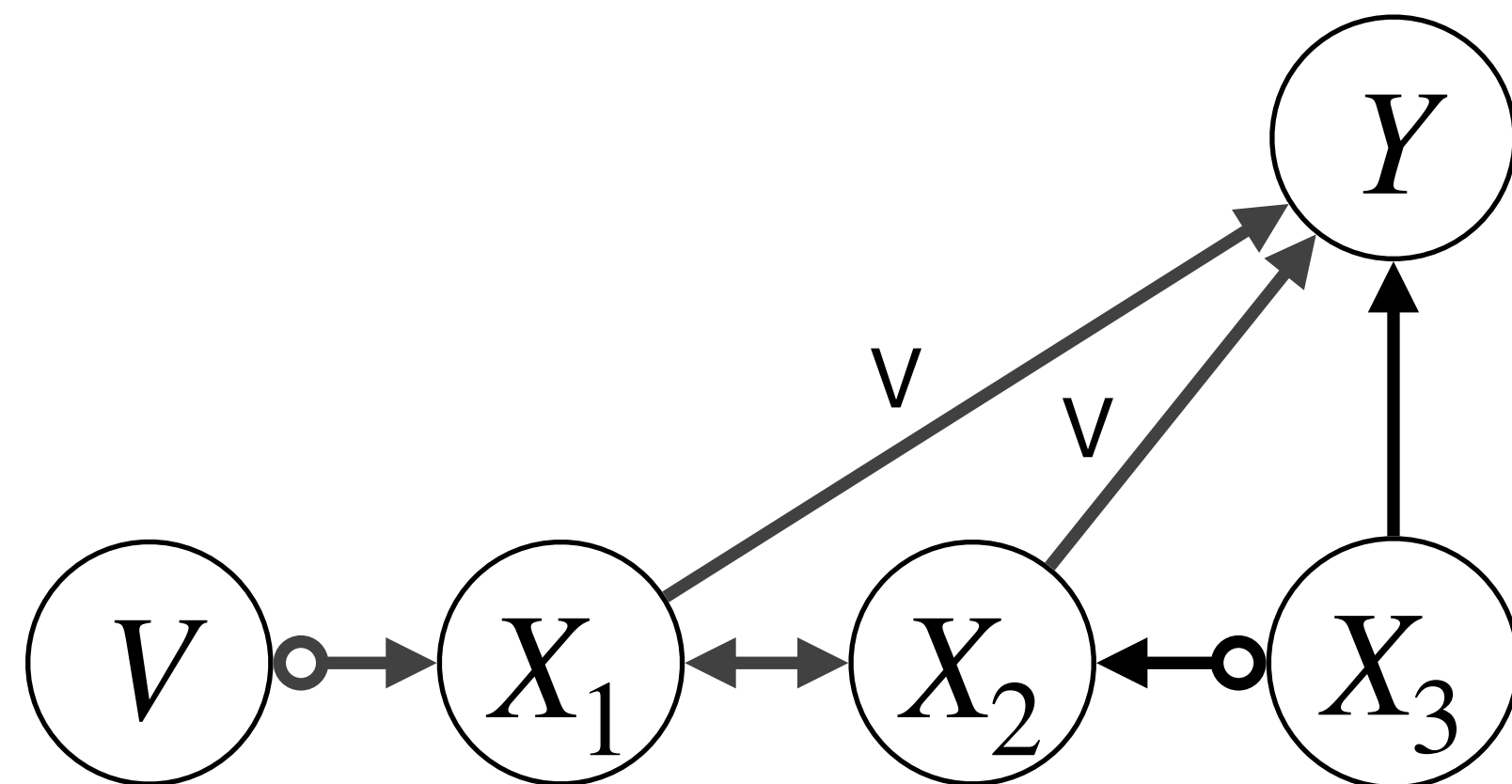
Visibility of an edge denotes the absence of a hidden confounder in every member of the equivalence class.



# Edge Visibility

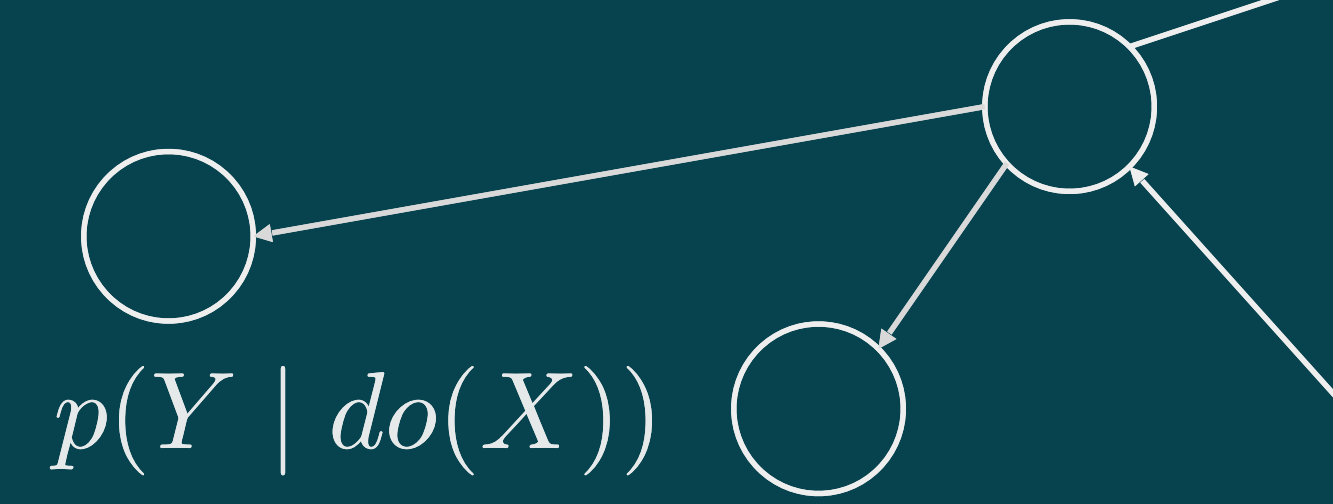
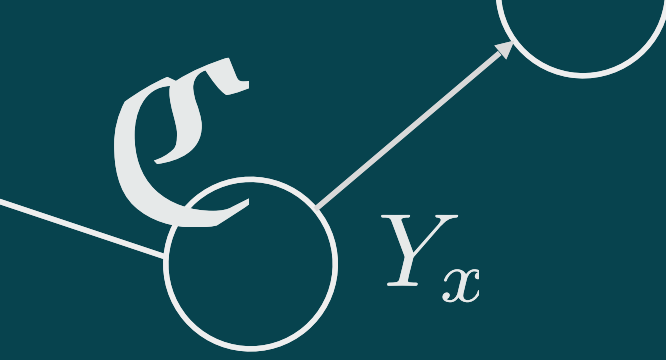
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Edges labeled with 'v' are referred to as visible edges

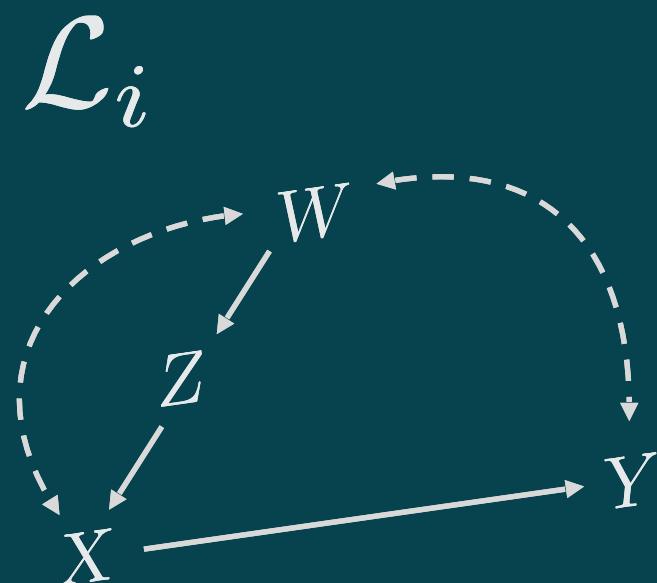
Visibility of an edge denotes the absence of a hidden confounder in every member of the equivalence class.



# 4

## Causal Discovery

### Fast Causal Inference (FCI) Algorithm



ESSAI & ACAI 2023  
LJUBLJANA, SLOVENIA

Machines Climbing Pearl's Ladder of Causation

# Fast Causal Inference (FCI) Algorithm

**Fast Causal Inference (FCI) Algorithm:** Learn a graphical representation of the Markov Equivalence Class of causal diagrams (ADMGs) from observational data.

**Assumptions:** the observed distribution is the marginal of a distribution  $P$  that satisfies the following conditions for the true causal diagram  $G$  (an **ADMG**):

1) **I-Map / Semi-Markov Condition:** for any disjoint subsets  $\mathbf{X}$ ,  $\mathbf{Y}$  and  $\mathbf{Z}$ :

$$(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G \Rightarrow (\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_P.$$

2) **Faithfulness Condition:** for any disjoint subsets  $\mathbf{X}$ ,  $\mathbf{Y}$  and  $\mathbf{Z}$ :

$$(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_P \Rightarrow (\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_G.$$

$G$  is an ***I-Map of  $P$***

$P$  is ***semi-Markov relative to  $G$*** .

$P$  is ***faithful to  $G$***

**Note:** Estimation of the marginal distribution from limited data requires and **additional assumption:**

3) An adequate *conditional independence test* is available.

# Conditional Independence Tests

Gaussian errors and independent observations: partial correlation test

Fisher, R.A. (1921). *On the " Probable Error" of a Coefficient of Correlation Deduced from a Small Sample*.

R package: <https://cran.r-project.org/web/packages/pcalg/>

Kernel-based non-parametric test:

Zhang, K., Peters, J., Janzing, D., & Schölkopf, B. (2012). *Kernel-based conditional independence test and application in causal discovery*. In: Uncertainty in artificial intelligence. AUAI Press; 2011. p.804–13

R package: <https://cran.r-project.org/web/packages/CondIndTests>

Continuous (conditional Gaussian) or Discrete (Binary, Ordinal, Multinomial) - Linear Regression

- Tsagris, M., Borboudakis, G., Lagani, V. *et al.* (2018) Constraint-based causal discovery with mixed data. *Int J Data Sci Anal* **6**, 19–30. ([Link](#))
- R package: <https://cran.r-project.org/web/packages/MXM/>

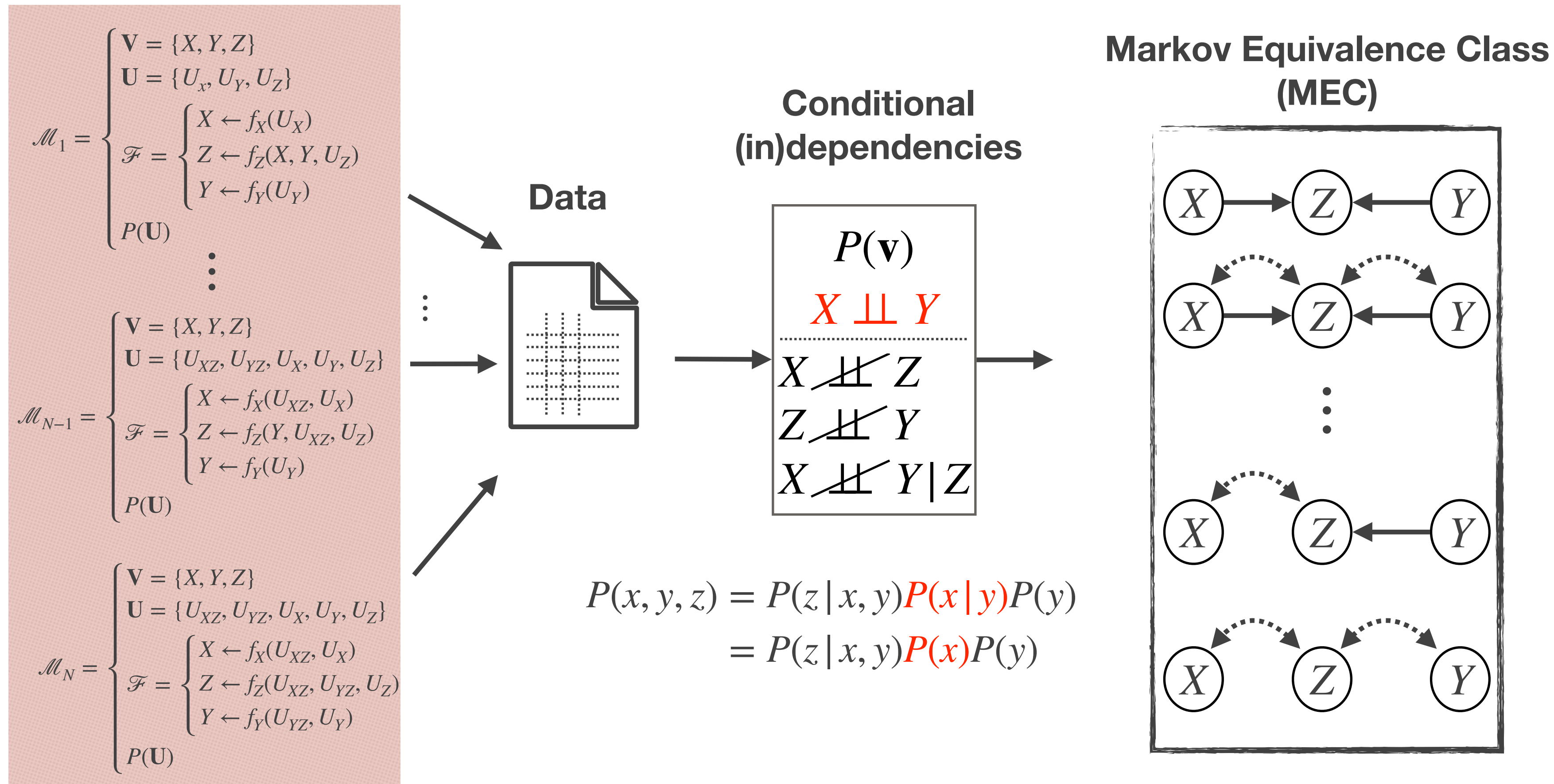
Gaussian errors and correlated observations (family data) :

Ribeiro A.H., Soler J.M.P. (2020). *Learning Genetic and environmental graphical models from family data*, Statistics in Medicine.

R package: <https://github.com/adele/FamilyBasedPGMs>

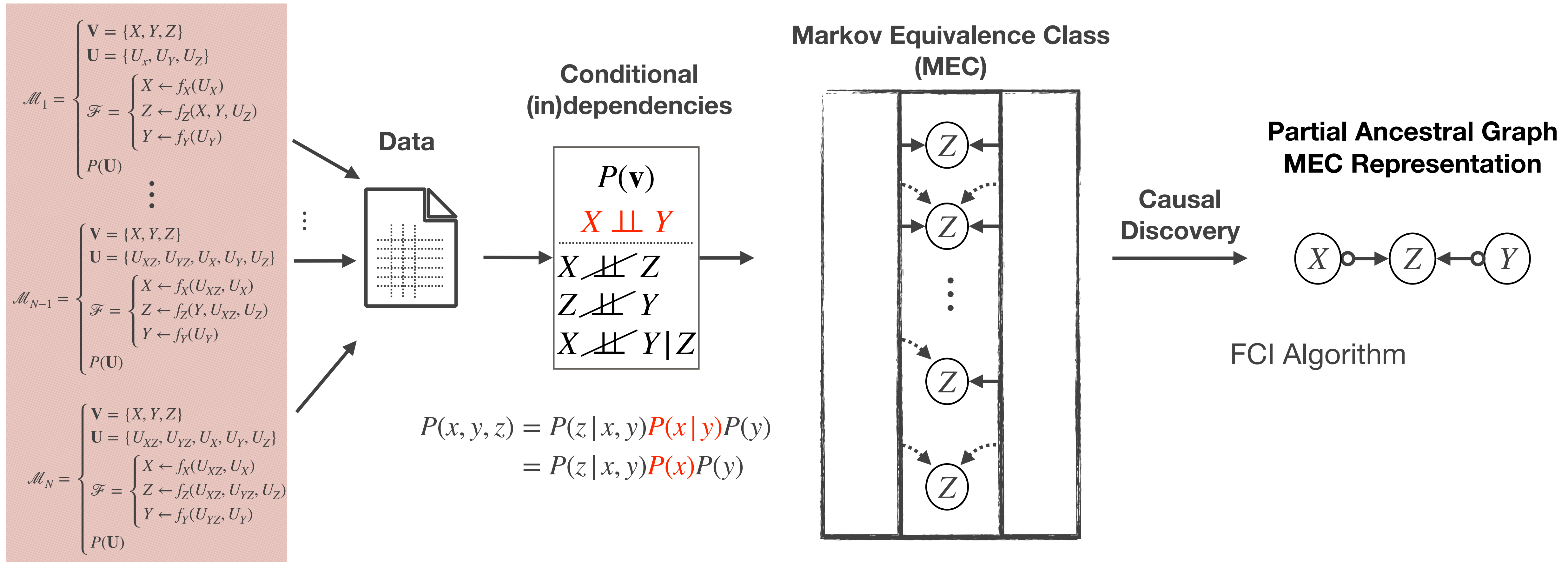


# Learning Structural Invariances





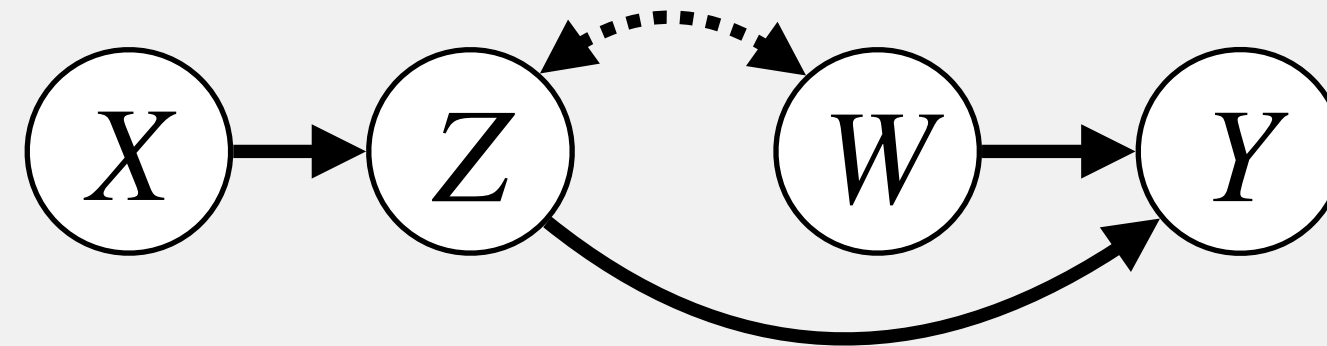
# Learning Structural Invariances



# FCI Algorithm - Pipeline

## Unknown Reality

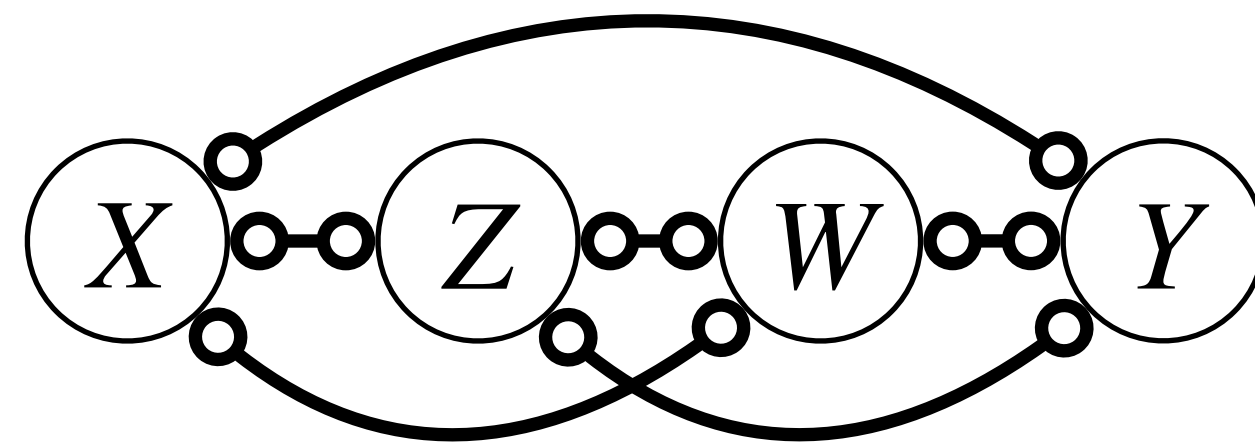
True causal diagram



$$X \perp\!\!\!\perp W$$

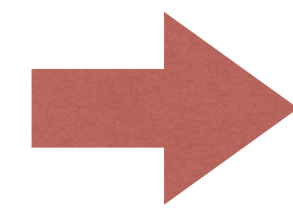
$$X \perp\!\!\!\perp Y | Z, W$$

Implied by the ADMG using d-separation



Complete Graph

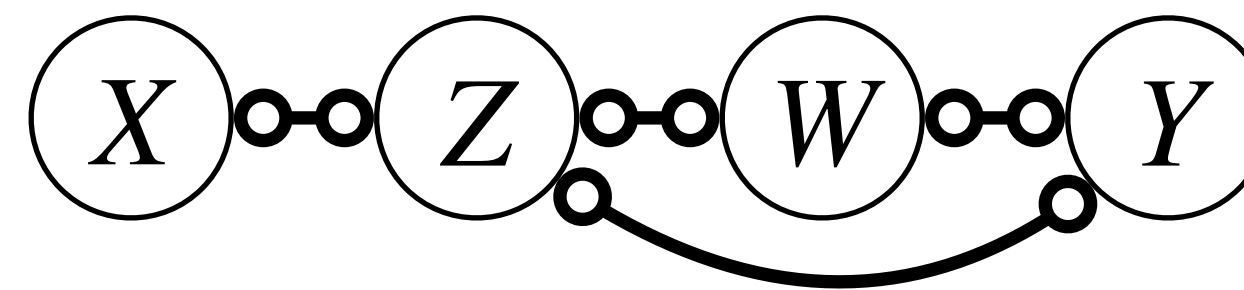
Conditional Independence Tests



$$X \perp\!\!\!\perp W$$

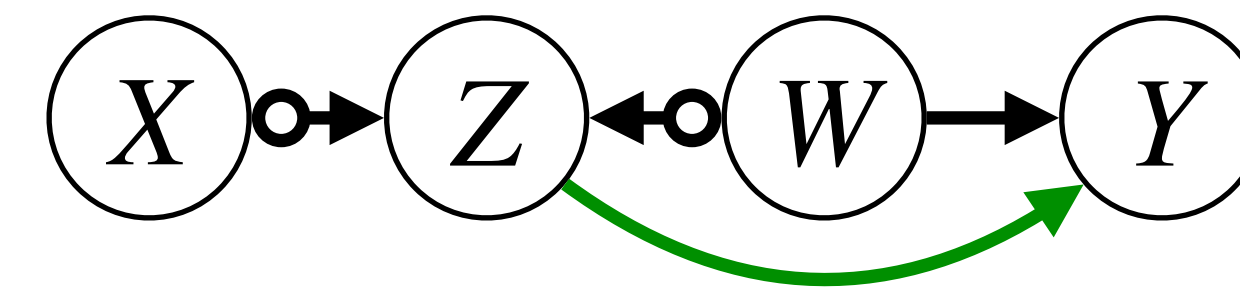
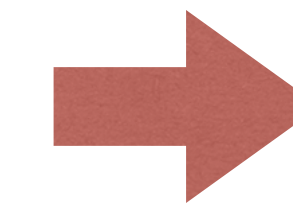
$$X \perp\!\!\!\perp Y | Z, W$$

By faithfulness, are observed in the data



Skeleton

FCI Rules (R1) – (R10)



Partial Ancestral Graph (PAG)

Implied by the PAG using m-separation

$$X \perp\!\!\!\perp W$$

$$X \perp\!\!\!\perp Y | Z, W$$

$A \longrightarrow B \implies$  ancestrally

$A \circ \longrightarrow B \implies$  non-ancestrality

$A \longleftrightarrow B \implies$  spurious association

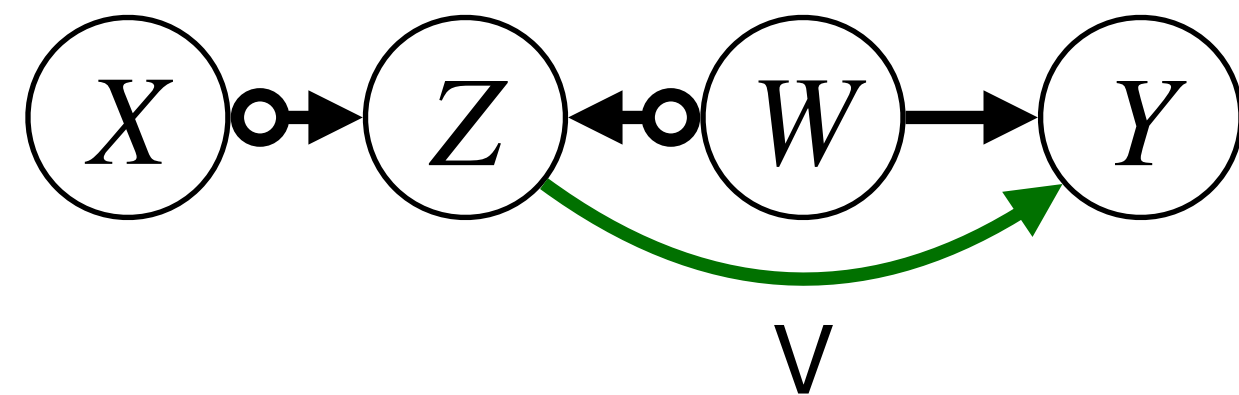
$A \dashv \longrightarrow B \implies$  selection bias

