

# CAUSAL DISCOVERY

- Taxonomy of causal discovery methods
- Peter-Clark
- Fast Causal Inference

# SCOPE

Conditional independence facts can be easily recovered from DAGs: can we recover a DAG from data?

Is conditional independence enough to establish a causal DAG? Under which assumptions?

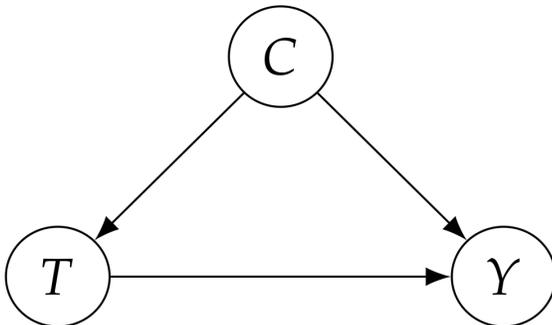


Causal Discovery's primary aim is to recover a causal DAG (or its equivalence class) from data!

# TWO MAIN ASSUMPTIONS

## Causal sufficiency:

A set of observed variables  $V$  is **Causally Sufficient** if every common cause of any two variables in  $V$  is also in  $V$ . In other words, there are no unobserved confounders (latent variables) that influence more than one variable in the set.



Example:

$V = \{T, Y, C\}$  is causal sufficient

$V = \{T, Y\}$  is not causal sufficient

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## Intuition

A set of variables is **Causally Sufficient** if the **Markov Blanket** of every variable is 'fully observable'.

- If you can block all influence on a variable  $X$  using only its observed neighbors, you have sufficiency.
- If  $X$  continues to 'talk' to  $Y$  despite conditioning on all potential observed parents/children, there is a ghost in the machine (**a latent confounder**) and your set is not causally sufficient.

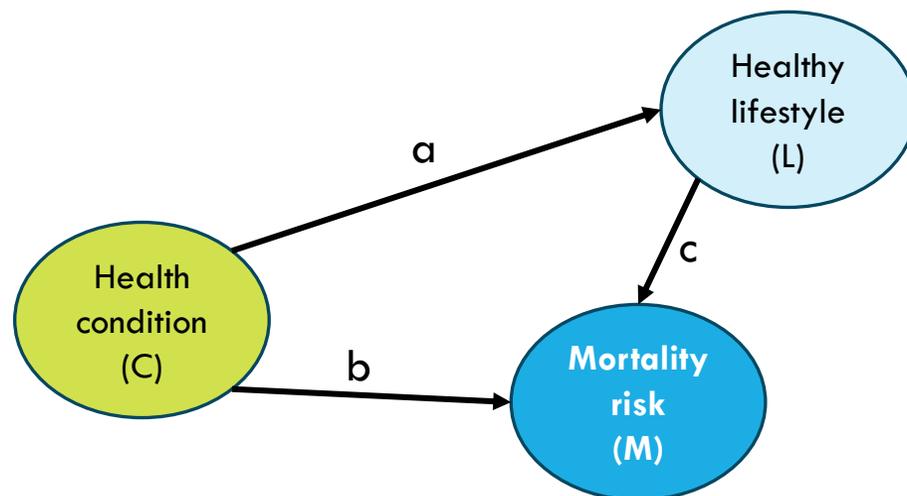
# TWO MAIN ASSUMPTIONS

## Faithfulness:

Given a graph over a set of observed variables  $V$ , and a joint distribution  $\mathbb{P}(V)$ , the **Faithfulness Condition** is satisfied iff the only conditional independencies in  $\mathbb{P}$  are the ones entailed by d-separation.