**Z is not an ancestor of X or W.**

**Z and W are ancestors of Y.**

**Z is not confounded with Y.**

# PAG: Representation of the Markov Equivalence Class

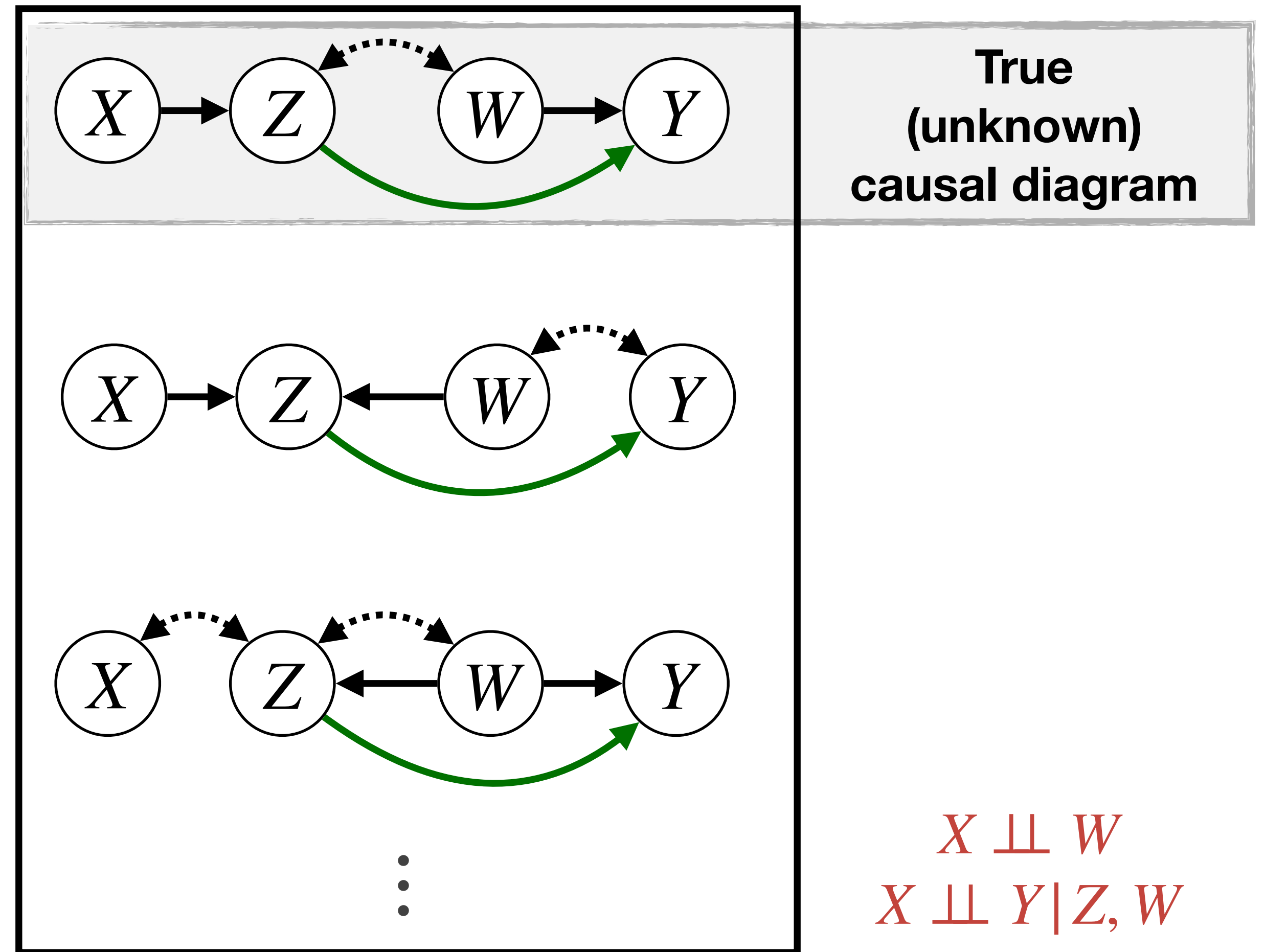


Partial Ancestral Graph  
(PAG)

$Z$  is not an ancestor of  $X$  or  $W$ .

$Z$  and  $W$  are ancestors of  $Y$ .

$Z$  is not confounded with  $Y$ .

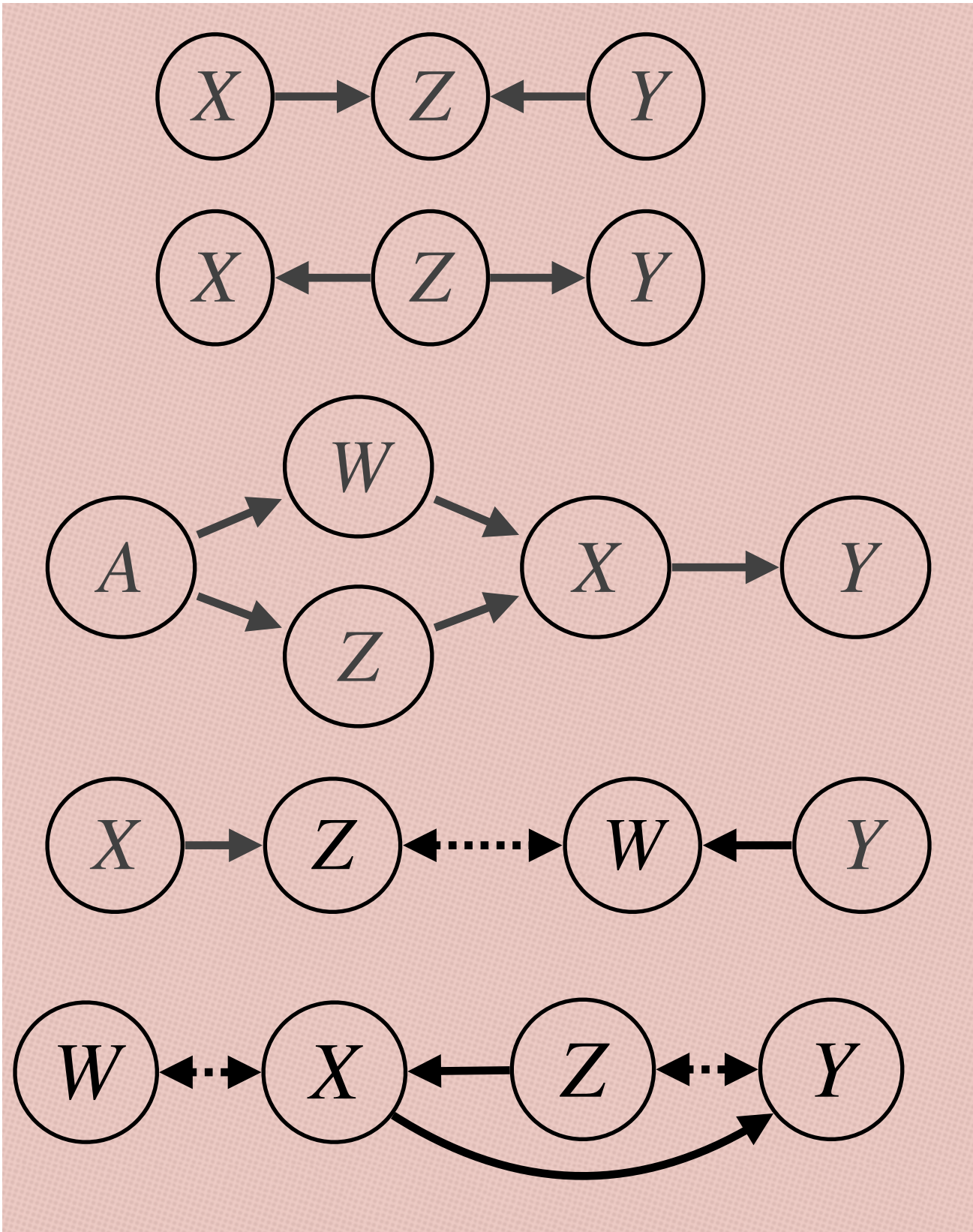


$X \perp\!\!\!\perp W$   
 $X \perp\!\!\!\perp Y | Z, W$

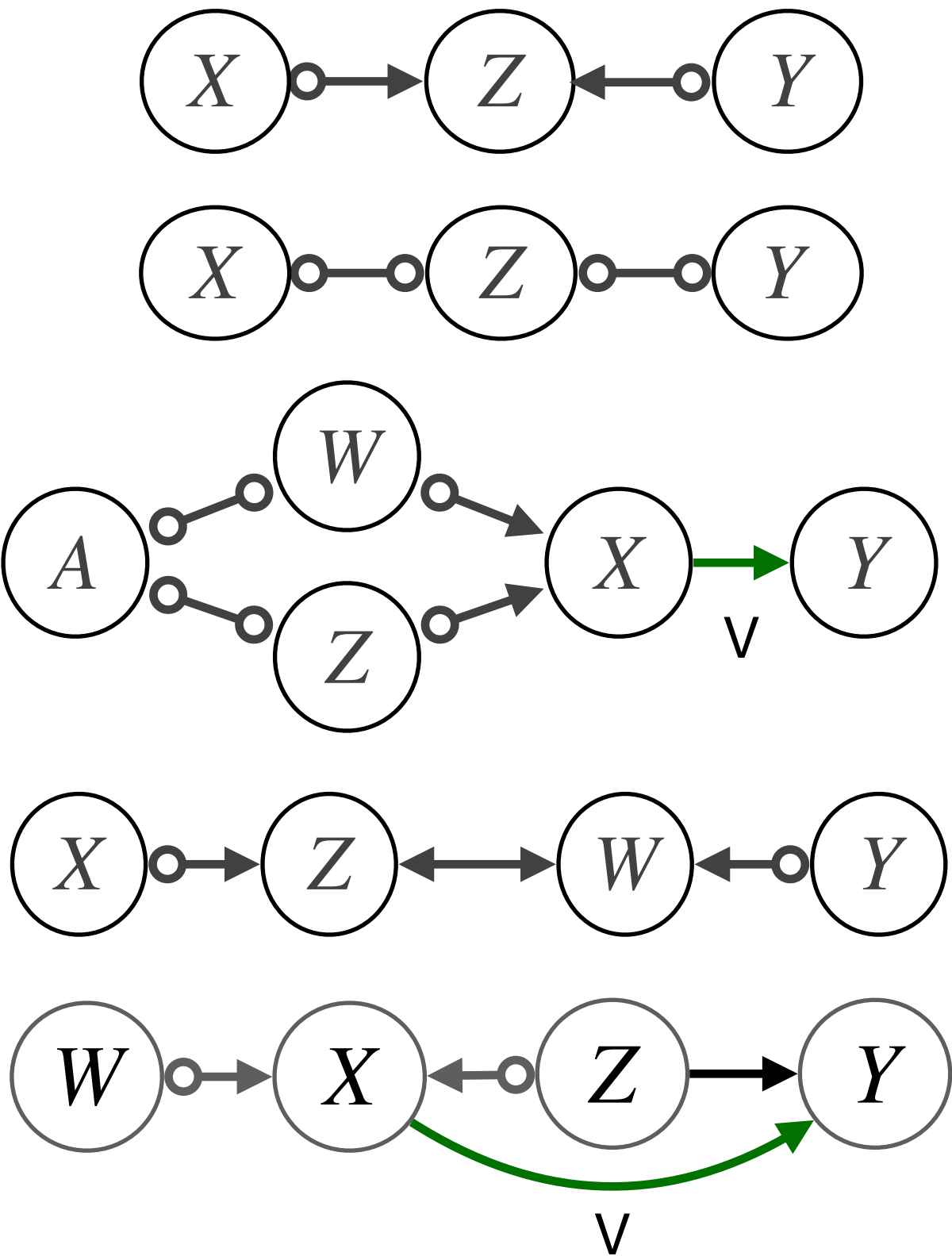


# Other Examples

Underlying Causal Diagram

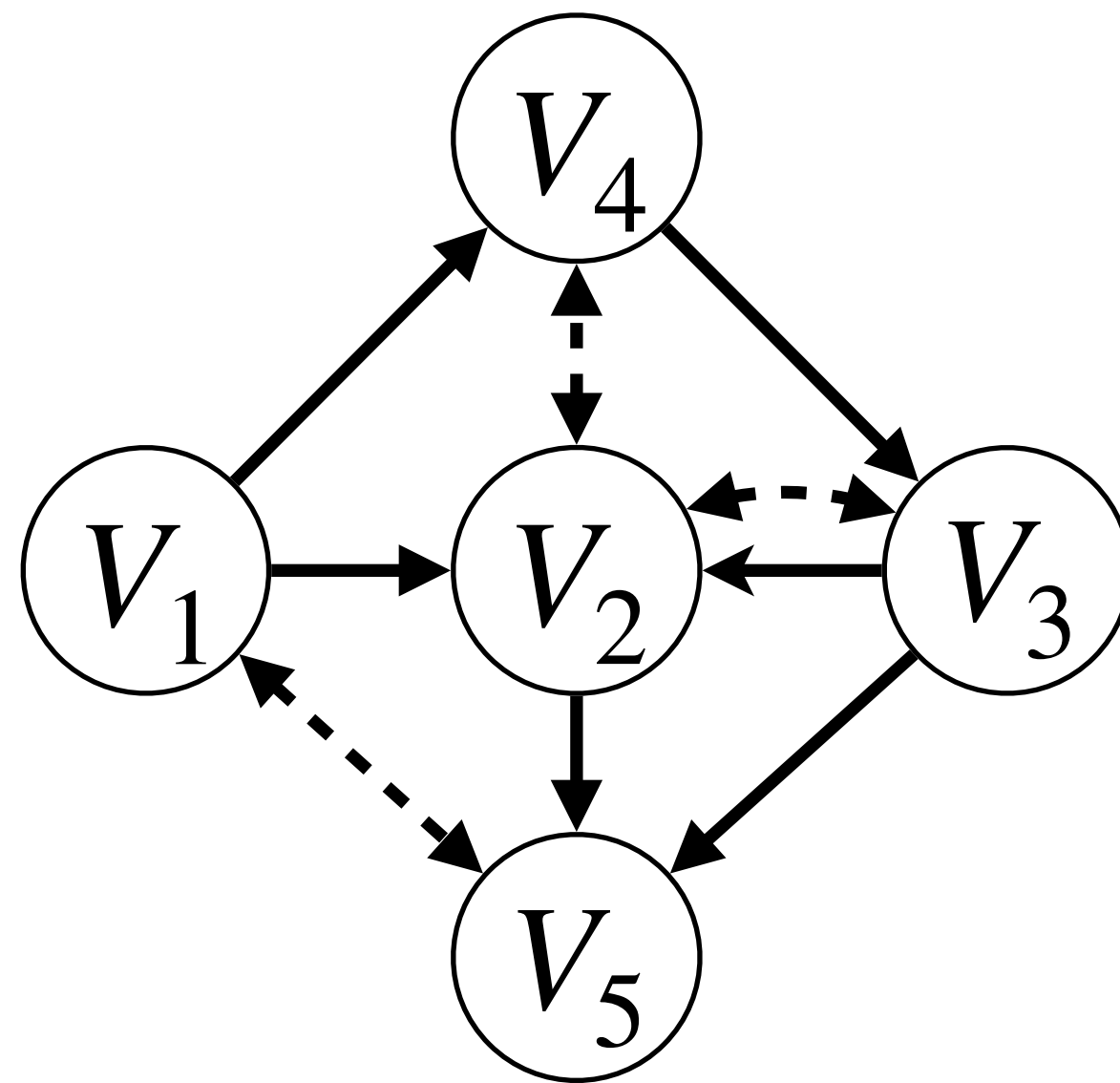


Partial Ancestral Graph

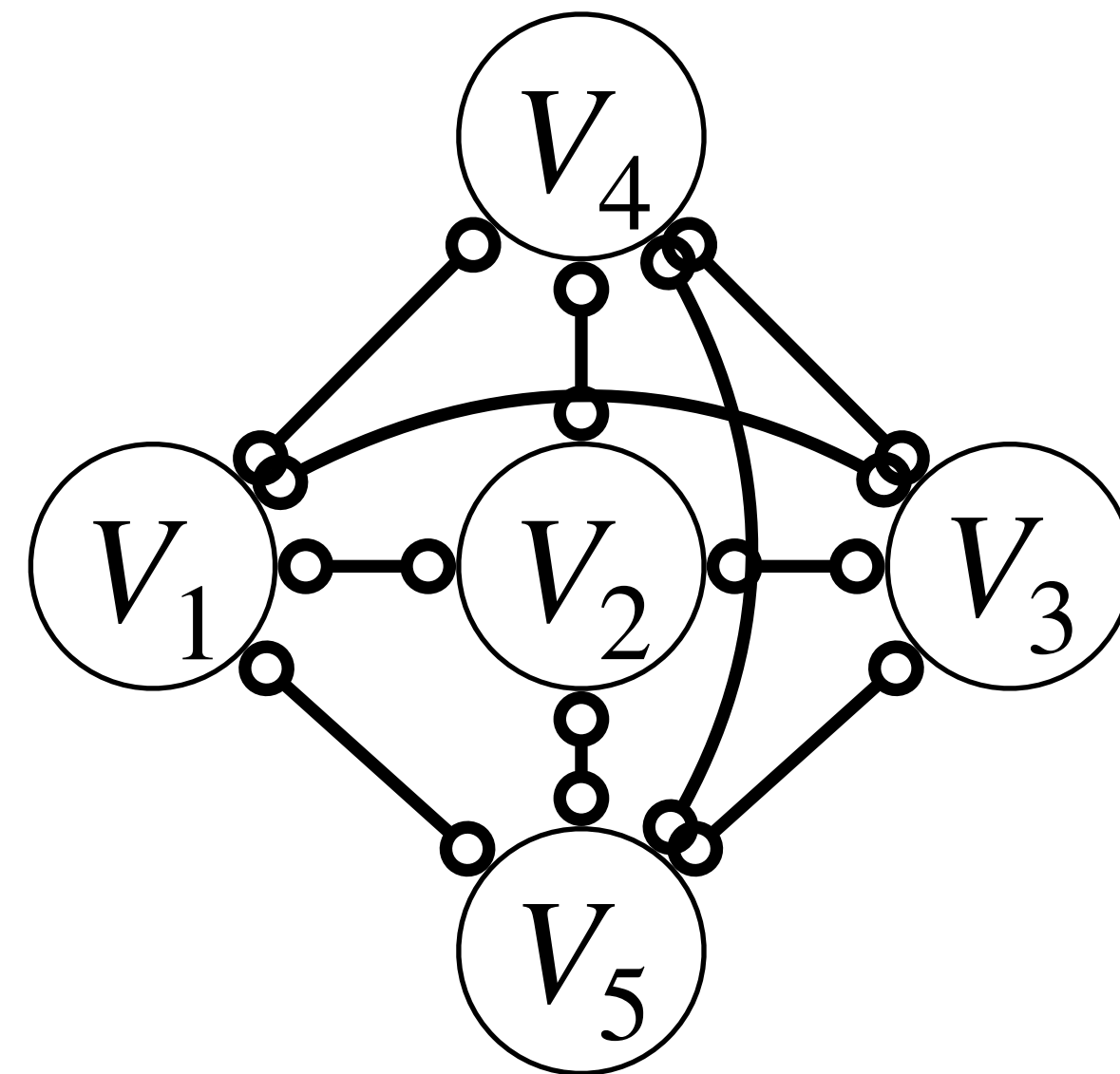


# FCI - Skeleton

Form a complete graph on the set of variables, in which there is a circle-circle edge between every pair of variables;

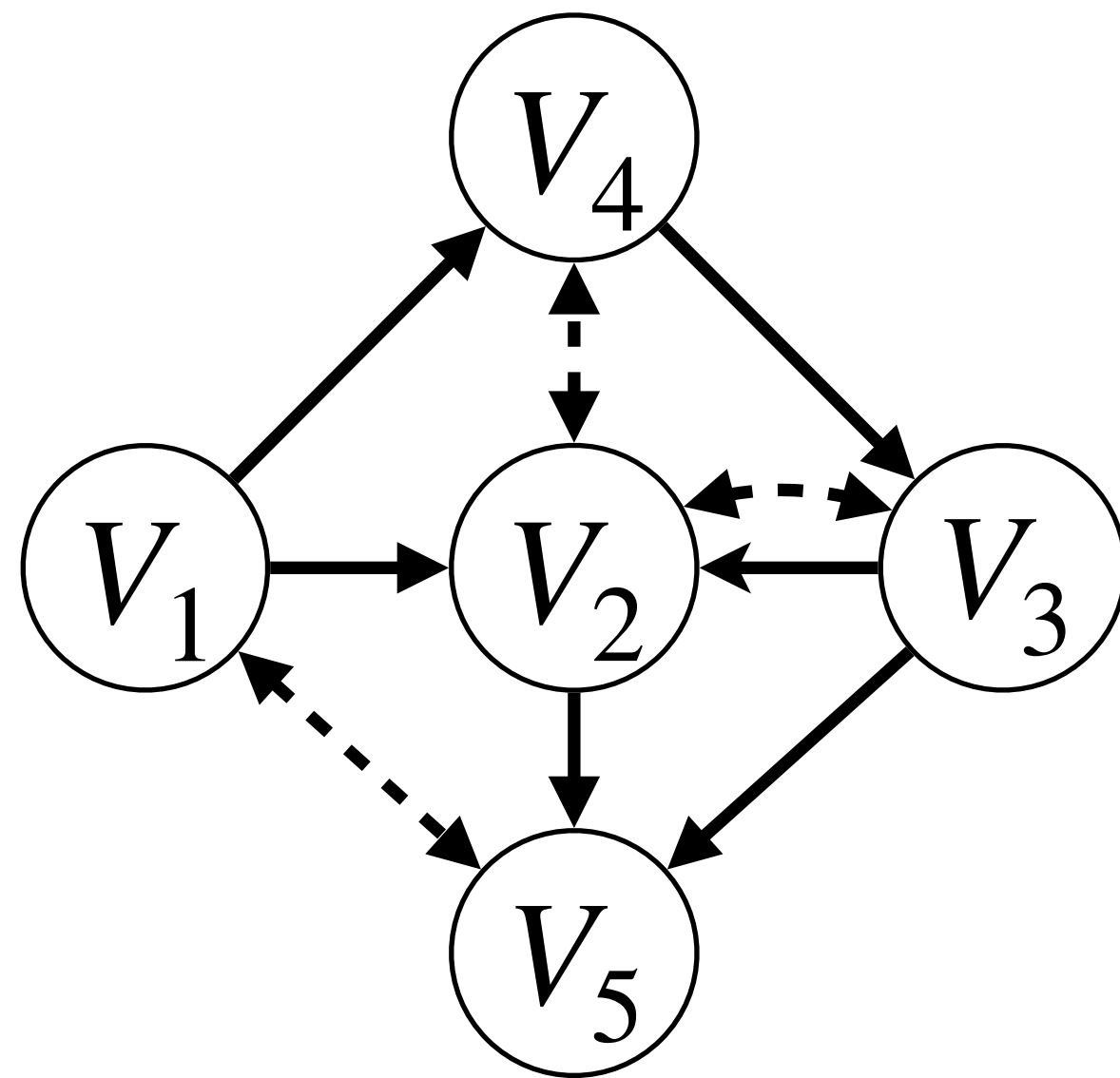


True, unknown ADMG

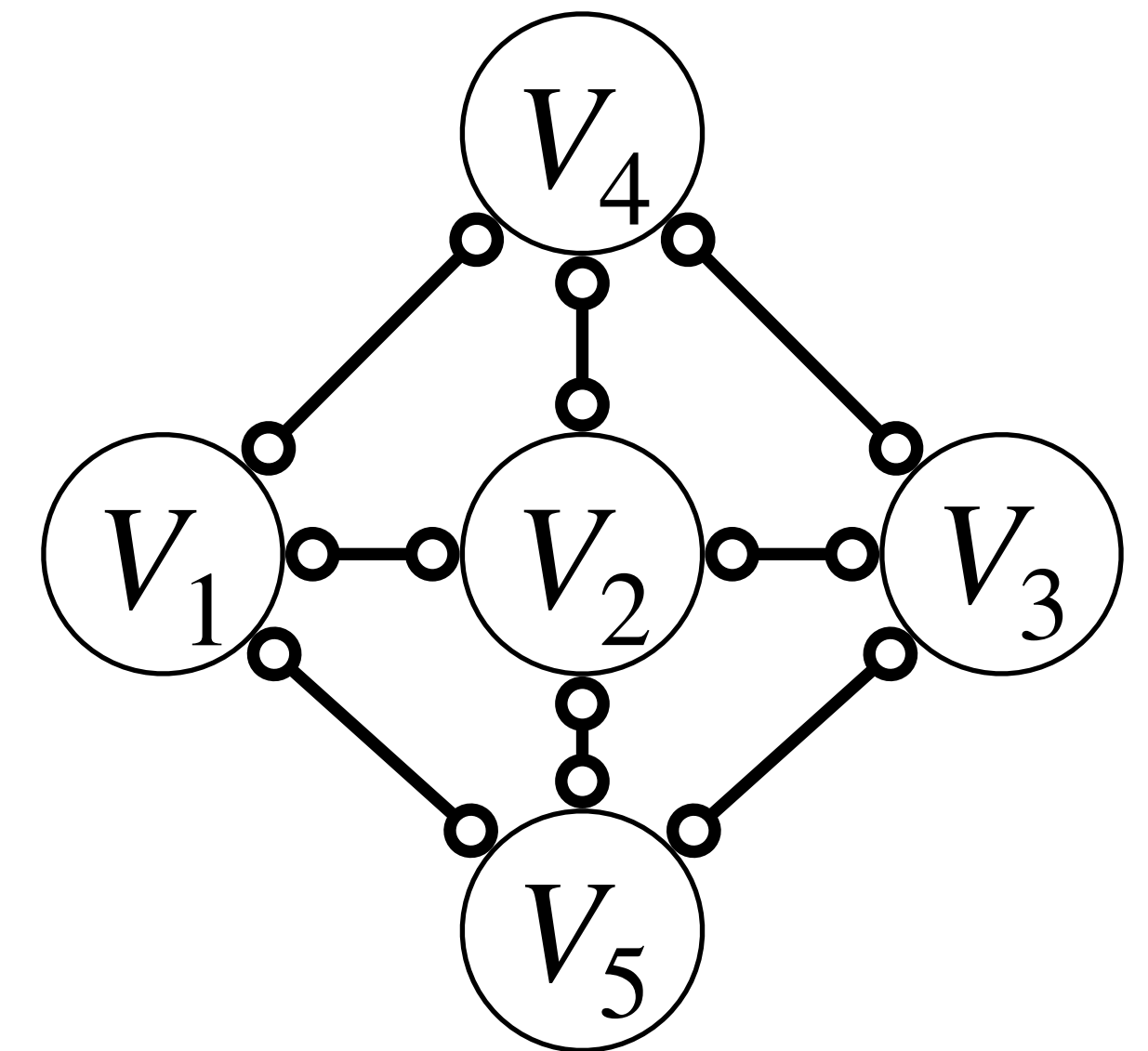
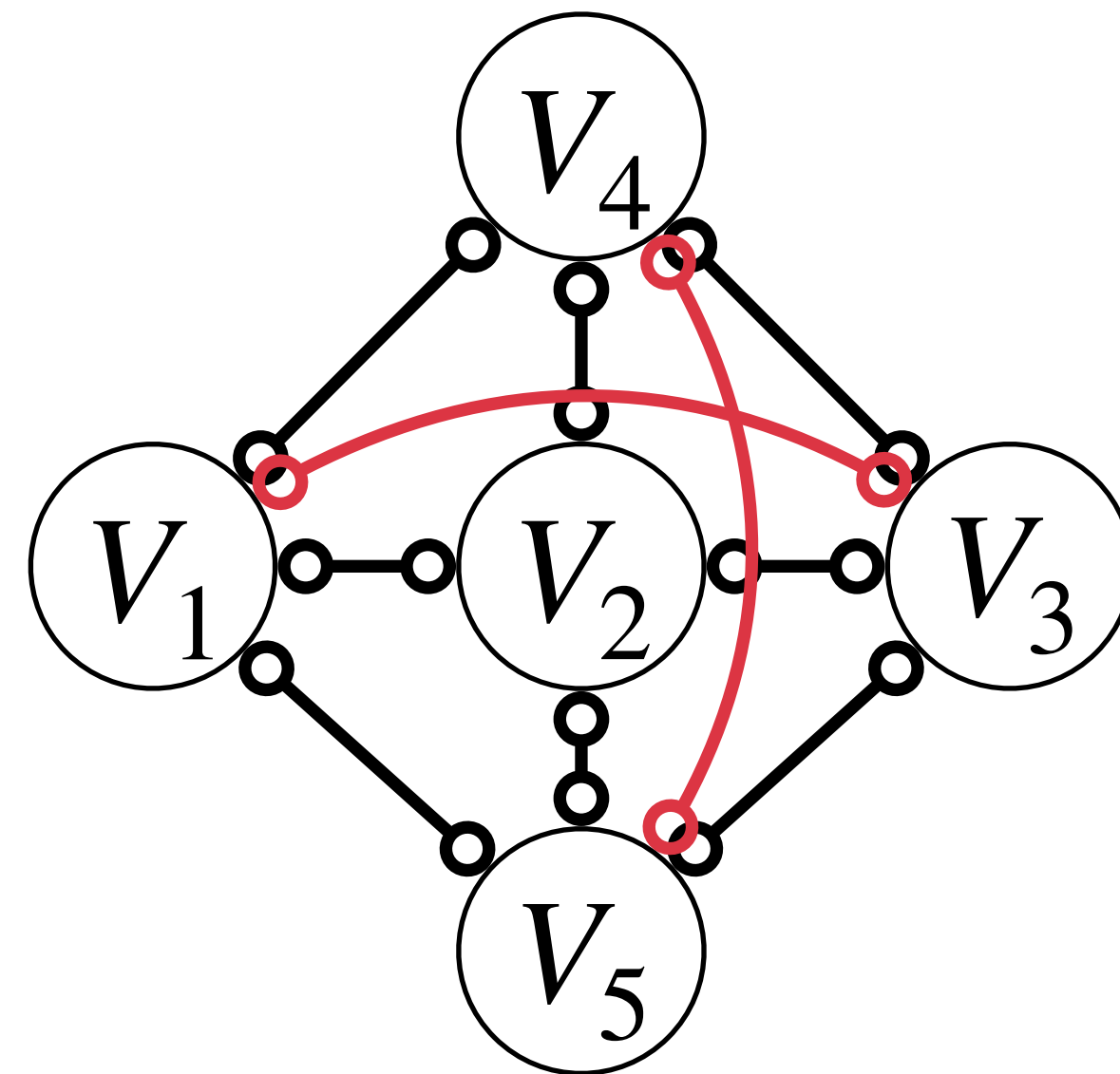


# FCI - Skeleton

For every pair of variables  $V_1$  and  $V_2$ , if exists a set  $\mathbf{S}_{1,2}$  such that  $V_1 \perp\!\!\!\perp V_2 \mid \mathbf{S}_{1,2}$ , then remove the edge between  $V_1$  and  $V_2$  and add  $\mathbf{S}_{1,2}$  in  $\text{Sepset}(V_1, V_2)$ .



True, unknown ADMG

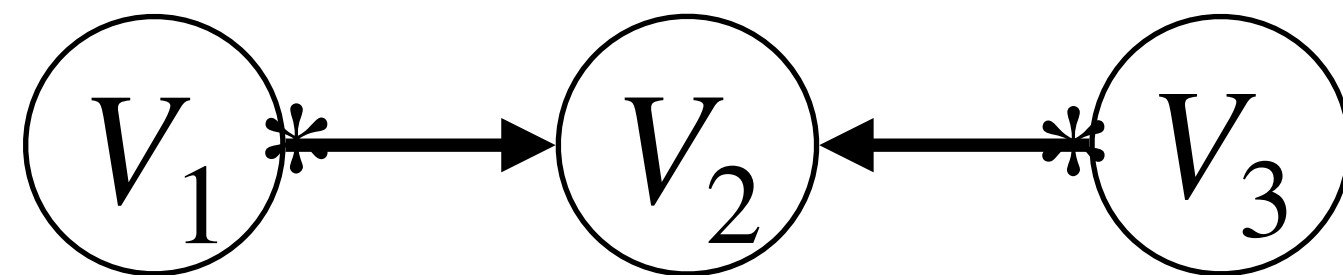


$$V_1 \perp\!\!\!\perp V_3 \mid V_4 \text{ and } V_4 \perp\!\!\!\perp V_5 \mid V_1, V_2, V_3$$

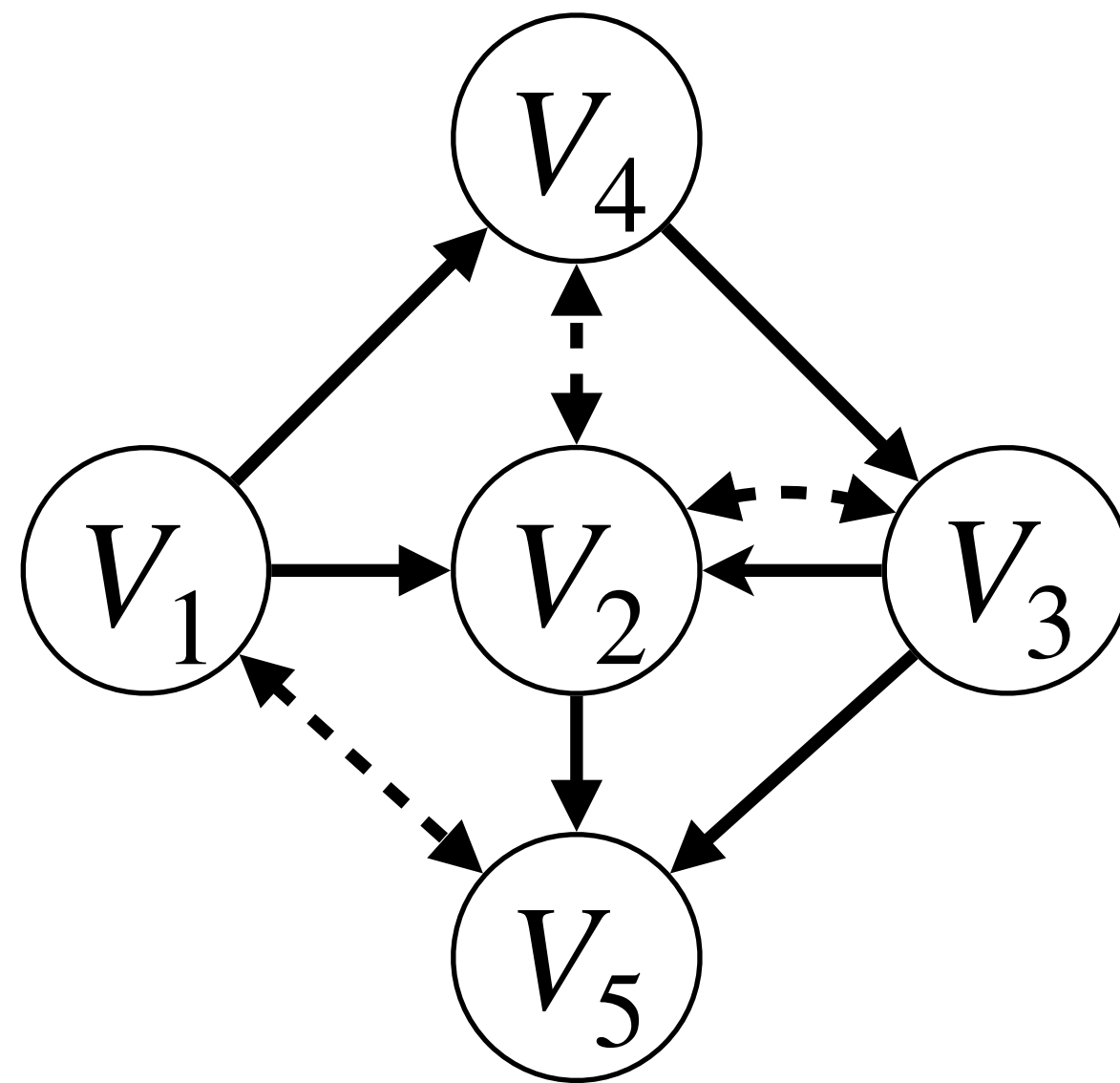


# FCI - Orienting the Colliders

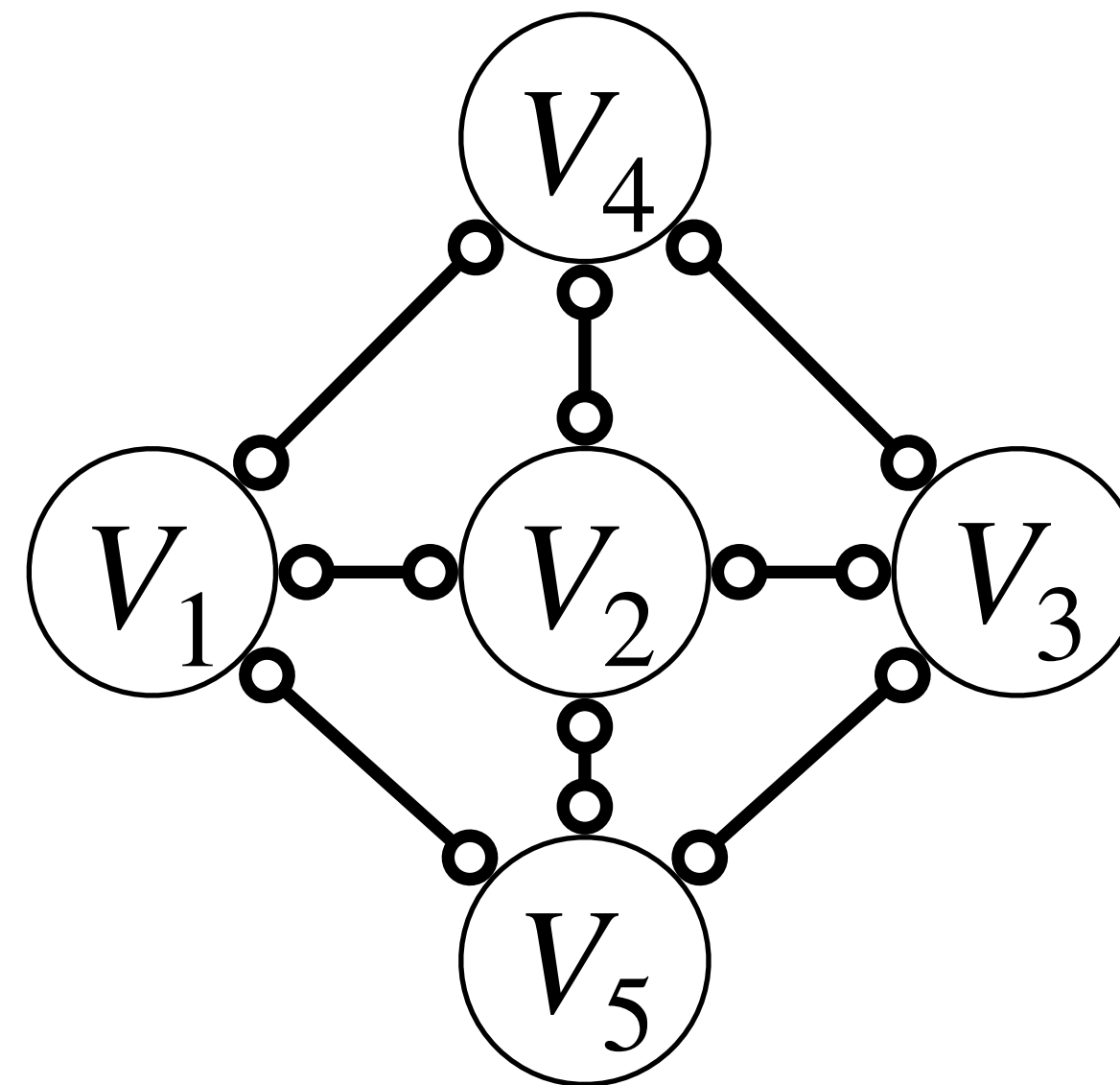
**R0:** If  $\langle V_1, V_2, V_3 \rangle$  is unshielded and  $V_2 \notin \text{Sepset}(V_1, V_3)$ , then



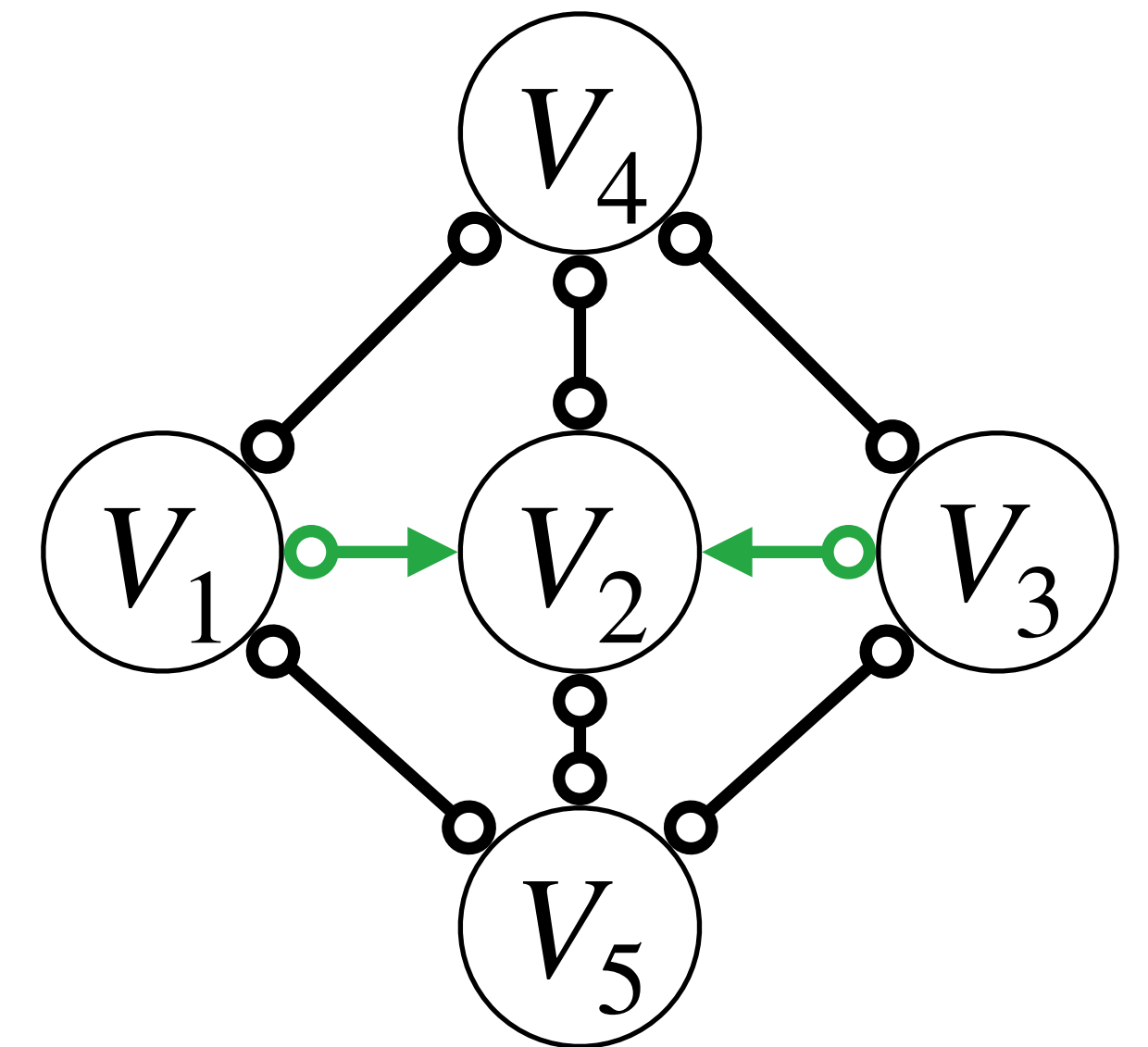
That is the only way for the path between  $V_1$  and  $V_3$  to be blocked when not conditioning on  $V_2$



True, unknown ADMG

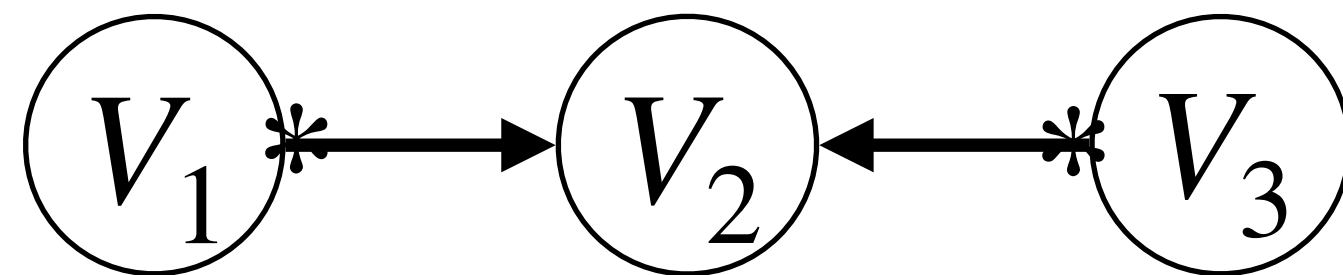


$V_1 \perp\!\!\!\perp V_3 \mid V_4$  and  $V_1 \not\perp\!\!\!\perp V_3 \mid V_4, V_2$

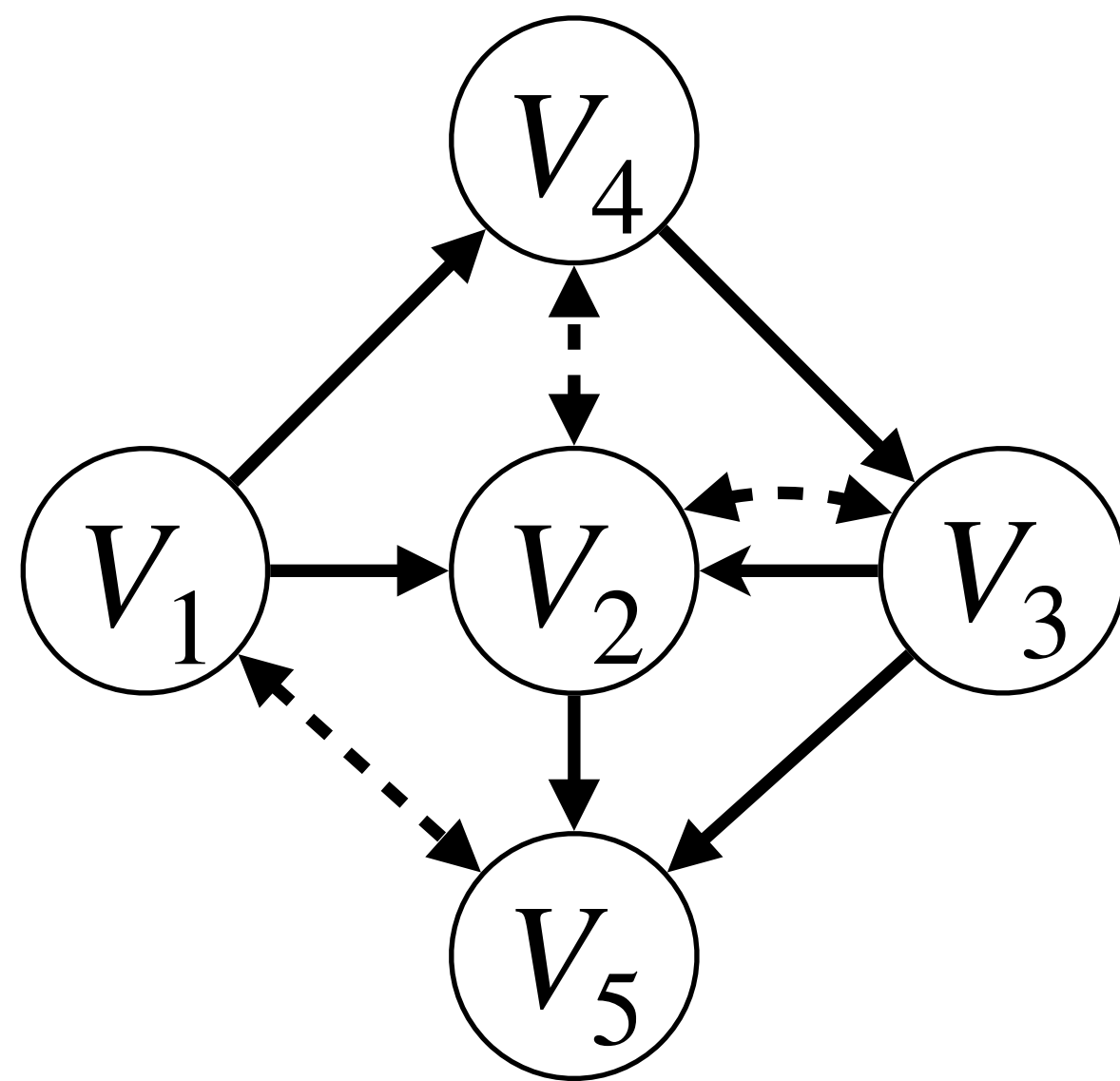


# FCI - Orienting the Colliders

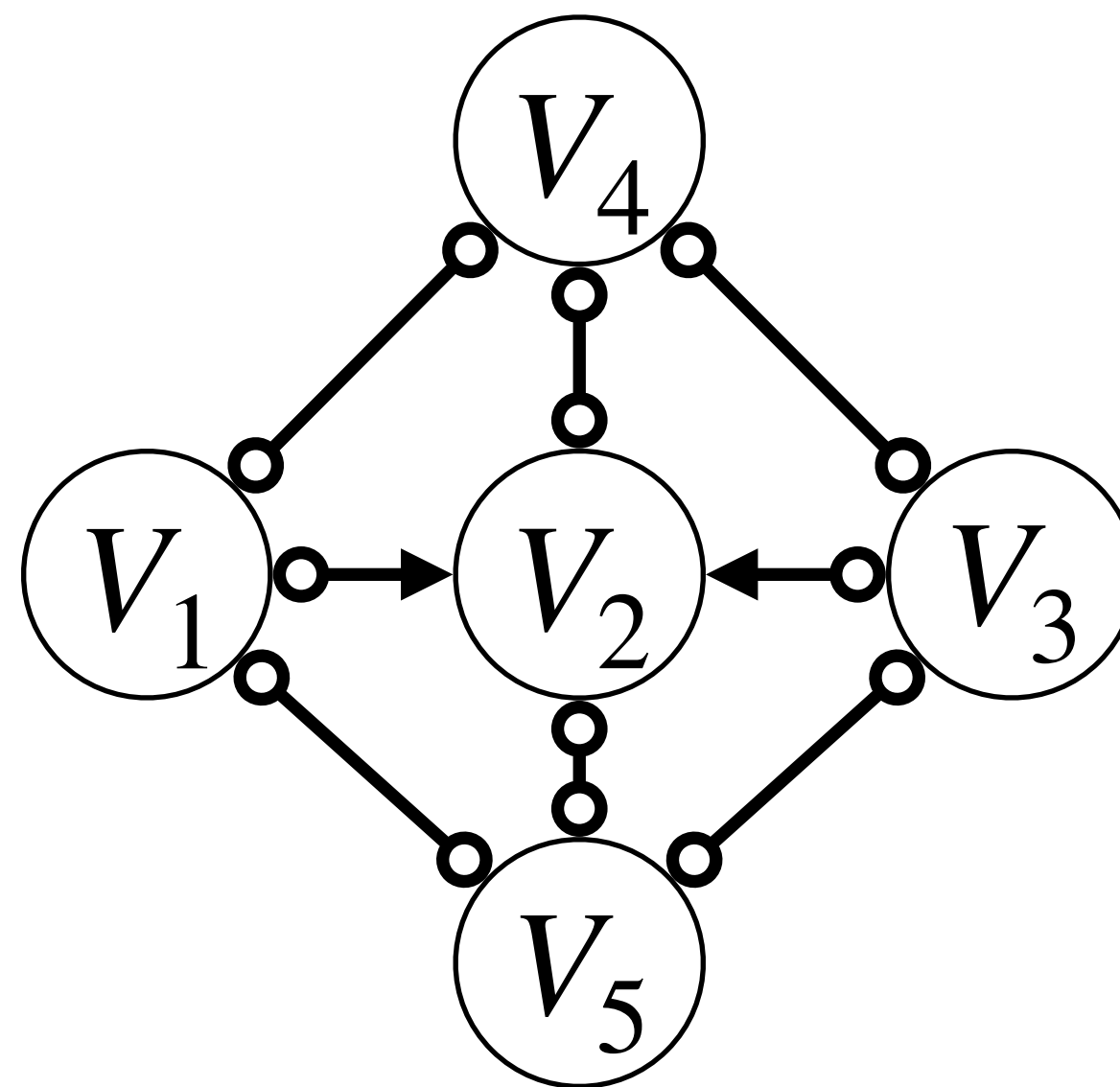
**R0:** If  $\langle V_1, V_2, V_3 \rangle$  is unshielded and  $V_2 \notin \text{Sepset}(V_1, V_3)$ , then