**conditional independence  $\Rightarrow$  d-separation**

Example of faithfulness violation:



Suppose that they are Gaussian variable linearly related as:

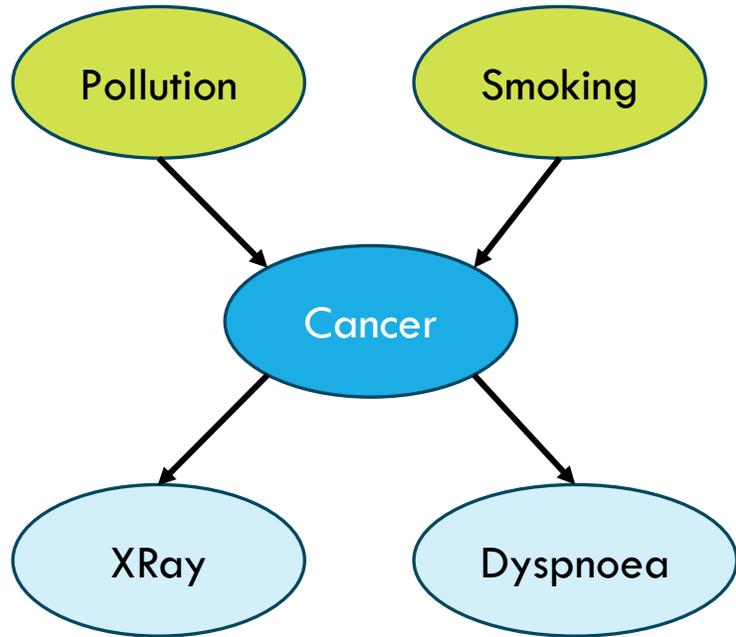
$$\begin{cases} L = a \times C \\ M = b \times C + c \times L \end{cases}$$

$$\Rightarrow M = (b+ac) C$$

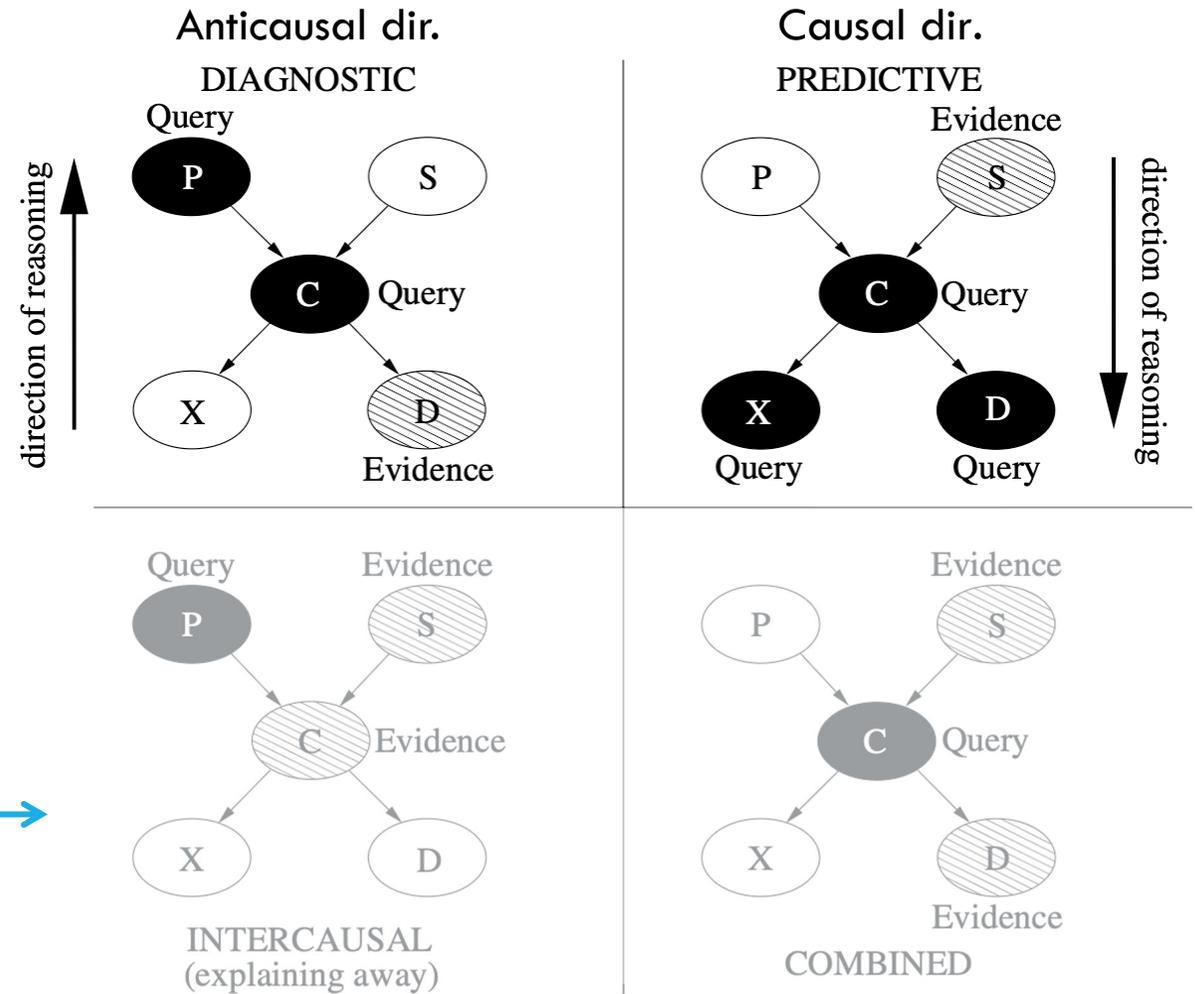
$\Rightarrow$  if  $b+ac=0$ , the mortality risk is independent of the health condition!