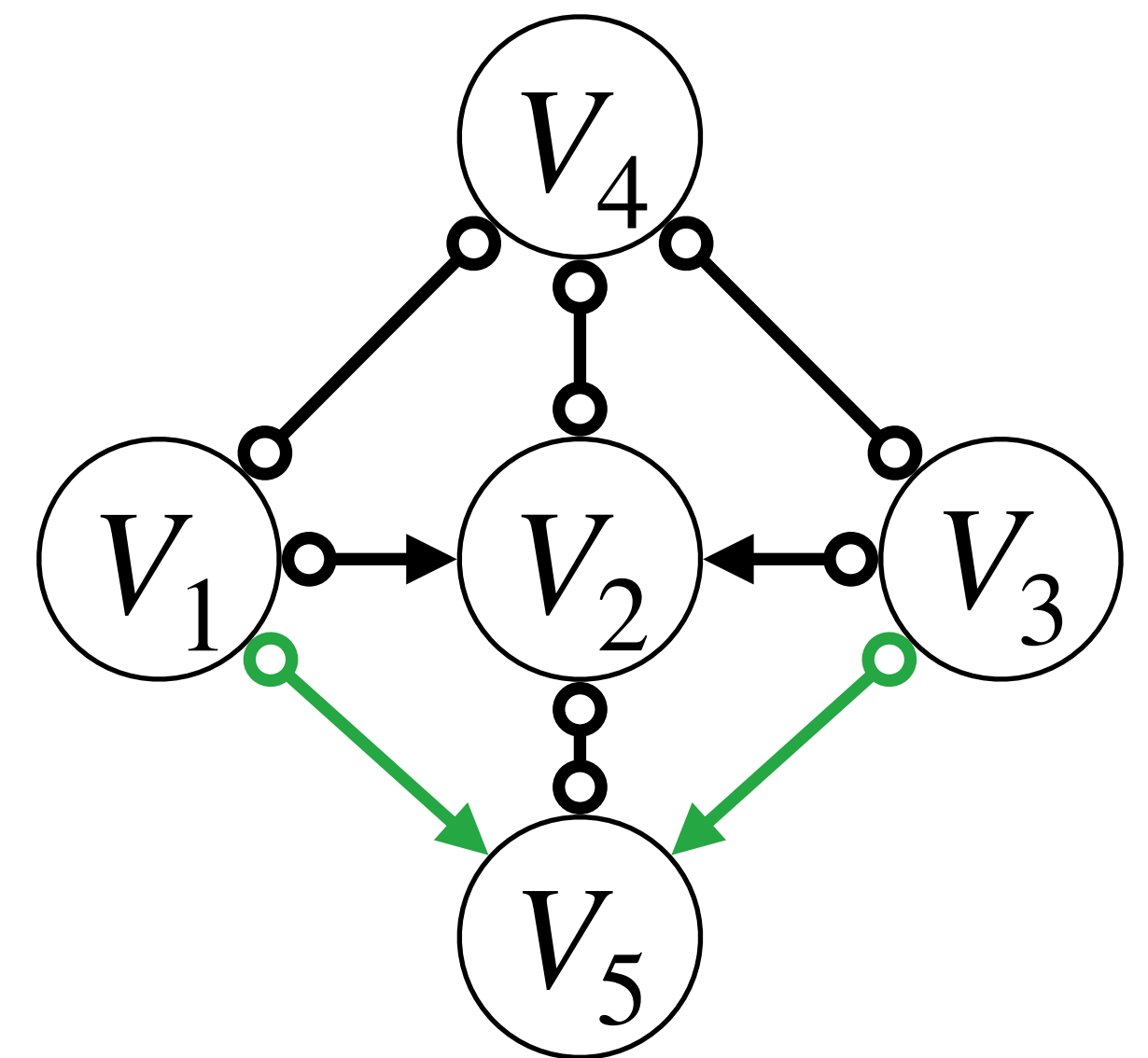
We apply R0 until no more collider can be oriented!



True, unknown ADMG

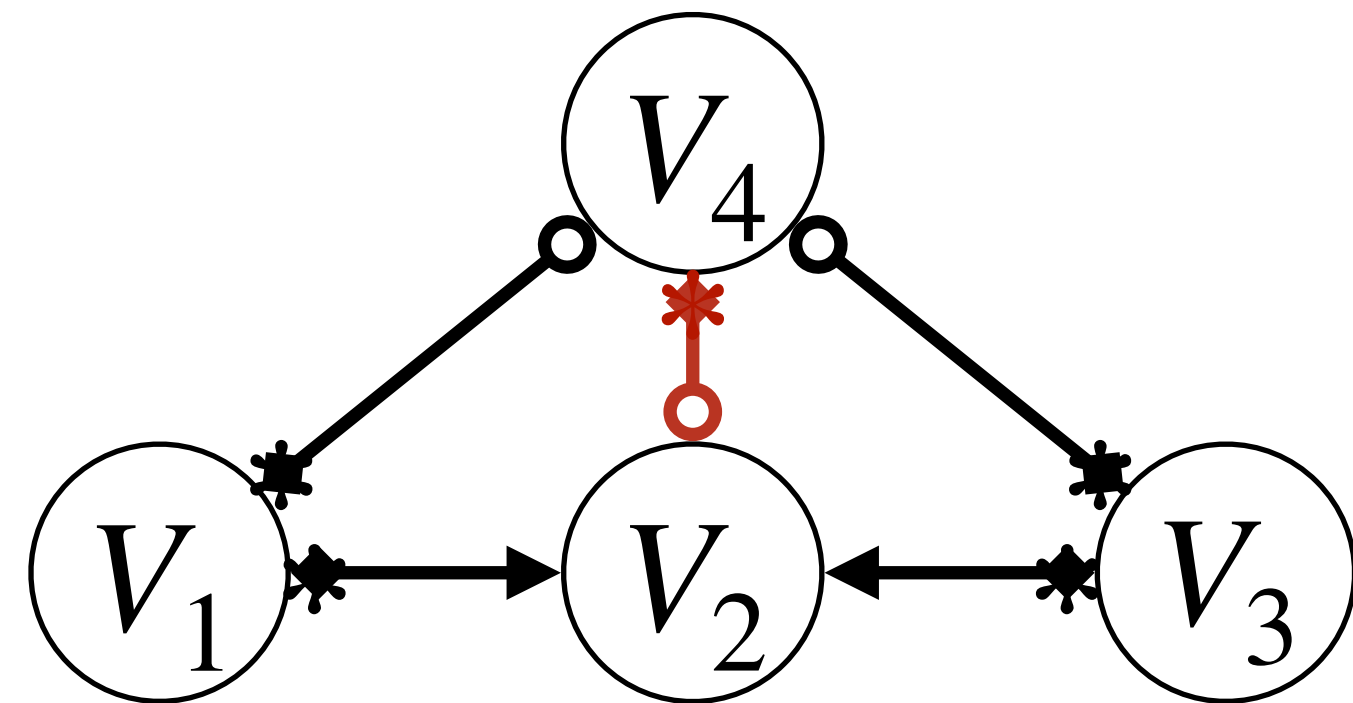


$V_1 \perp\!\!\!\perp V_3 \mid V_4$  and  $V_1 \not\perp\!\!\!\perp V_3 \mid V_4, V_5$

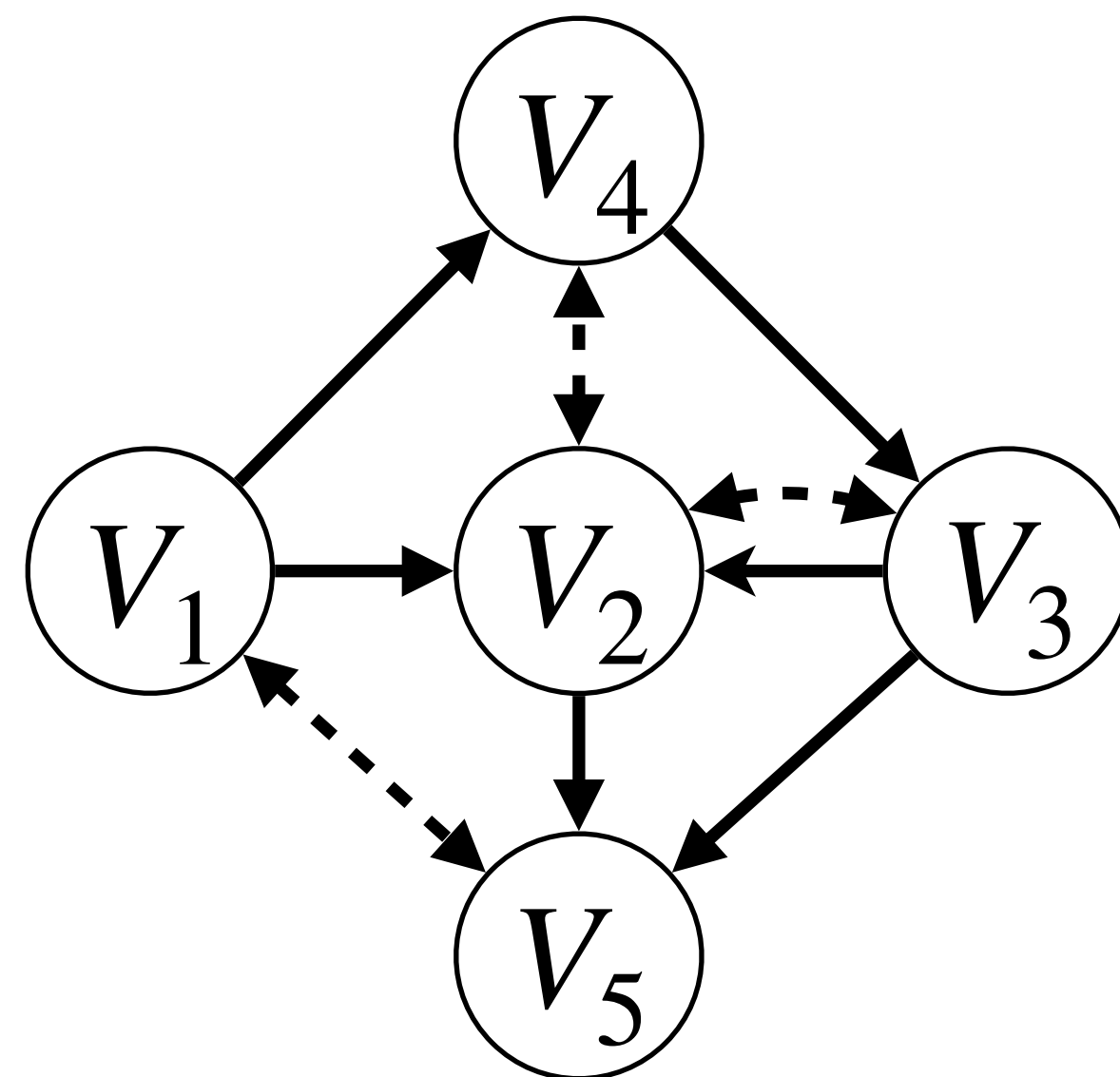
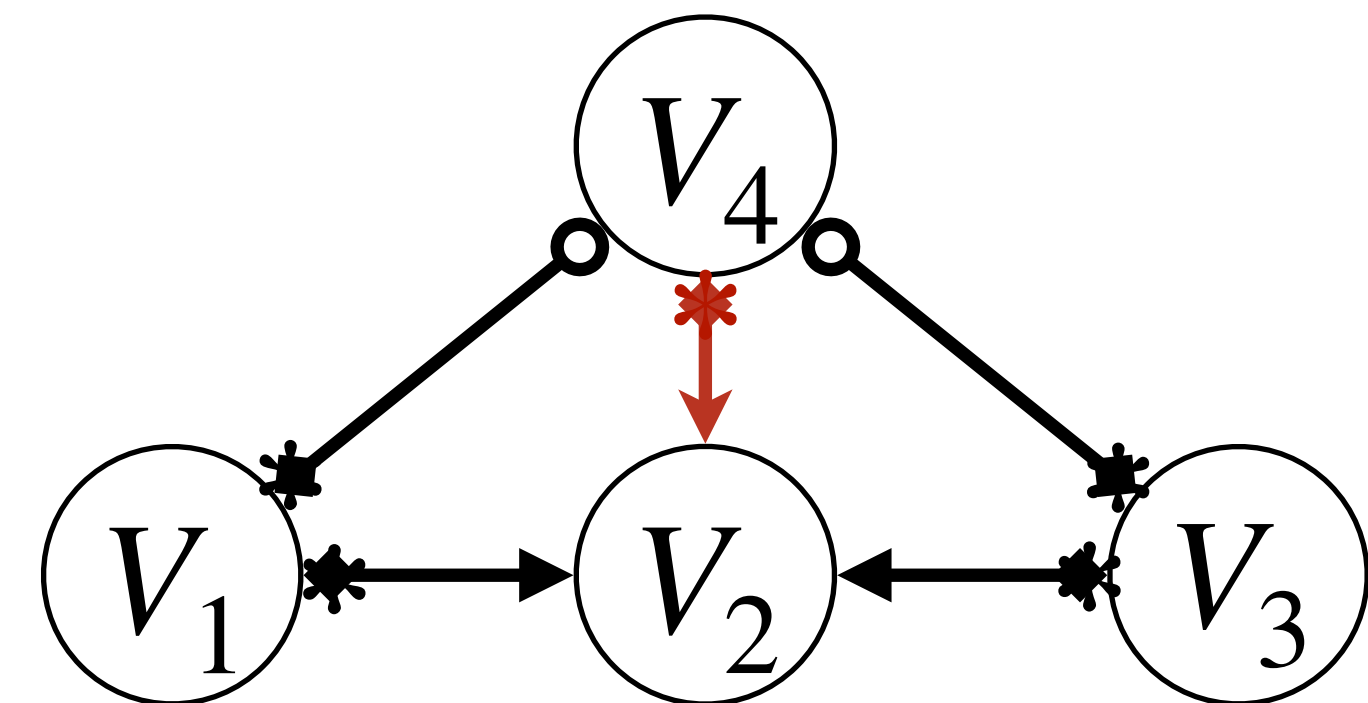


# Applying Mark Inference Rules

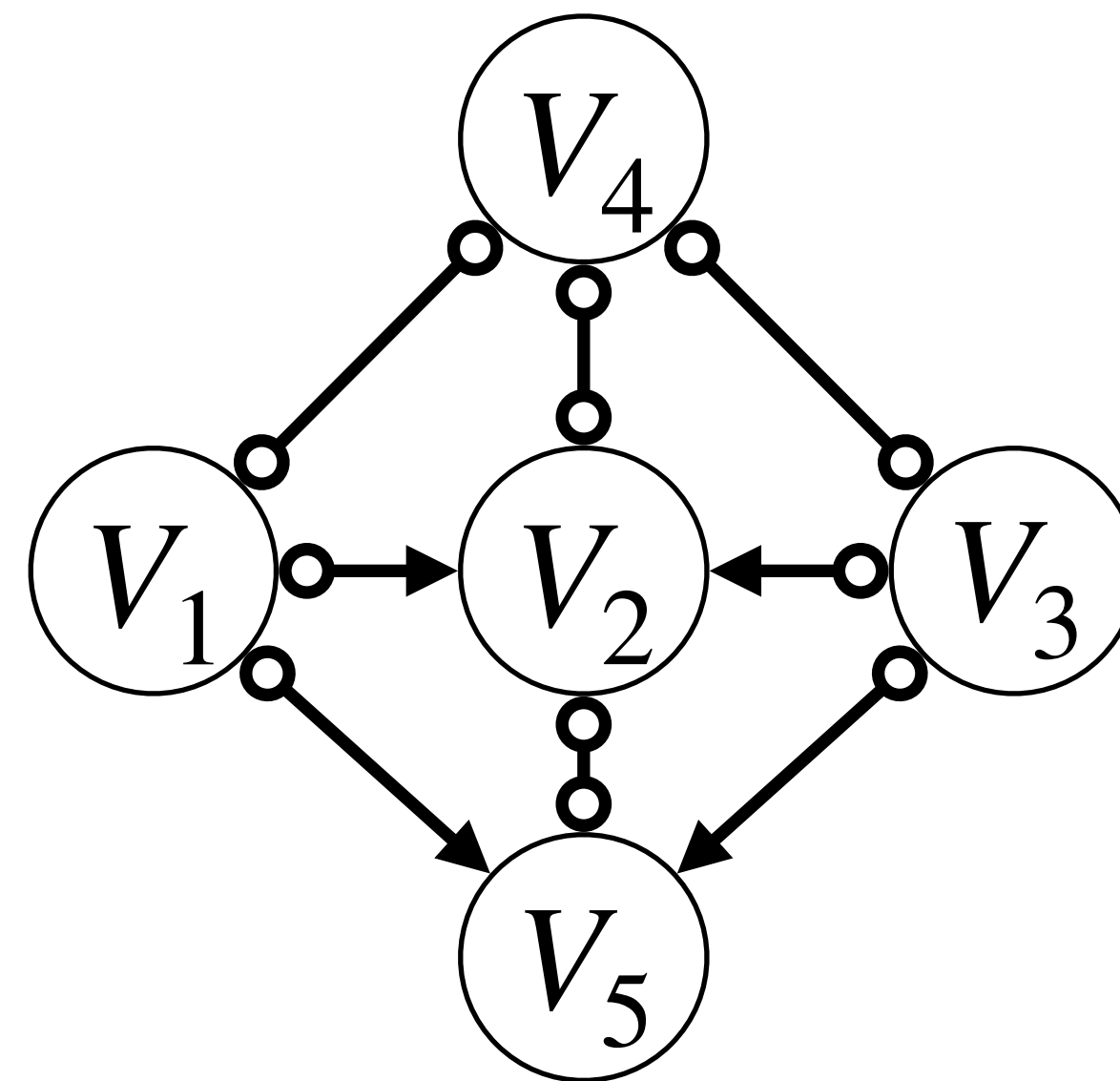
**R3:**



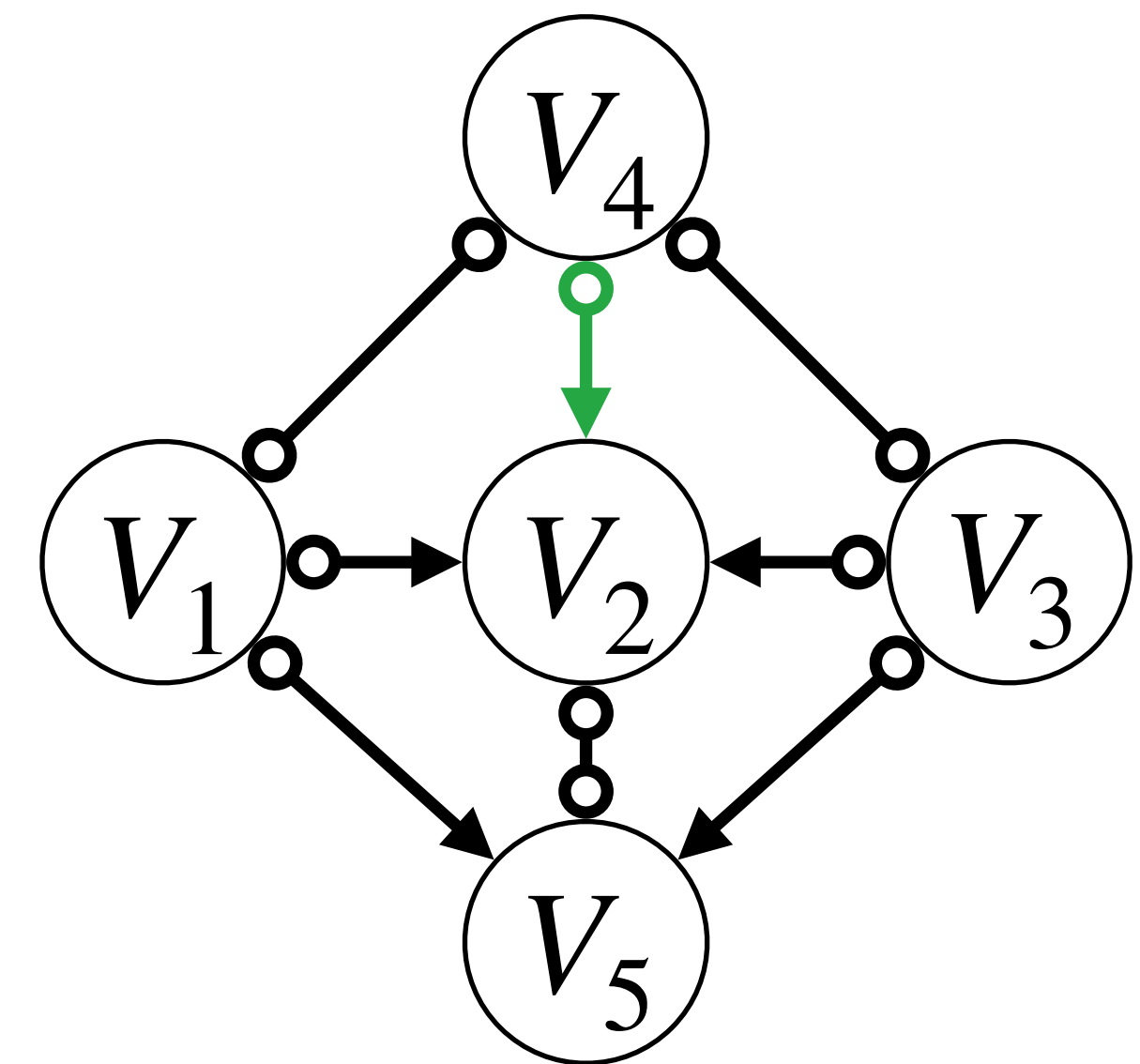
where  $V_1$  and  $V_3$  are not adjacent



True, unknown ADMG



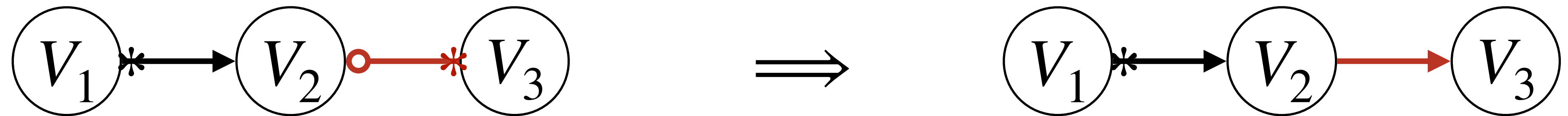
After Skeleton + R0



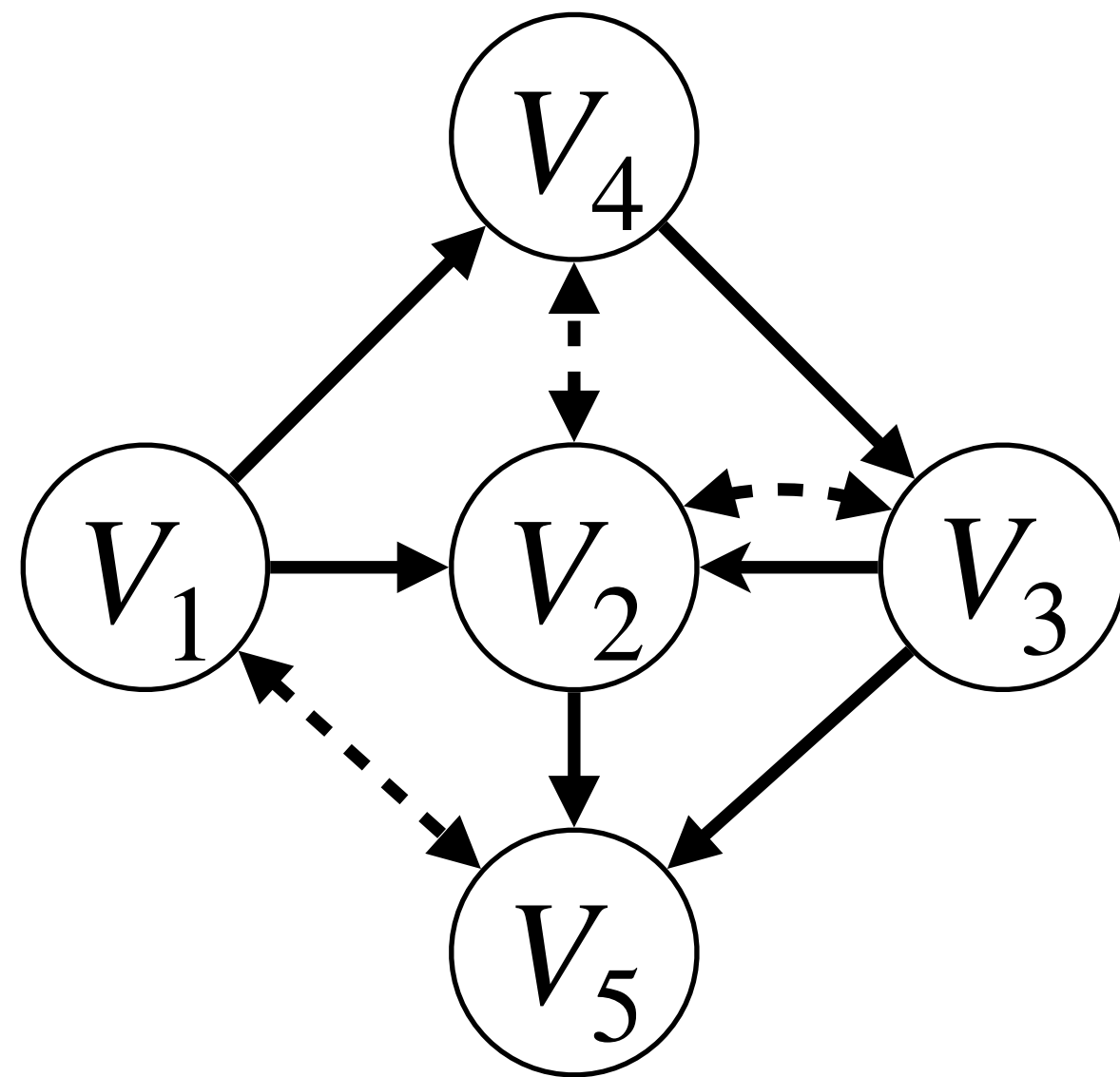
Applying R3

# Applying Mark Inference Rules

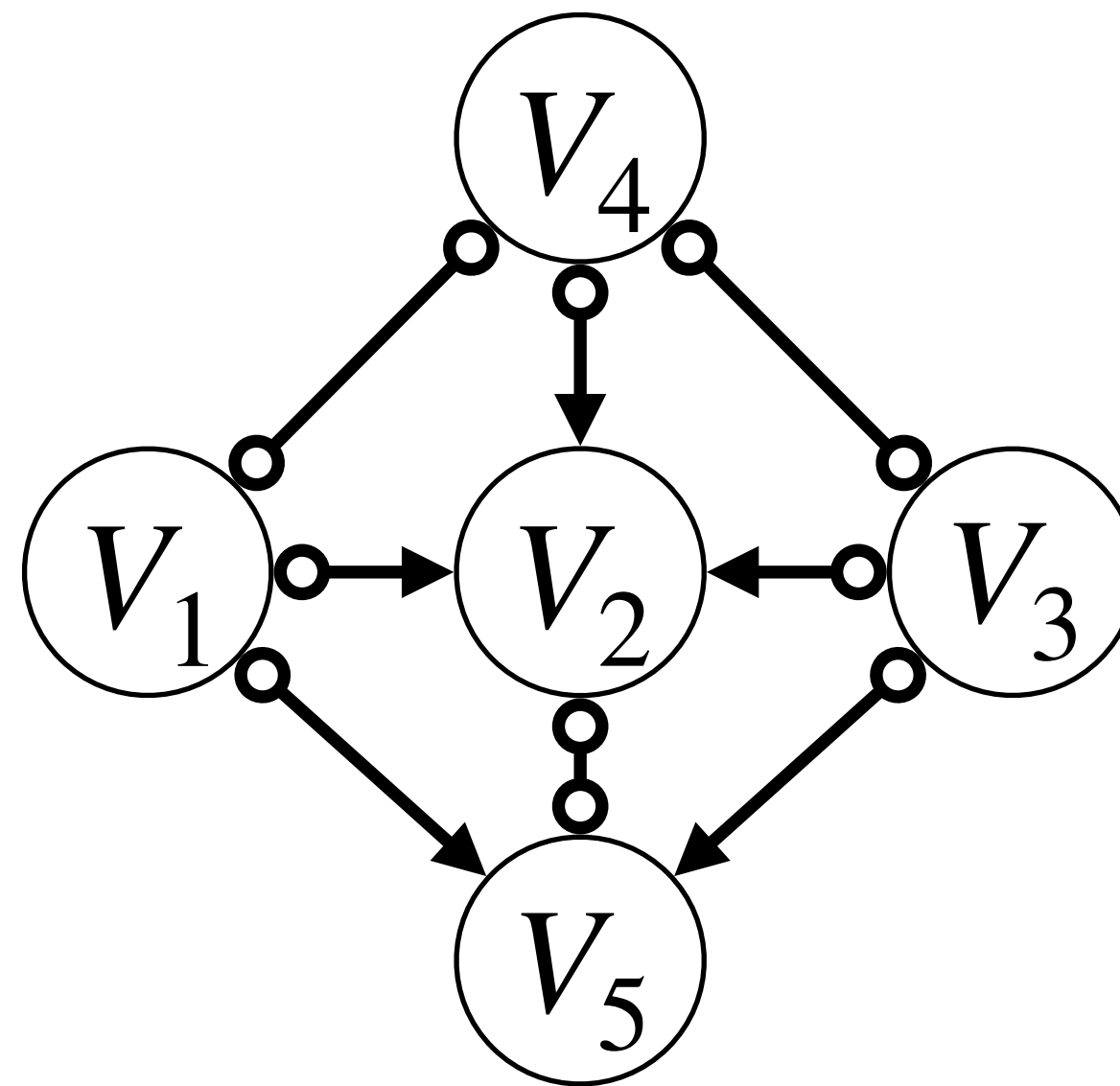
**R1:**



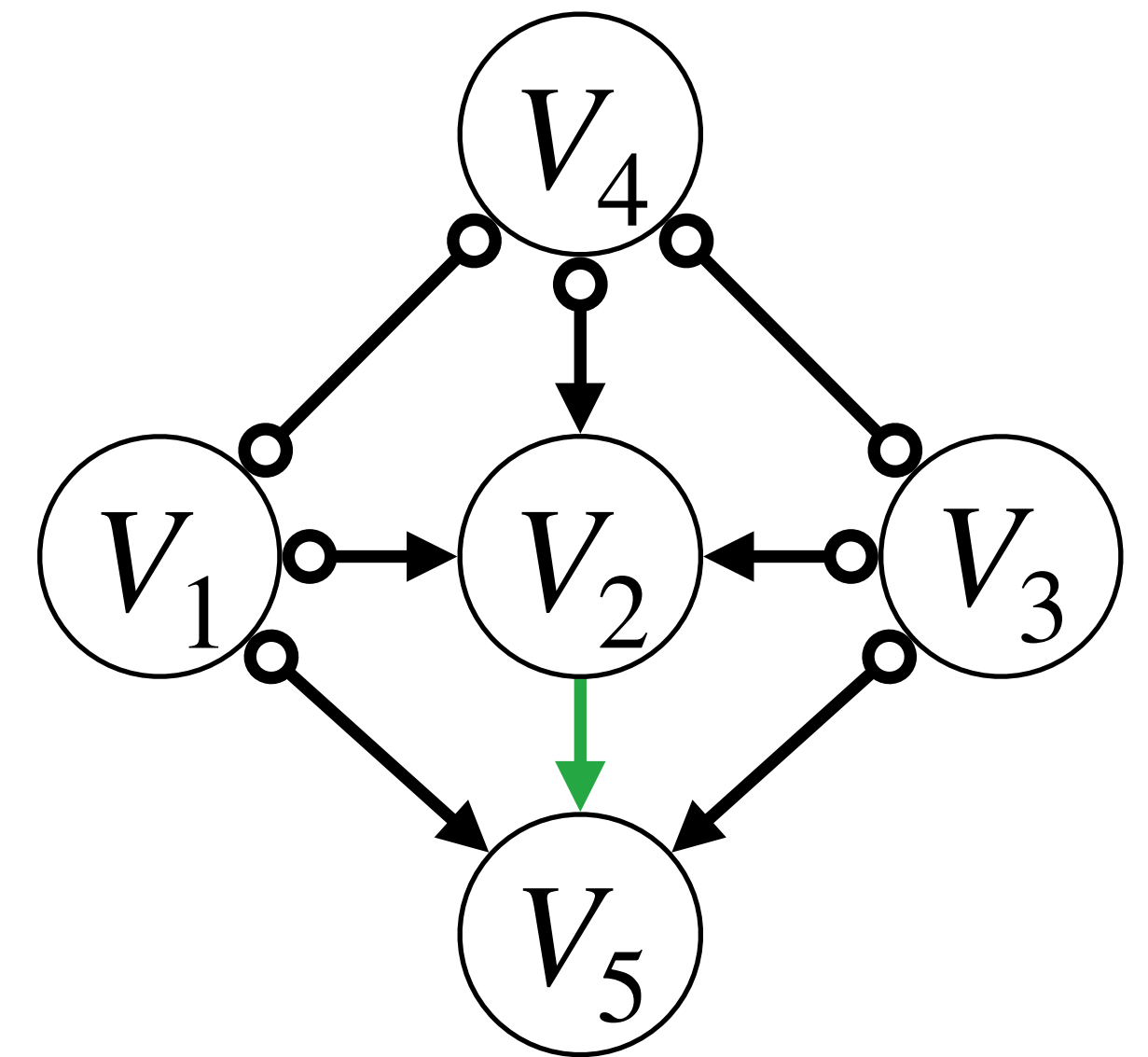
where  $V_1$  and  $V_3$  are not adjacent



True, unknown ADMG

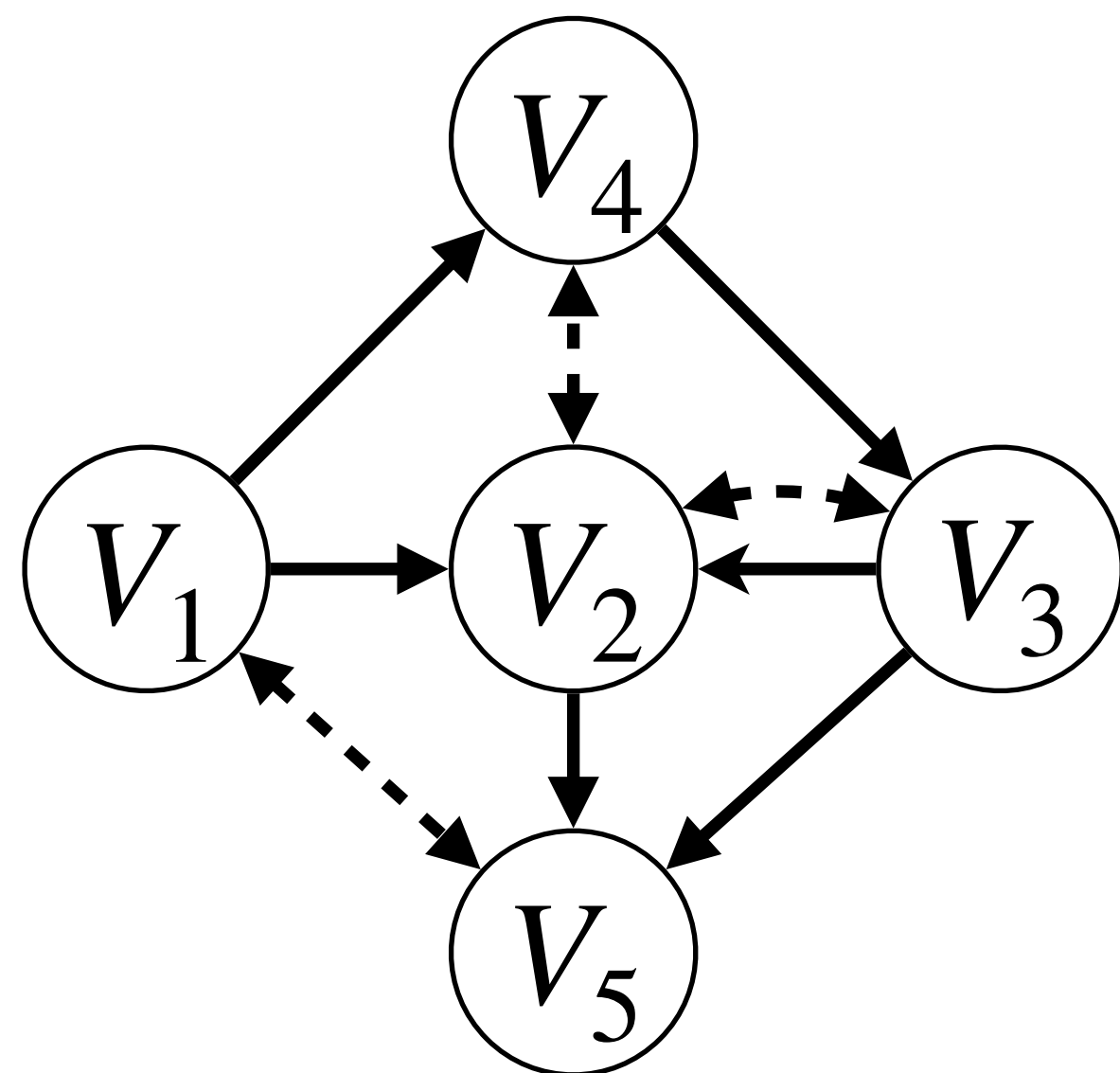
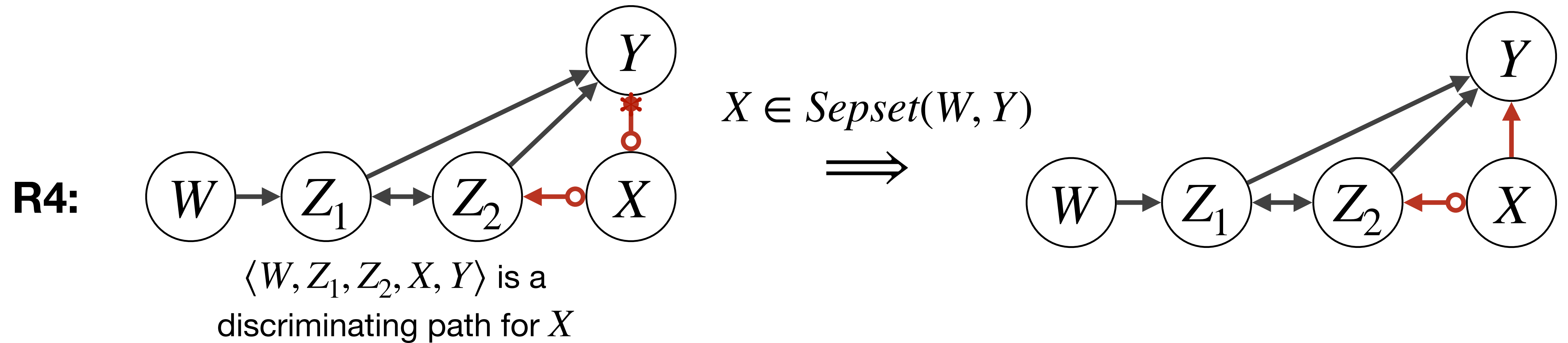