# CAUSAL DATA STRUCTURING AND REASONING

Let us suppose the following (simplified) Lung-cancer problem<sup>1</sup>, for which a causal DAG has been established.



Full representation of the probability distribution allows to explain the type of reasoning we can perform through conditioning.



# CAUSAL DISCOVERY METHODS — A TAXONOMY



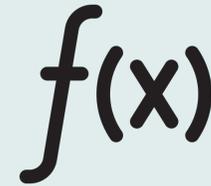
## Constraint

- Uses statistical independence tests to prune edges from a fully connected graph.
- Examples: PC, FCI,...



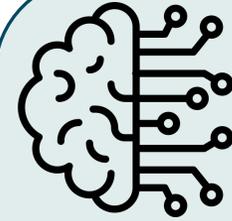
## Score-based

- Searches the space of possible DAGs and optimizes a goodness-of-fit score (like BIC).
- Examples: GES, Hill climbing,...



## Functional-based

- Assumes a specific functional model to describe the causal flow. Exploits noise properties to establish/orient edges.
- Examples: LiNGAM, ANM,...



## Continuous

- DL/ML approach framing discovery as a continuous optimization problem (NNs + gradient descent).
- Examples: NOTEARS, Dag-GNN,...

# CAUSAL DISCOVERY METHODS — A TAXONOMY



## Constraint

- Uses statistical independence tests to prune edges from a fully connected graph.
- Examples: **PC**, **FCI**,...



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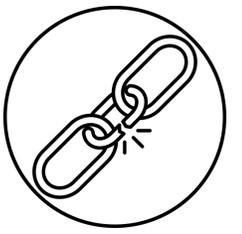
# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED



## We focus on Constraint-based methods:

- ✓ **Interpretability:** Every edge removed is backed by a statistical test.
- ✓ **Reliability:** Well-understood theoretical limits in small samples/provably identifiable (under certain assumptions).
- ✓ **Latent Handling:** FCI is one of the few methods that detects unobserved confounders.

# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED



**Constraint-based methods rely on (conditional) independence tests to recover the DAG:**

- Markov condition
  - Faithfulness condition
- } To smoothly go from independence to d-separation to DAG

**Causal sufficiency** is also required most of the time, to ensure completeness → all possible conditional independence facts can be actually tested!

# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED



## Intuition on conditional independence testing – the linear Gaussian case

If  $X_2, X_3$  are jointly normally distributed, then:  $X_2 \perp\!\!\!\perp X_3 \Leftrightarrow \text{Corr}(X_2, X_3) = 0$

ⓘ  
x2

ⓘ  
x3

Zero correlation can be tested e.g. with the Fisher's z test:

1. Calculate sample correlation (statistic): 
$$r_{X_1, X_2} = \frac{\widehat{\text{Cov}}(X_1, X_2)}{\hat{\sigma}_{X_1} \hat{\sigma}_{X_2}} = \frac{\sum_i (X_{1i} - \bar{X}_1)(X_{2i} - \bar{X}_2)}{\sqrt{\sum_i (X_{1i} - \bar{X}_1)^2} \sqrt{\sum_i (X_{2i} - \bar{X}_2)^2}}$$
2. Under H0 (zero correlation): 
$$z := \frac{1}{2} \ln \left( \frac{1 + r_{X_1, X_2}}{1 - r_{X_1, X_2}} \right) \sim \mathcal{N} \left( 0, \frac{1}{N - 3} \right)$$

# samples
3. Given the statistic and its null distribution, we can find the p-value.



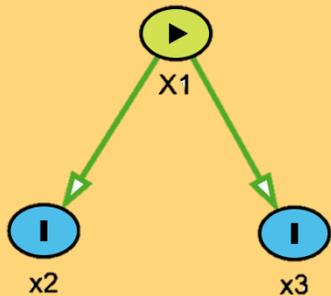
# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED

## Intuition on conditional independence testing – the linear Gaussian case

Conditional independence  $\leftrightarrow$  partial correlation: can be tested by using the residuals!

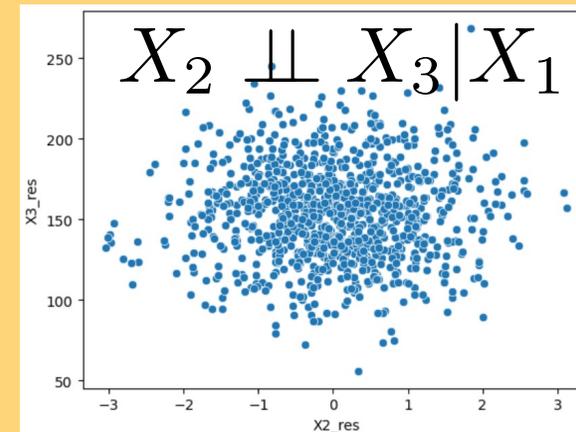
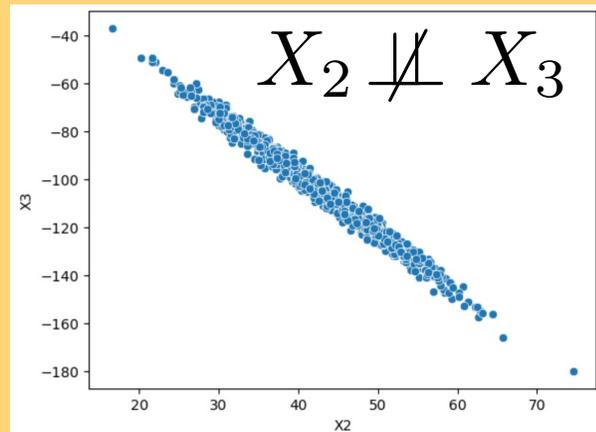
1. Regress  $X_2$  on  $X_1$  and  $X_3$  on  $X_1$ :  $\hat{X}_2(X_1); \hat{X}_3(X_1)$
2. Calculate the residuals ( $\rightarrow$  noise):  $\text{res}_{X_2} = X_2 - \hat{X}_2(X_1); \text{res}_{X_3} = X_3 - \hat{X}_3(X_1)$
3. If  $X_2 \perp\!\!\!\perp X_3 | X_1$  then the residuals are zero-correlated, which can be tested as before with Fisher-z!