After Skel + R0 + R3

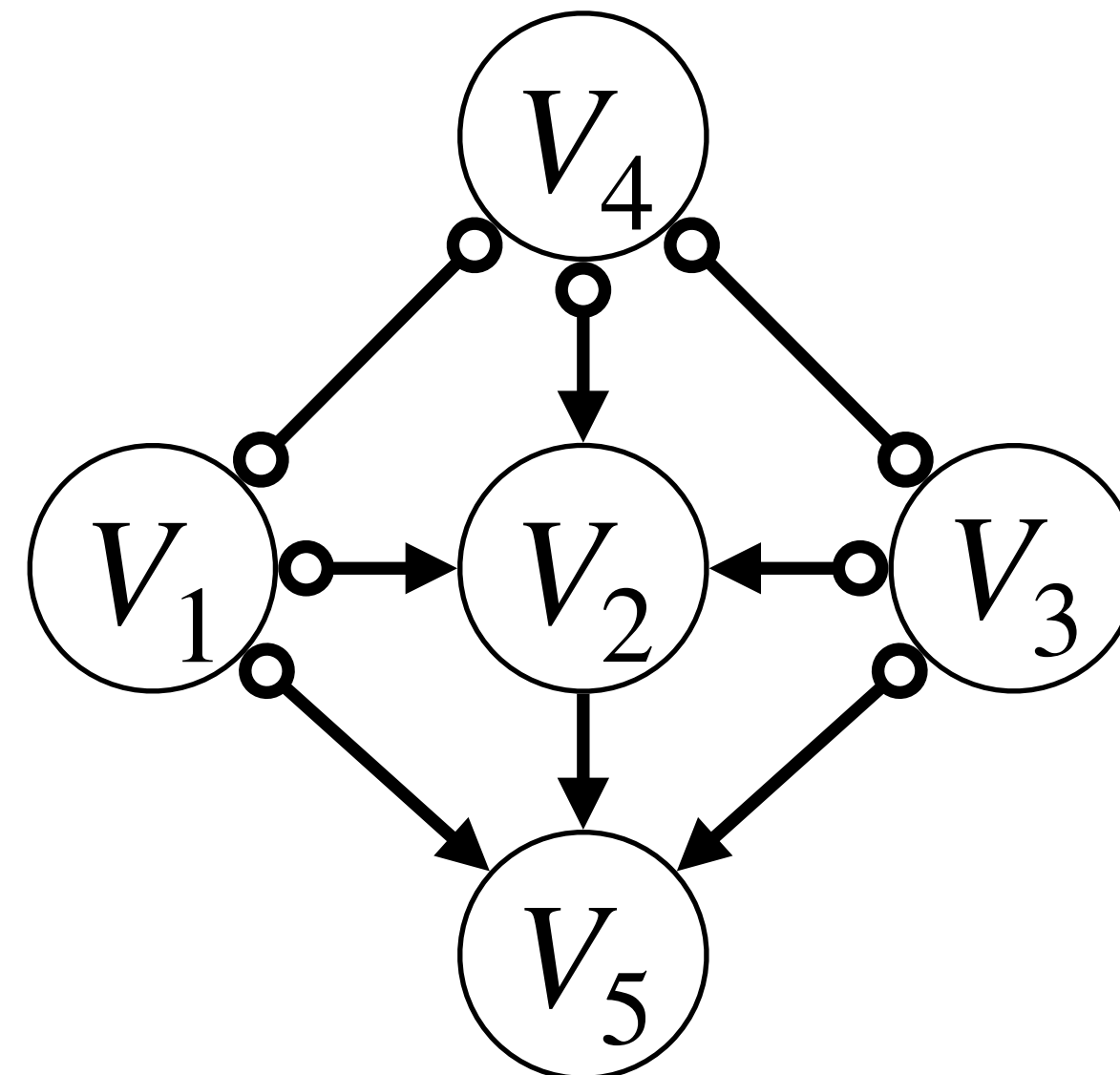


Applying R1

# Applying Mark Inference Rules



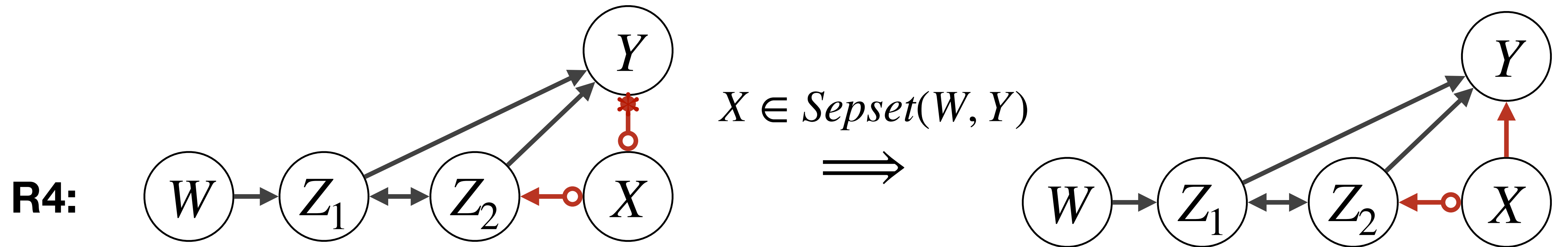
True, unknown ADMG



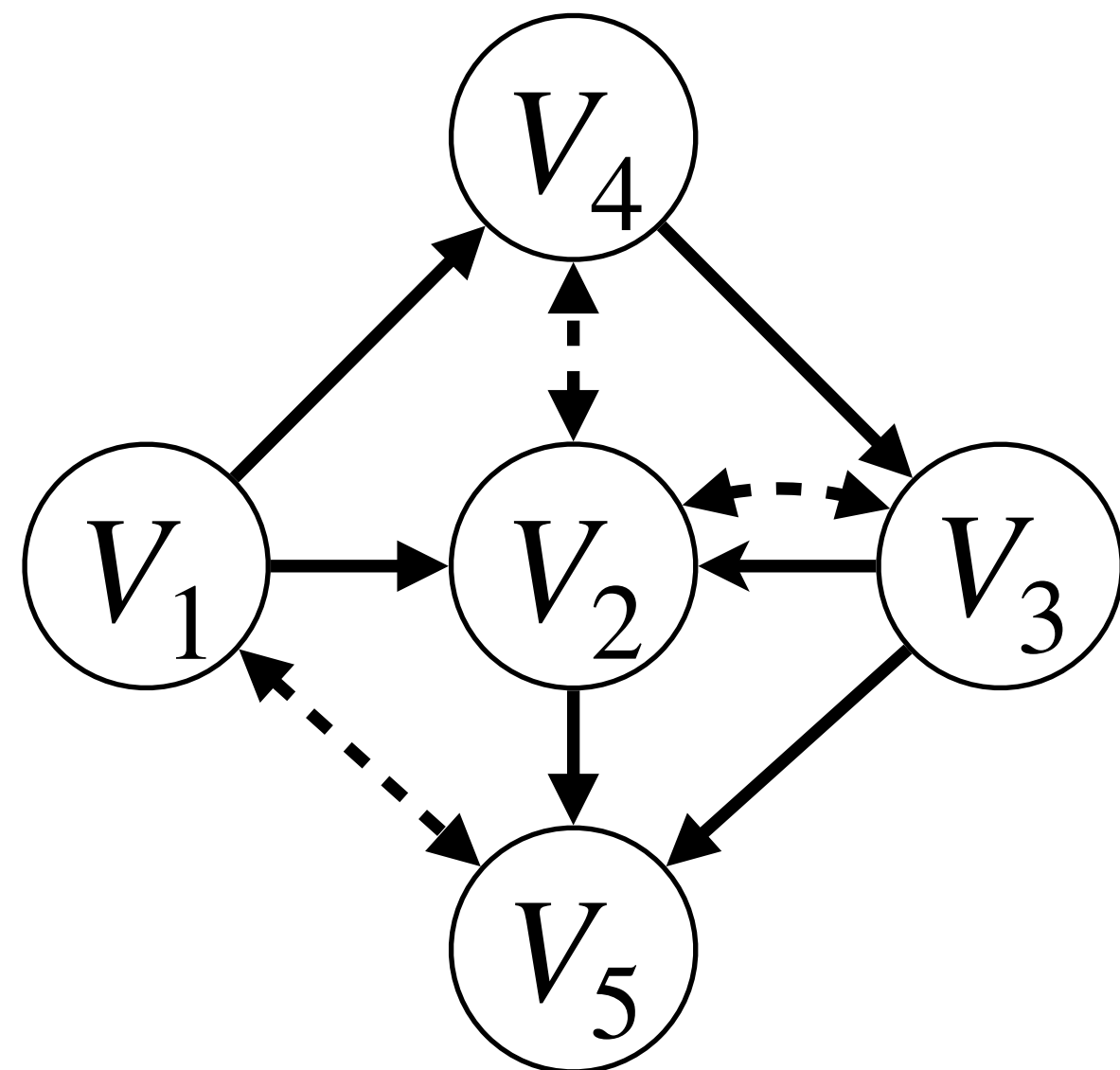
After Skel + R0 + R3 + R1



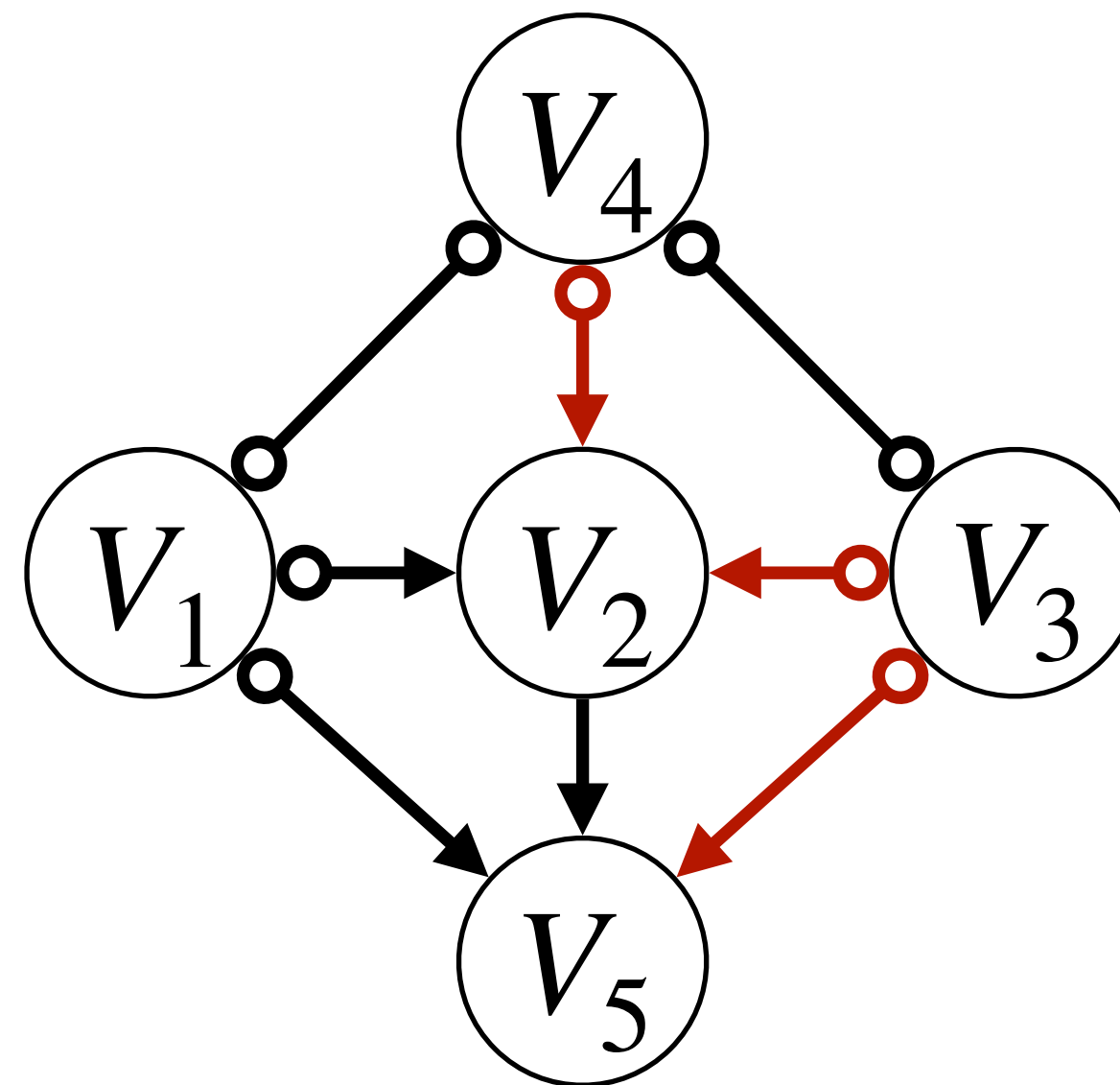
# Applying Mark Inference Rules



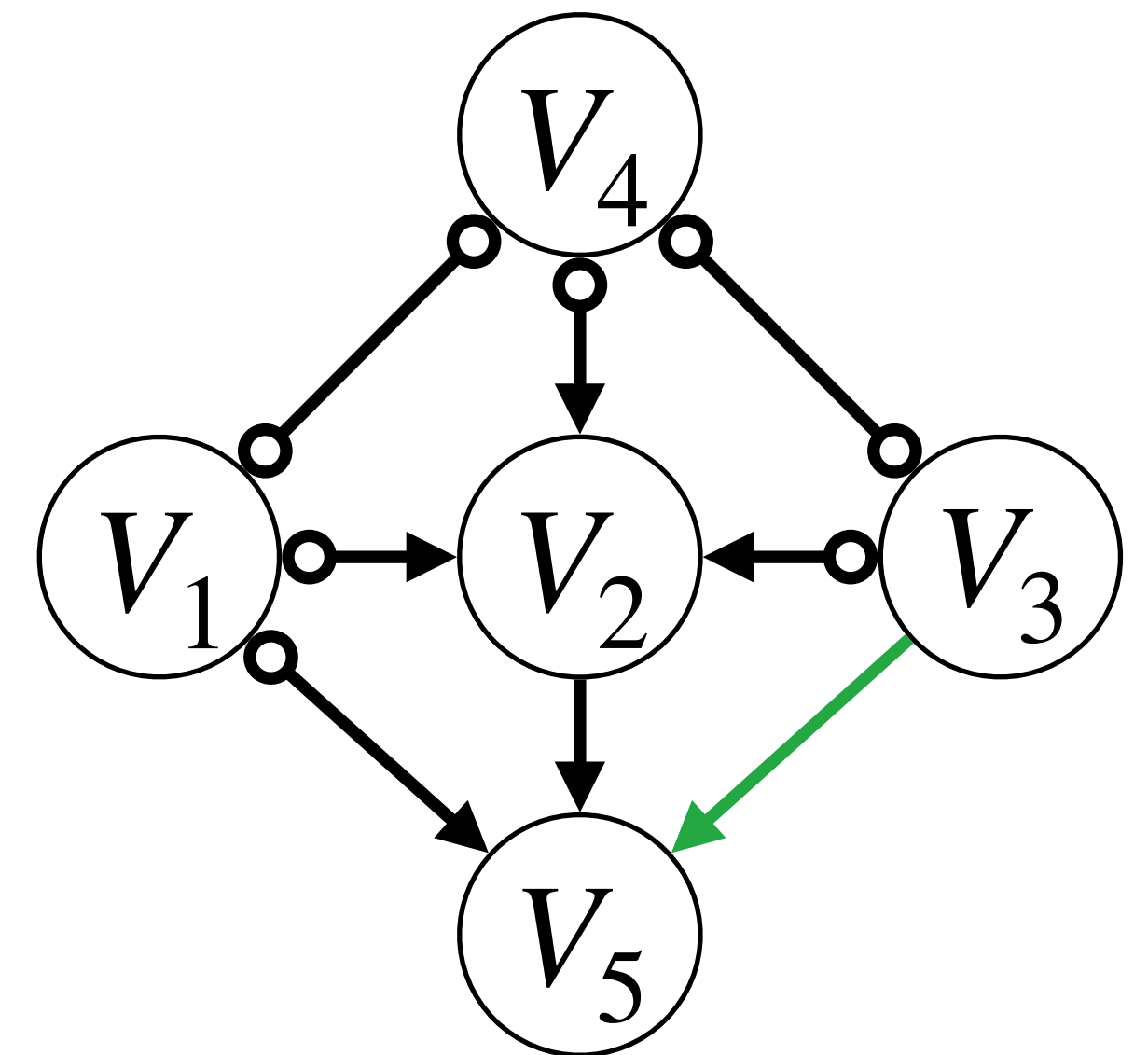
$\langle W, Z_1, Z_2, X, Y \rangle$  is a discriminating path for  $X$



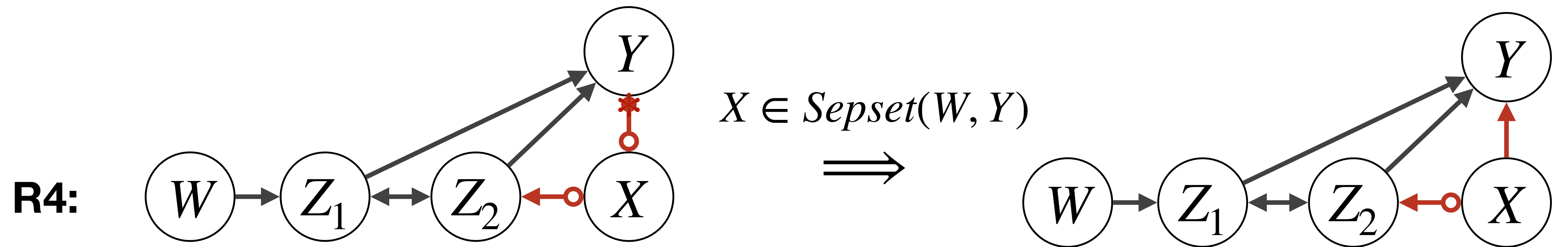
True, unknown ADMG



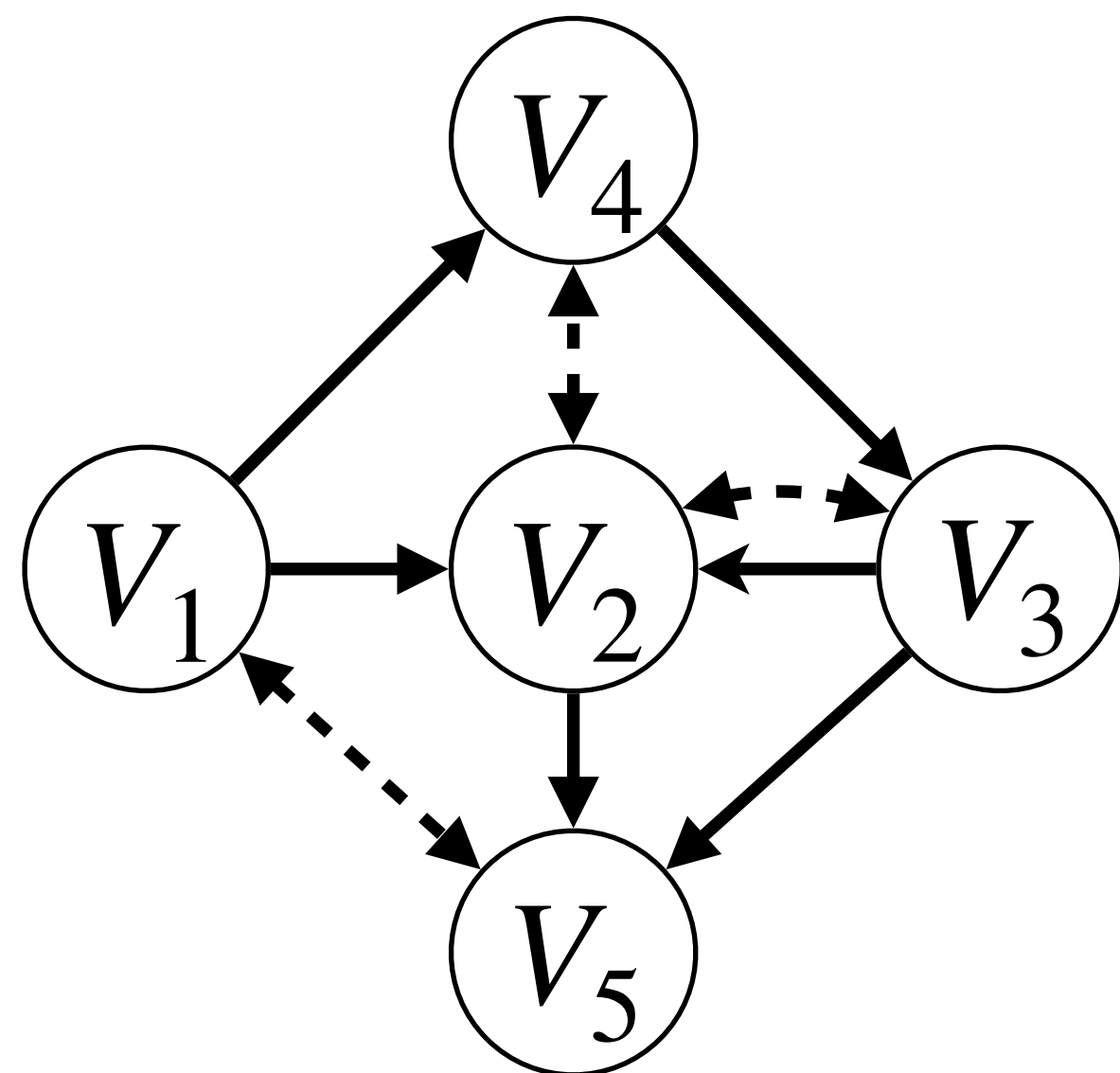
$\langle V_4, V_2, V_3, V_5 \rangle$  is a discriminating path for  $V_3$  and  
 $V_3 \in \text{Sepset}(V_4, V_5) - V_4 \perp\!\!\!\perp V_5 \mid V_1, V_2, V_3$



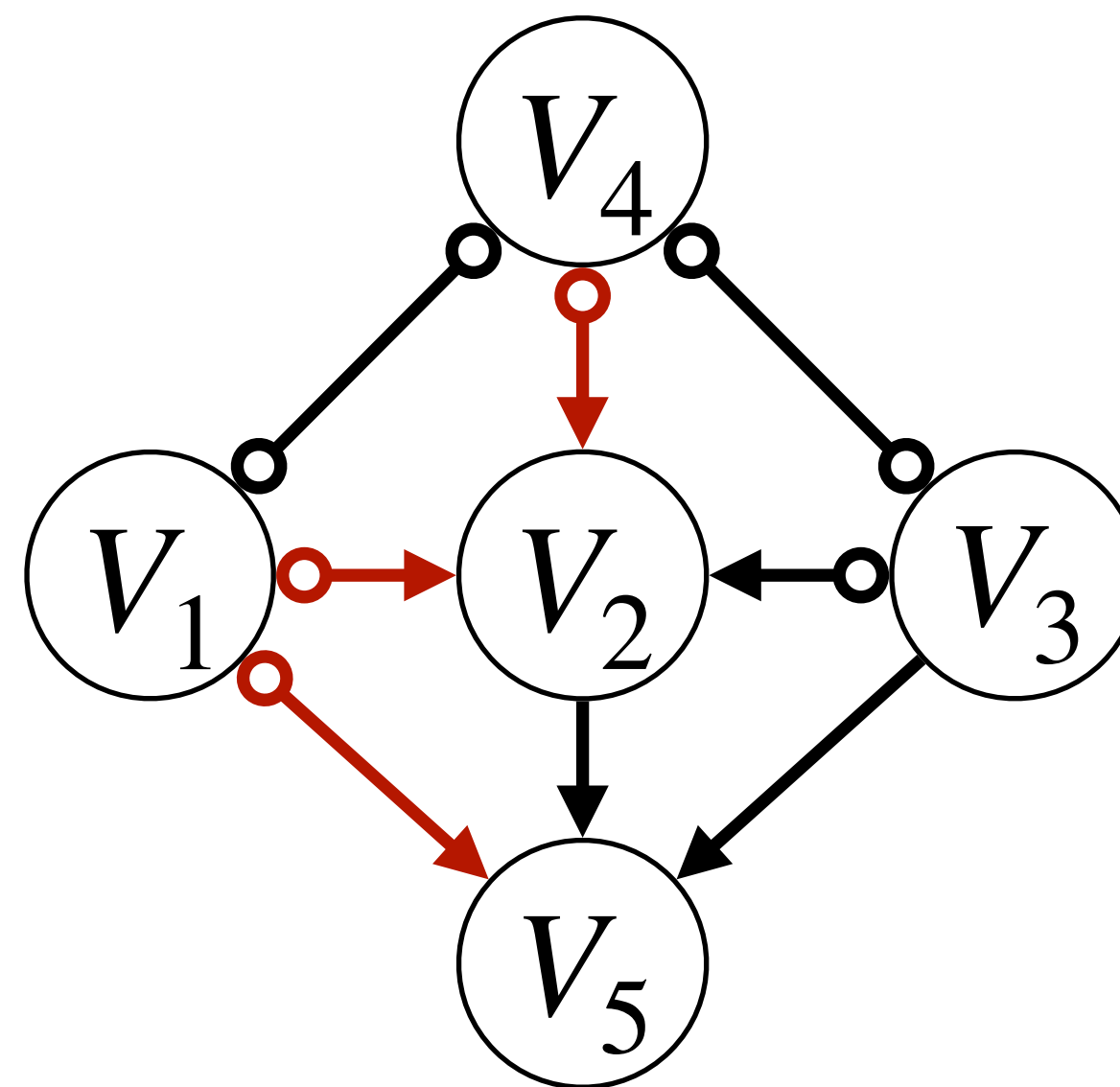
# Applying Mark Inference Rules



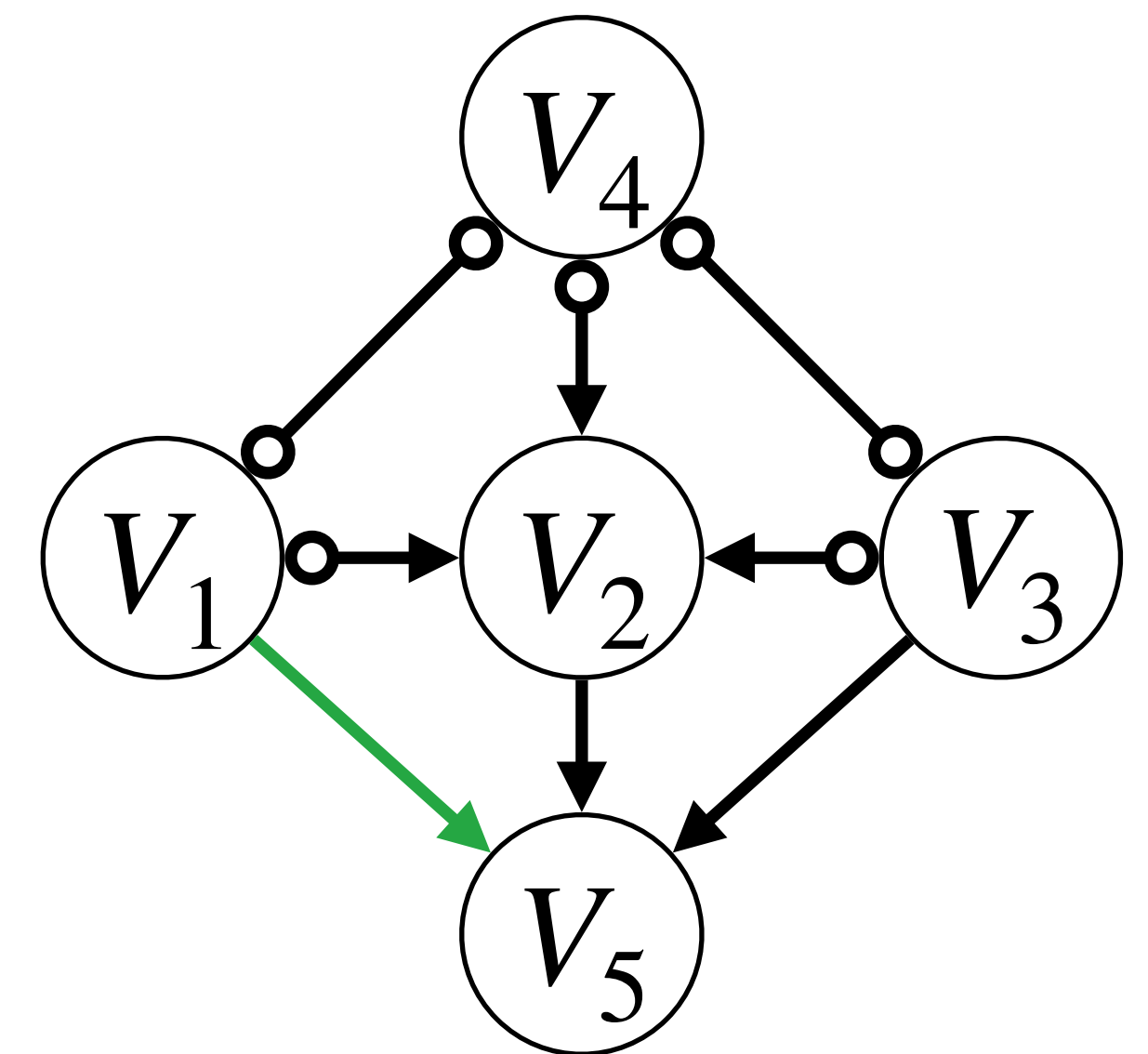
$\langle W, Z_1, Z_2, X, Y \rangle$  is a discriminating path for  $X$



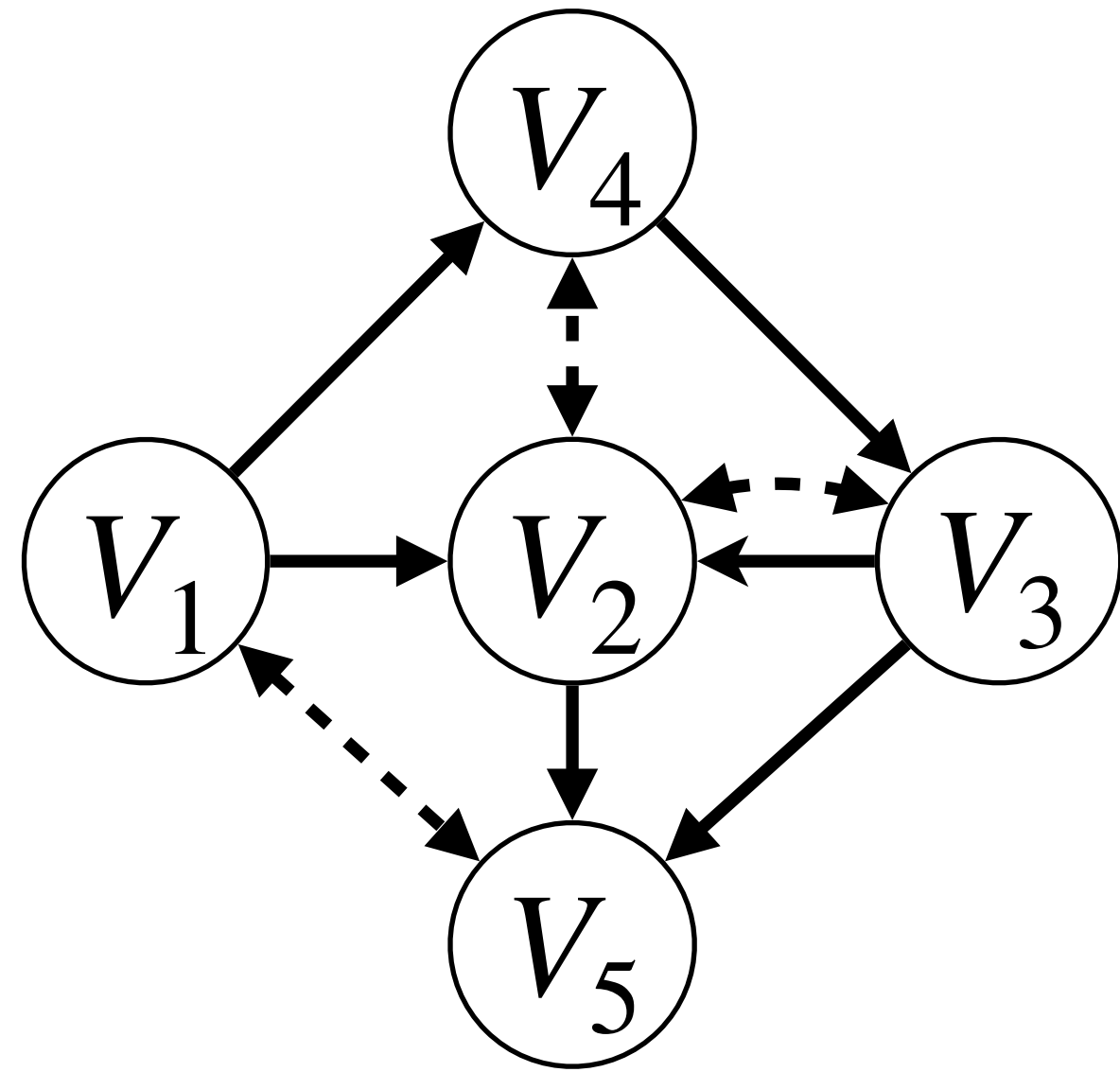
True, unknown ADMG



$\langle V_4, V_2, V_1, V_5 \rangle$  is a discriminating path for  $V_1$  and  $V_1 \in \text{Sepset}(V_4, V_5) - V_4 \perp\!\!\!\perp V_5 \mid V_1, V_2, V_3$



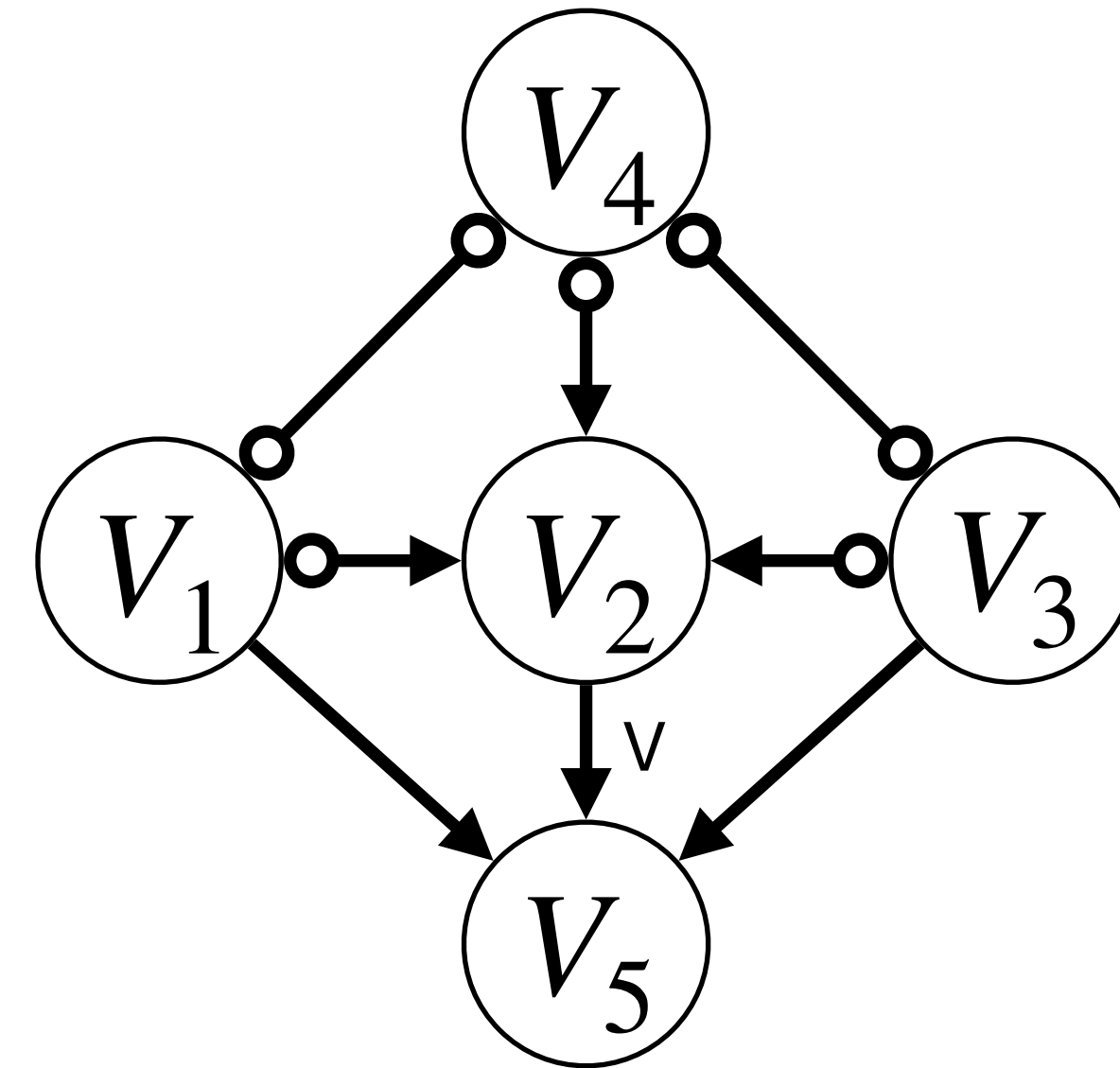
# Final PAG



True, unknown ADMG

$$V_1 \perp\!\!\!\perp V_3 \mid V_4$$

$$V_4 \perp\!\!\!\perp V_5 \mid V_1, V_2, V_3$$



Final PAG

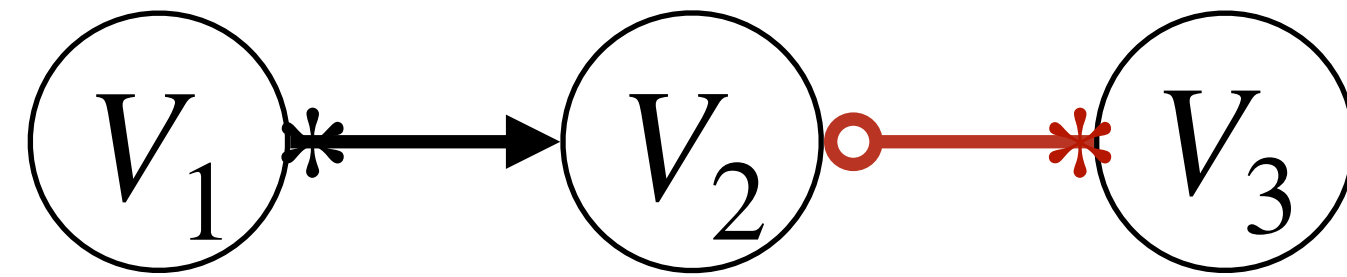
After Skel + R0 + R3 + R1 + R4 + R4

$$V_1 \perp\!\!\!\perp V_3 \mid V_4$$

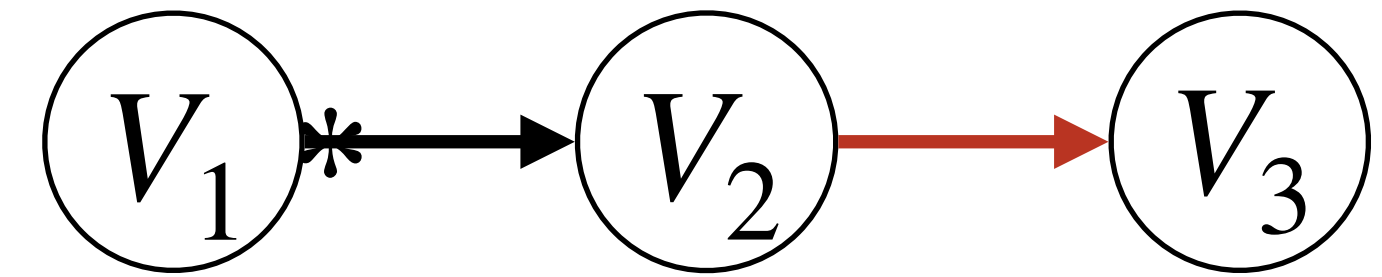
$$V_4 \perp\!\!\!\perp V_5 \mid V_1, V_2, V_3$$

# FCI - Complete Set of Mark Inference Rules

**R1:**

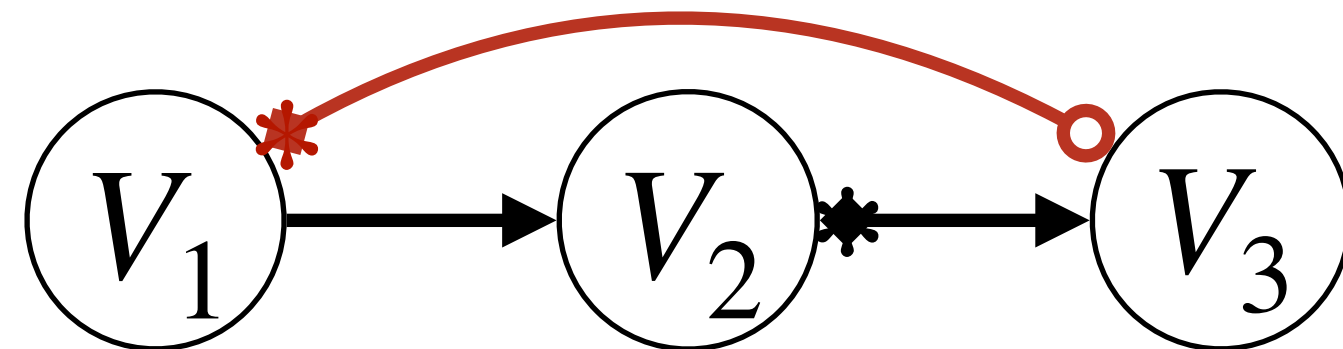


$\Rightarrow$

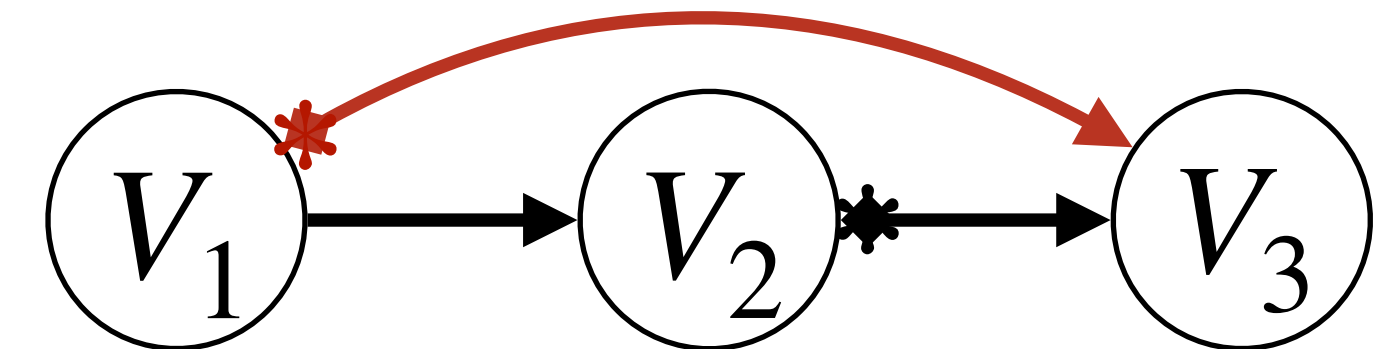


where  $V_1$  and  $V_3$  are not adjacent

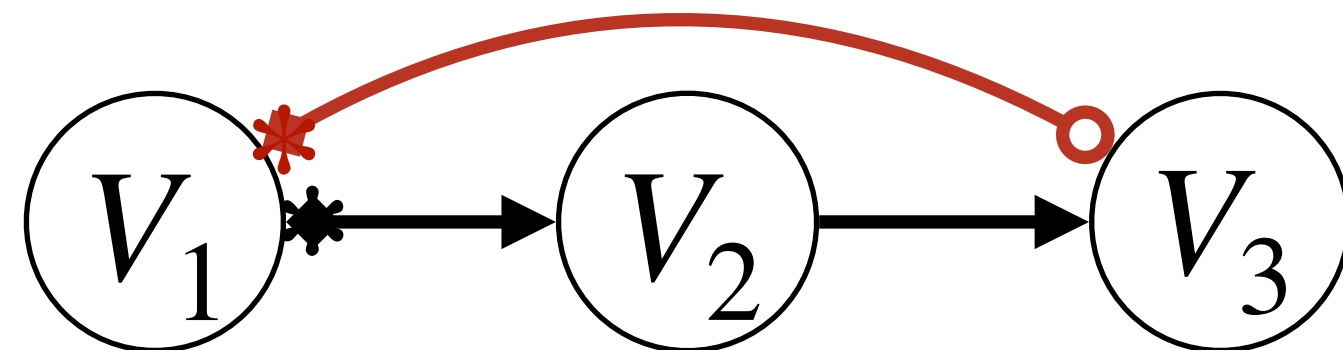
**R2:**



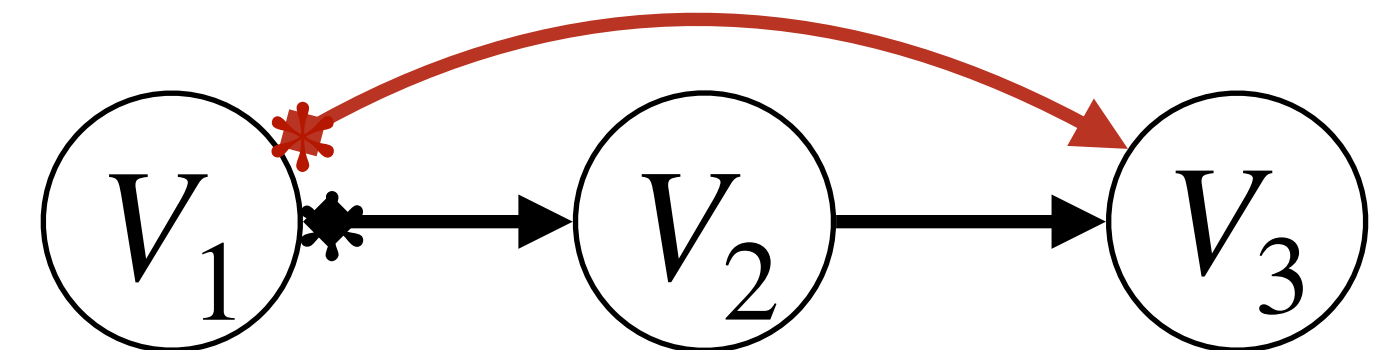
$\Rightarrow$



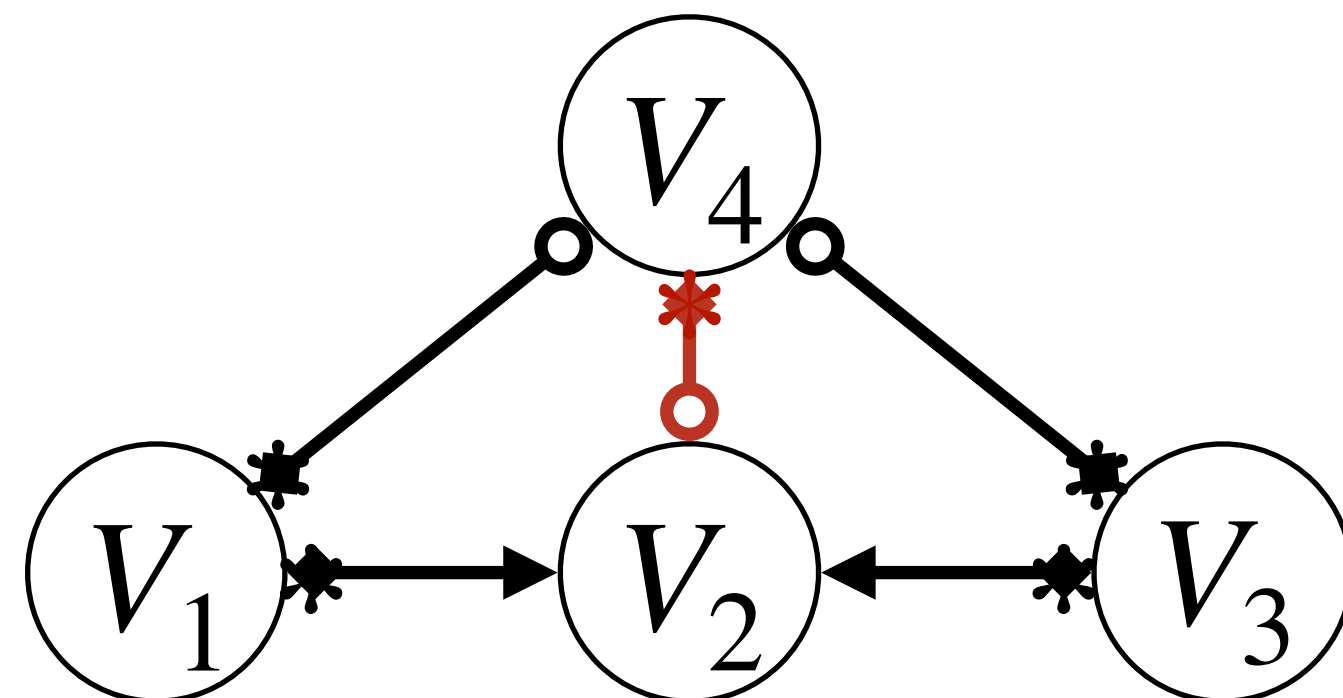
or



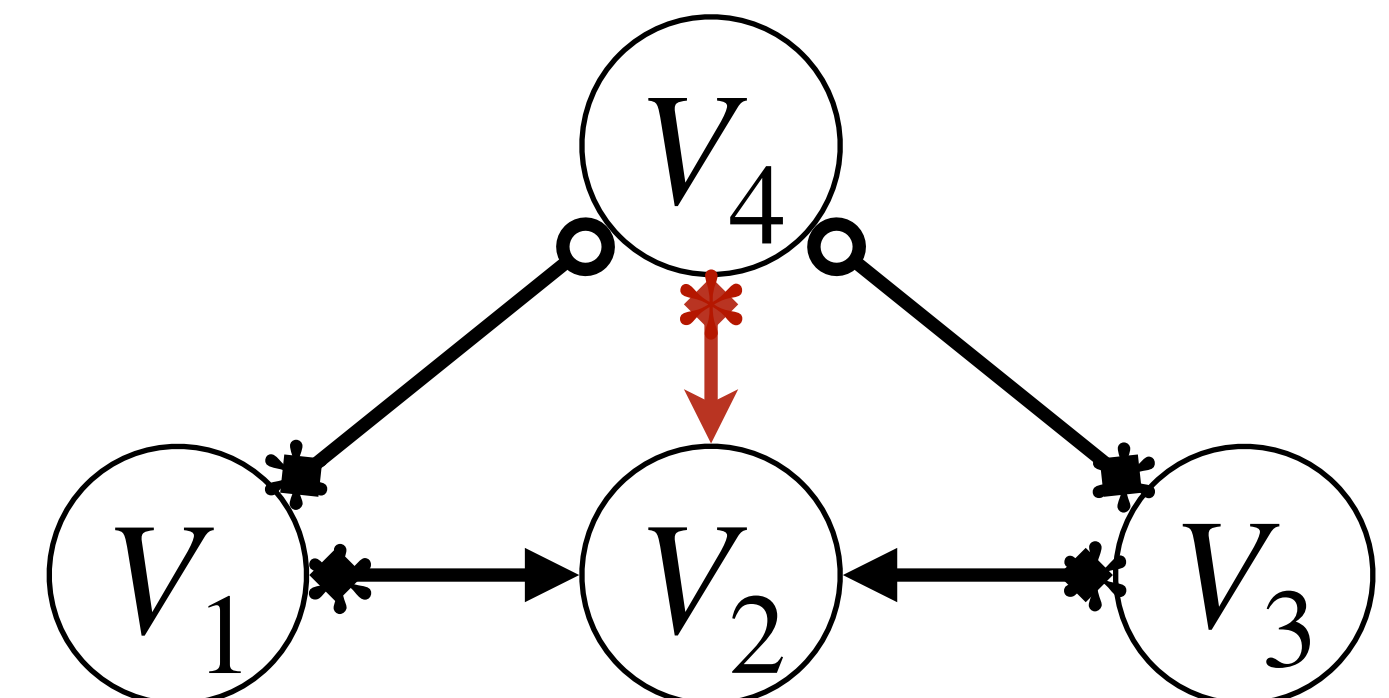
$\Rightarrow$



**R3:**



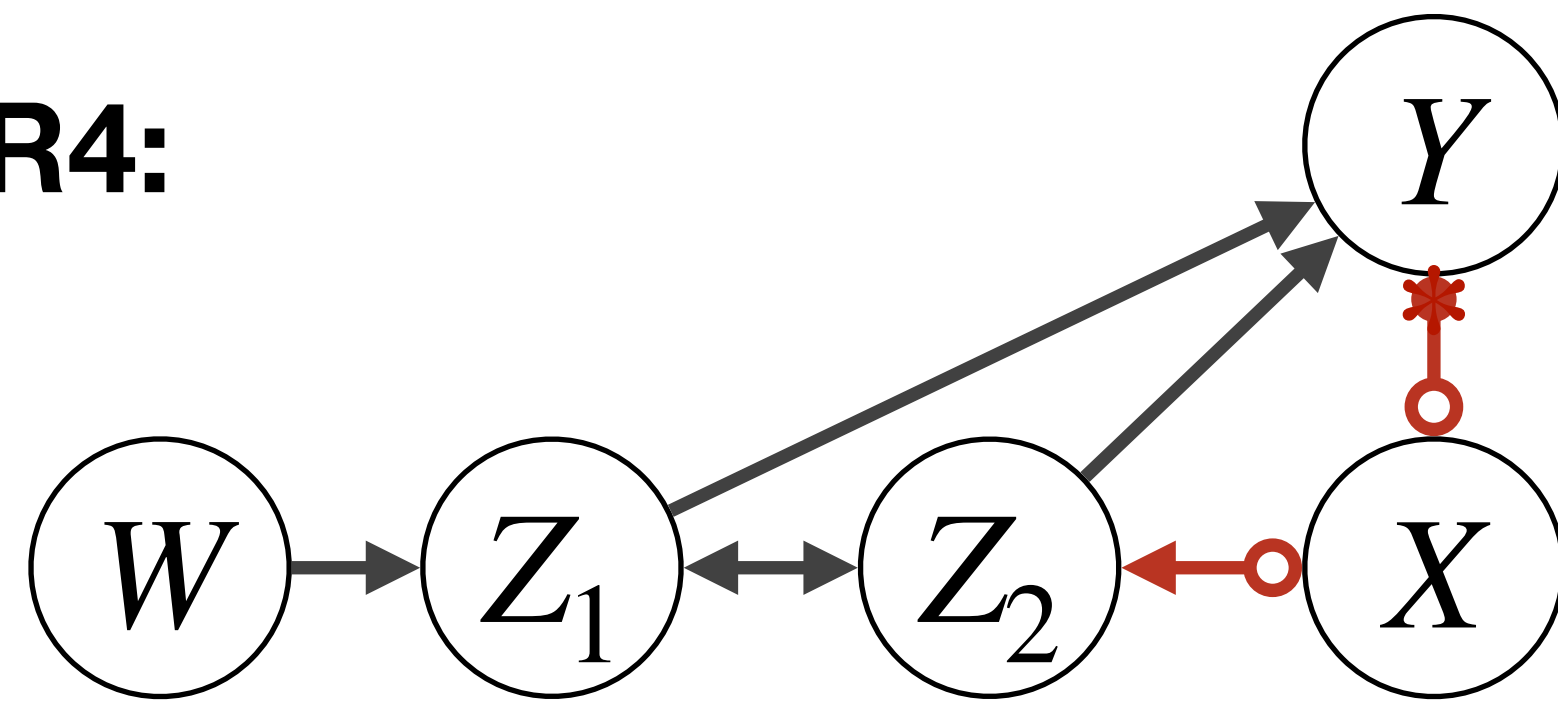
$\Rightarrow$



where  $V_1$  and  $V_3$  are not adjacent

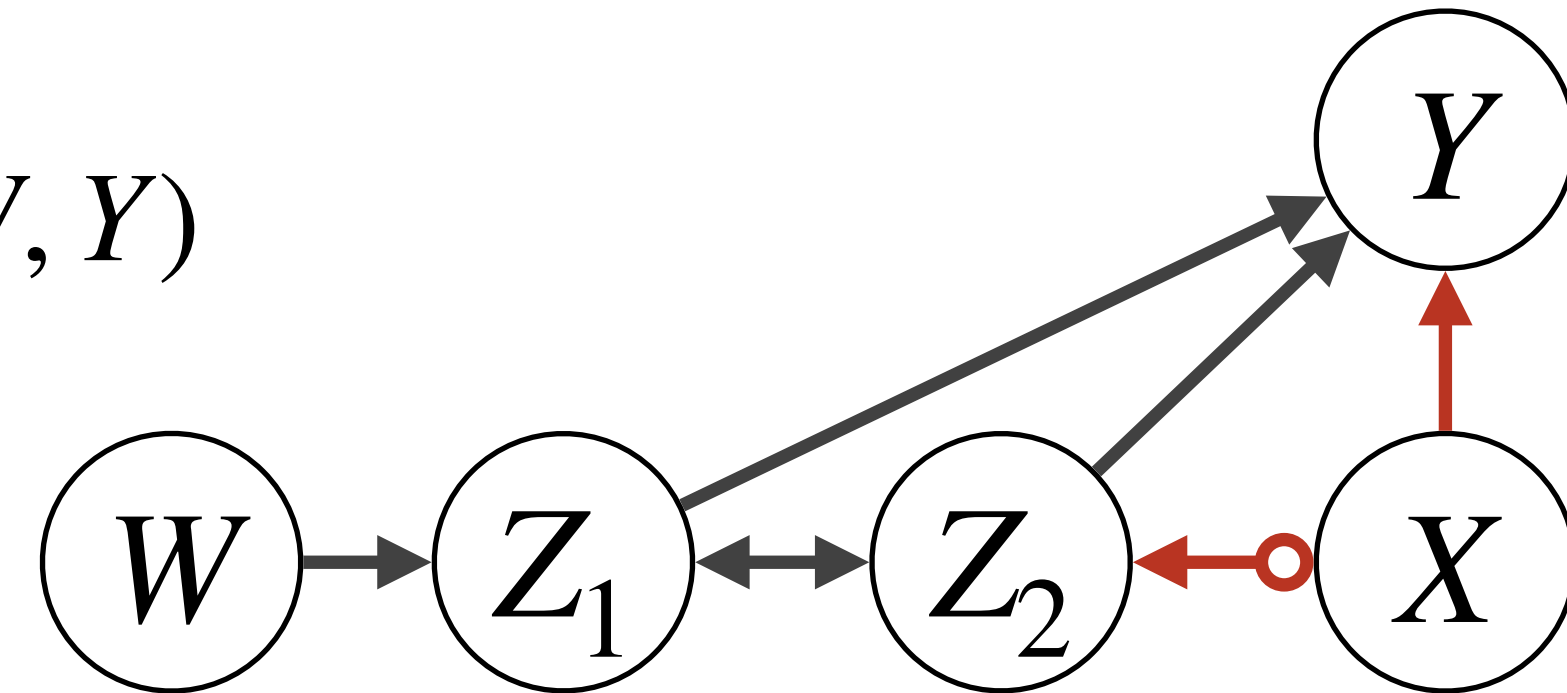
# FCI - Complete Set of Mark Inference Rules

**R4:**



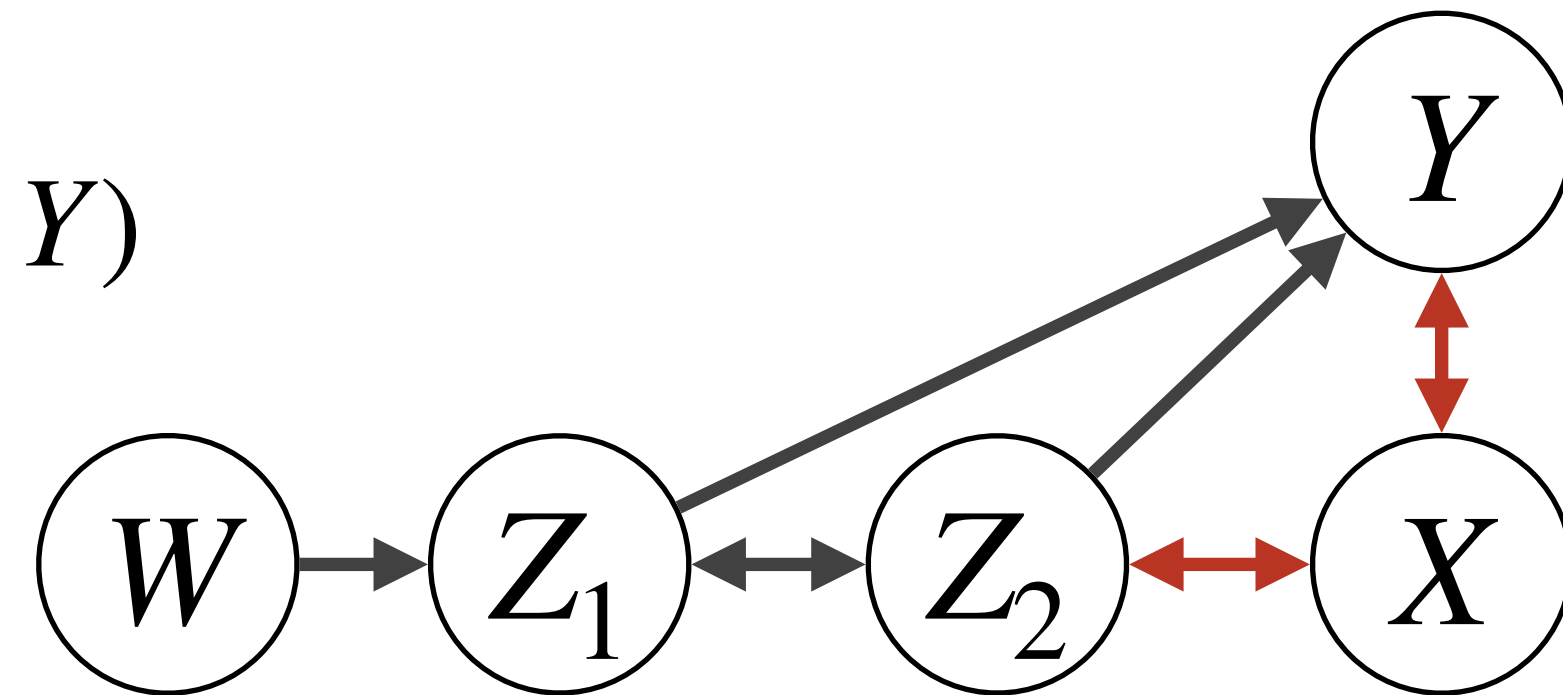
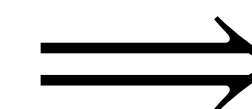
$\langle W, Z_1, Z_2, X, Y \rangle$  is a discriminating path for  $X$

$X \in \text{Sepset}(W, Y)$



$X$  is a non-collider in  $\langle Z_2, X, Y \rangle$

$X \notin \text{Sepset}(W, Y)$



$X$  is a collider in  $\langle Z_2, X, Y \rangle$

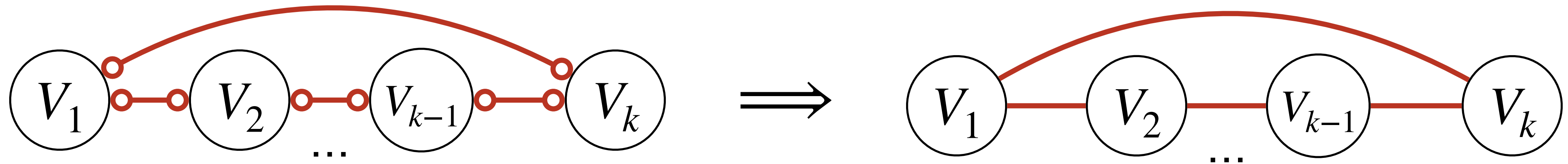
**Definition (discriminating path):** A path  $p = \langle X, \dots, W, V, Y \rangle$  in a MAG is a discriminating path for  $V$  if

- (i)  $p$  includes at least three edges;
- (ii)  $V$  is a non-endpoint vertex on  $p$ , and is adjacent to  $Y$  on  $p$ ; and
- (iii)  $X$  is not adjacent to  $Y$ , and every vertex between  $X$  and  $V$  is a collider on  $p$  and is a parent of  $Y$ .



# FCI - Complete Set of Mark Inference Rules

**R5:**

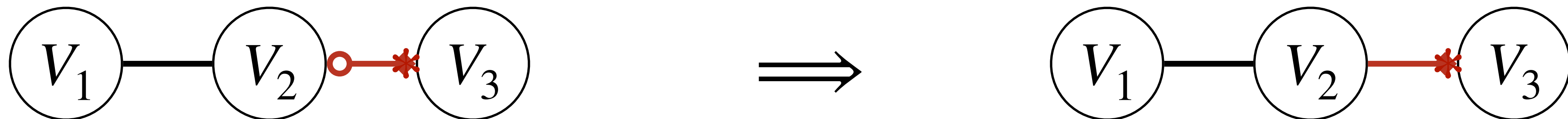


$\langle V_1, V_2, \dots, V_{k-1}, V_k \rangle$  is an  
uncovered circle path

$V_1$  and  $V_{k-1}$  are not adjacent

$V_2$  and  $V_k$  are not adjacent

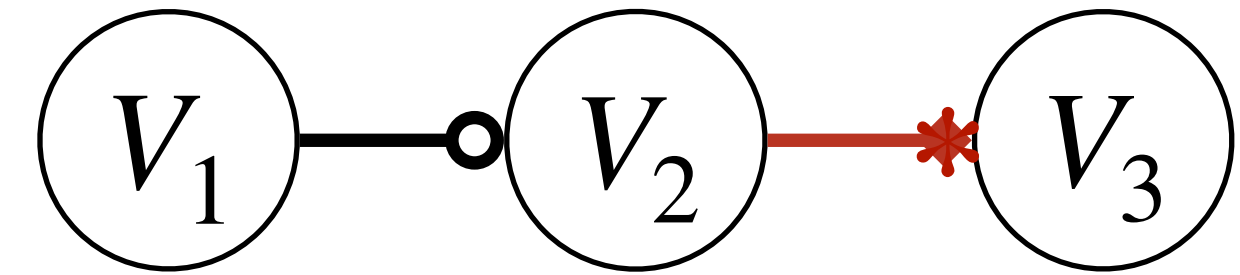
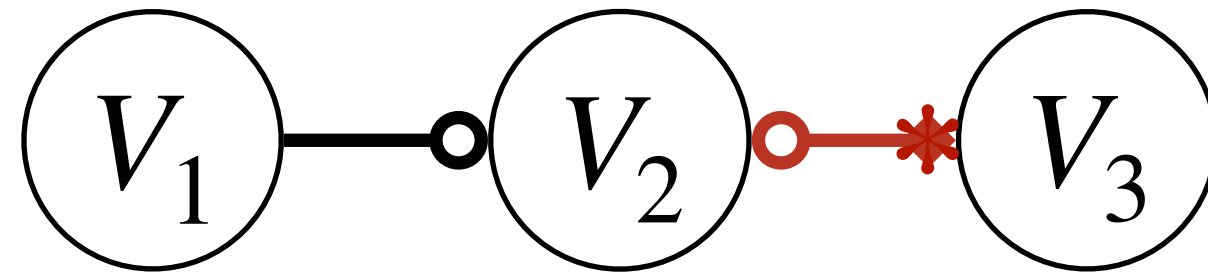
**R6:**



$V_1$  and  $V_3$  may or may  
not be adjacent

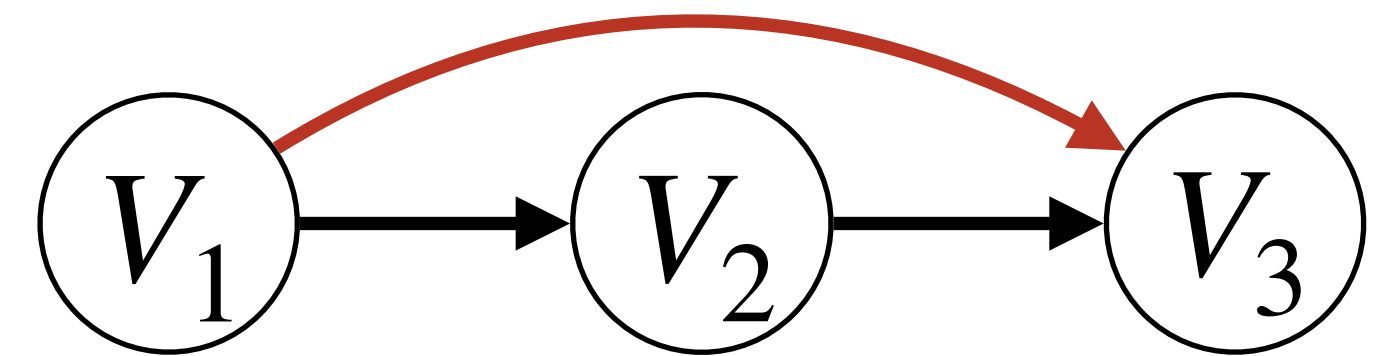
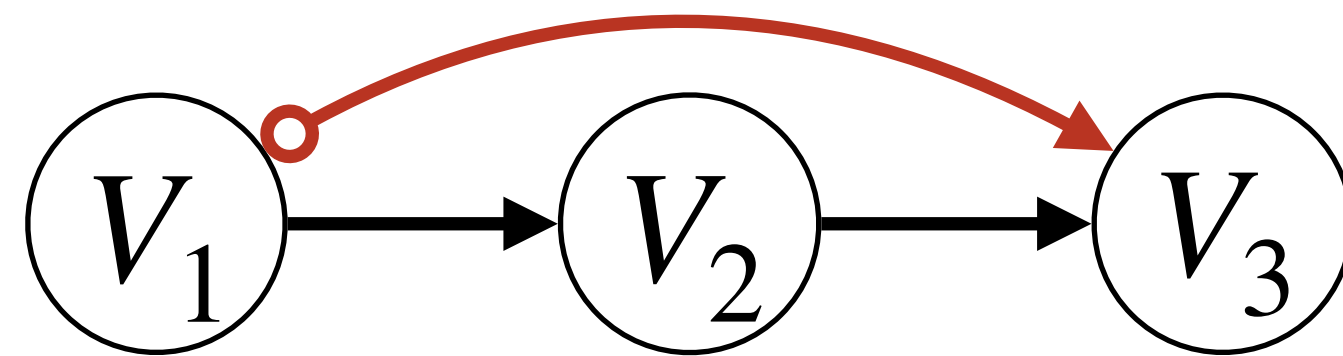
# FCI - Complete Set of Mark Inference Rules

**R7:**

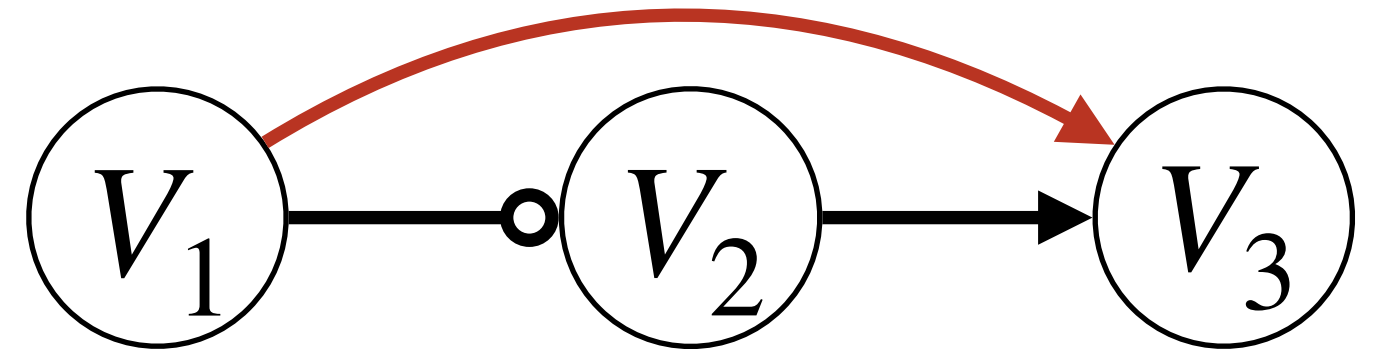
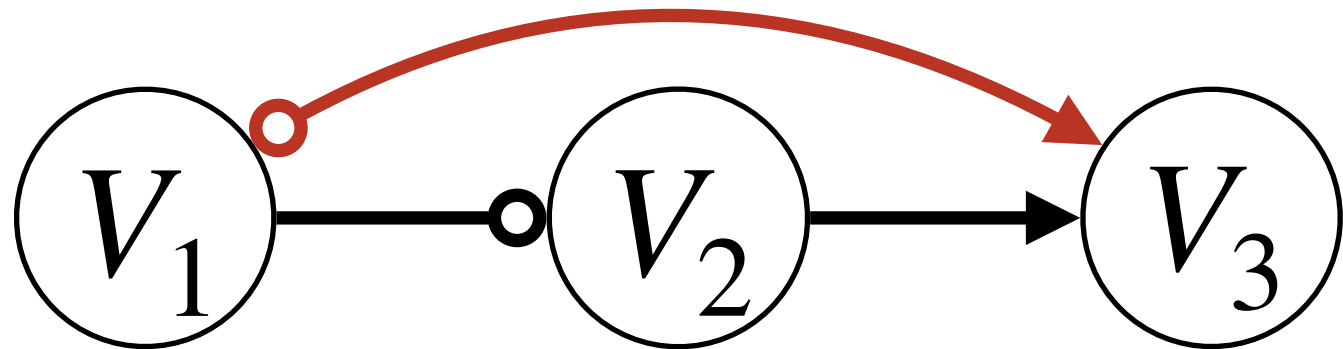


$V_1$  and  $V_3$  are not adjacent

**R8:**

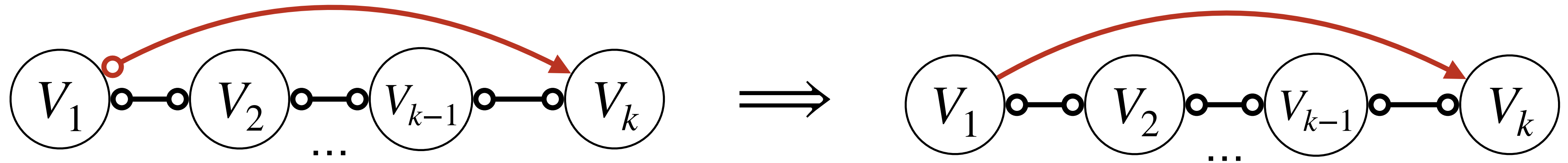


or



# FCI - Complete Set of Mark Inference Rules

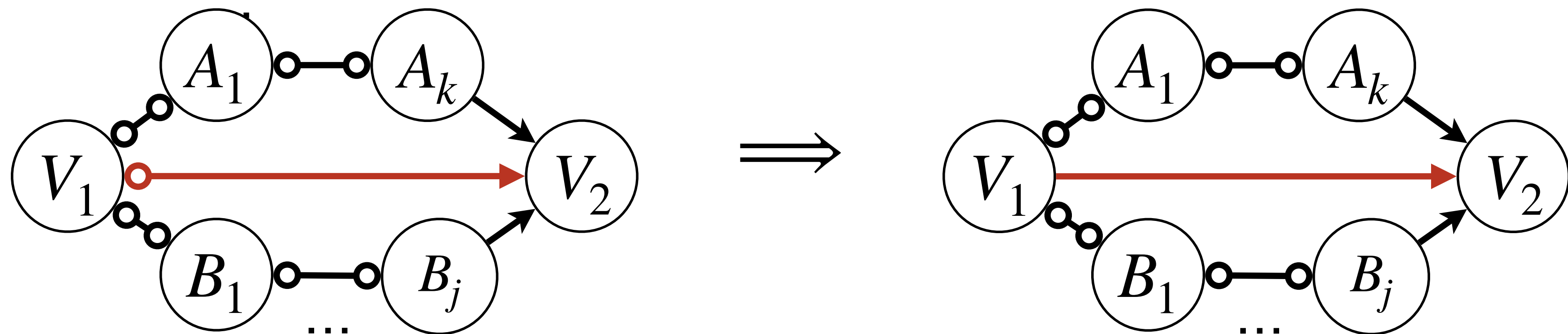
**R9:**



$\langle V_1, V_2, \dots, V_{k-1}, V_k \rangle$  is an uncovered potentially directed path from  $V_1$  to  $V_k$

$V_2$  and  $V_k$  are not adjacent

**R10:**

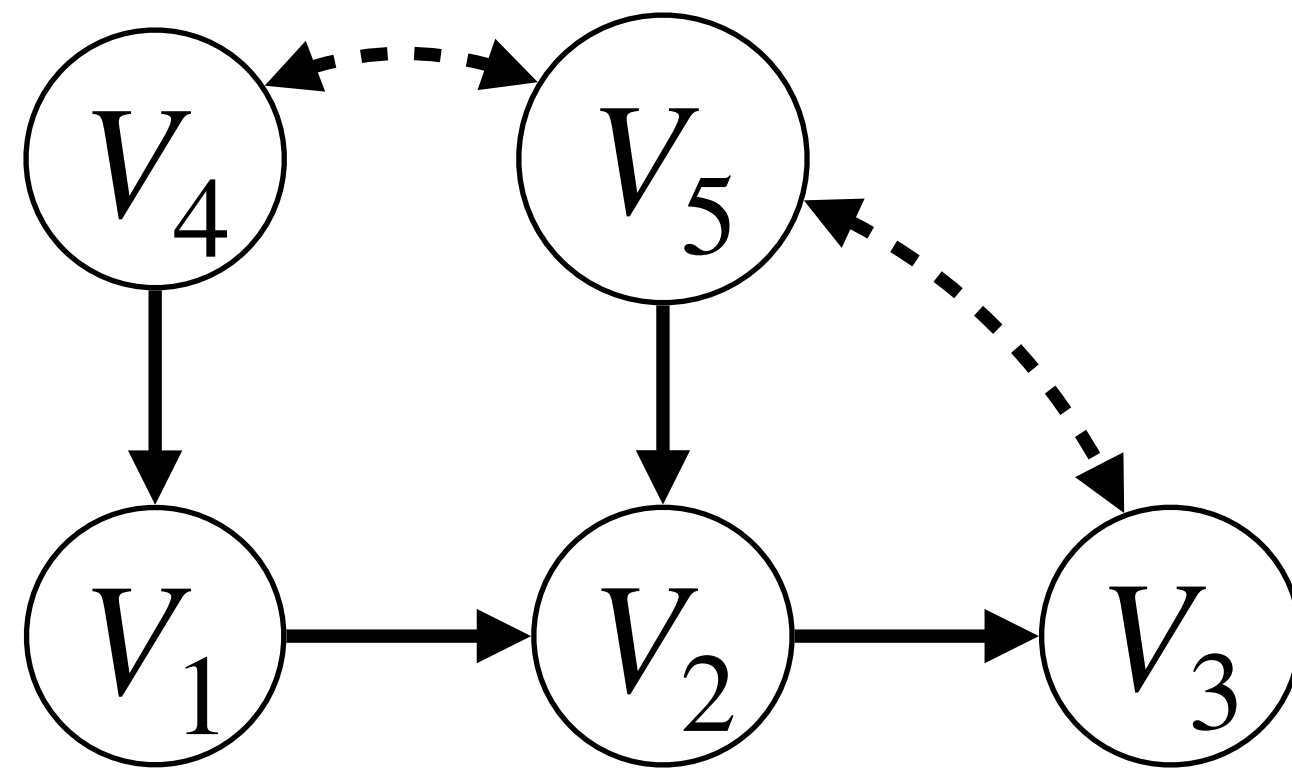


$\langle V_1, A_1, \dots, A_k \rangle$  is an uncovered potentially directed path from  $V_1$  to  $A_k$  ( $A_1$  may be  $A_k$ )

$\langle V_1, B_1, \dots, B_k \rangle$  is an uncovered potentially directed path from  $V_1$  to  $B_k$  ( $B_1$  may be  $B_k$ )

$A_1 \neq B_1$  and  $A_1$  and  $B_1$  are not adjacent

# Another Example

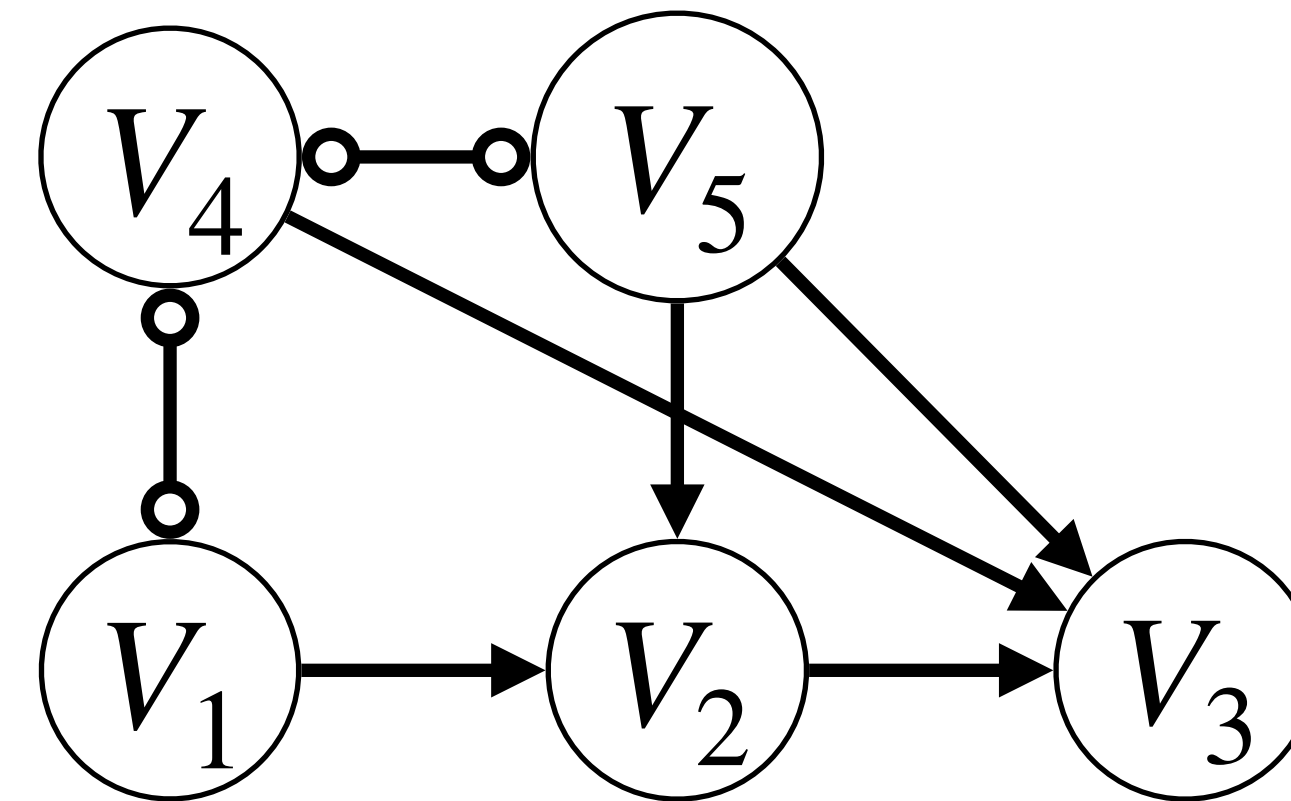


True, unknown  
Causal Diagram

$$V_1 \perp\!\!\!\perp V_3 \mid V_2, V_4, V_5$$

$$V_1 \perp\!\!\!\perp V_5 \mid V_4$$

$$V_2 \perp\!\!\!\perp V_4 \mid V_1, V_5$$



Corresponding PAG

$$V_1 \perp\!\!\!\perp V_3 \mid V_2, V_4, V_5$$

$$V_1 \perp\!\!\!\perp V_5 \mid V_4$$

$$V_2 \perp\!\!\!\perp V_4 \mid V_1, V_5$$

Hint: apply Rules 0, 1, 2, 4 and then Rule 9 three times.

# More on Causal Discovery and PAGs

## **Causal discovery from observational and experimental data:**

- Kocaoglu, M., Jaber, A., Shanmugam, K., Bareinboim, E. Characterization and Learning of Causal Graphs with Latent Variables from Soft Interventions. In Proceedings of the 33rd Annual Conference on Neural Information Processing Systems. 2019. (Link)
- Jaber, A., Kocaoglu, M., Shanmugam, K., Bareinboim, E. Causal Discovery from Soft Interventions with Unknown Targets: Characterization & Learning. In Advances in Neural Information Processing Systems 2020. (Link)

## **Causal effect identification from PAGs:**

- Jaber A., Ribeiro A. H., Zhang, J., Bareinboim, E. Causal Identification under Markov Equivalence - Calculus, Algorithm, and Completeness. In Proceedings of the 36th Annual Conference on Neural Information Processing Systems, NeurIPS 2022. (Link)



# Available Implementations of the FCI

## R Packages:

- pcalg R package:
  - <https://cran.r-project.org/web/packages/pcalg/>
  - <https://github.com/cran/pcalg/>
- RPy-Tetrad (Wrapper in R): <https://github.com/cmu-phil/py-tetrad/tree/main/pytetrad/R>

## Python Packages:

- Do-discover in PyWhy: <https://github.com/py-why/dodiscover>
- Causal-Learn: <https://causal-learn.readthedocs.io/en/latest/index.html>
- Py-Tetrad (Wrapper in Python): <https://github.com/bd2kccd/py-causal>

# Thank you for your attention!

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