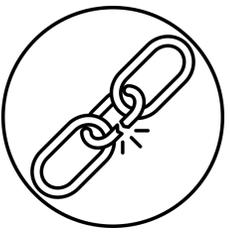
$$X_1 = \mathcal{N}(50, 10^2)$$



$$X_2 = 2 + 0.8X_1 + \mathcal{N}(0, 1)$$

$$X_3 = -3 - 2X_1 + \mathcal{N}(0, 1)$$





# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED

Are we always able to correctly recover the true DAG by testing for conditional independencies?

X1	X2	X3	X4	X5
2.099343	2.586254	-0.661093	8.039057	6.757995
1.972347	2.520444	-2.360024	10.356054	7.349395
2.129538	3.306731	-1.705014	8.162636	5.965670
2.304606	1.239023	-4.266158	7.896162	5.646977
1.953169	1.251667	-3.309183	9.865793	5.454375
1.953173	2.414299	-2.072563	7.364751	4.962531
2.315843	2.145090	-3.541617	8.782157	5.930440
2.153487	3.390991	-1.359504	6.208884	6.161564
1.906105	2.045028	-2.959345	7.353365	6.020301
2.108512	1.641952	-2.892420	9.086643	4.780281



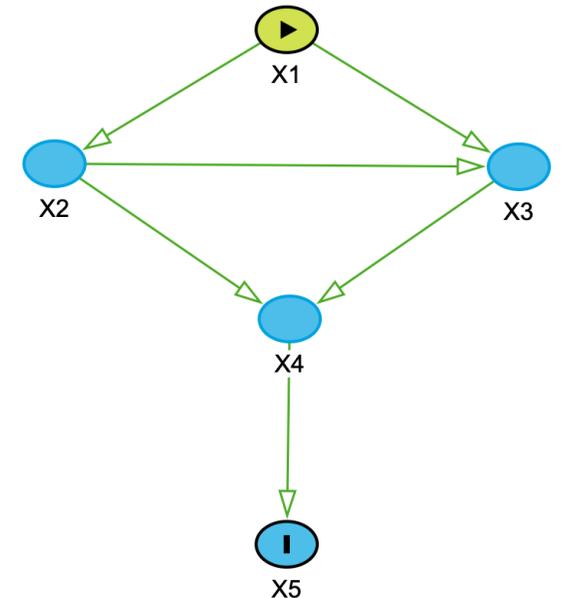
$$X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$$

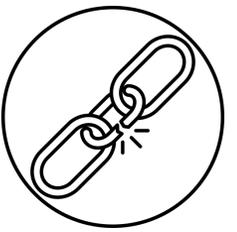
$$X_1 \perp\!\!\!\perp X_5 \mid X_4$$

$$X_1 \perp\!\!\!\perp X_5 \mid X_2, X_3$$

$$X_2 \perp\!\!\!\perp X_5 \mid X_4$$

$$X_3 \perp\!\!\!\perp X_5 \mid X_4$$





# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED

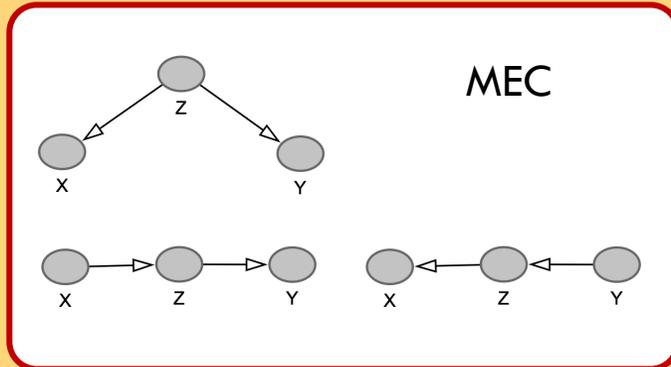
## Markov equivalence class (MEC):

A set of DAGs that have the same skeleton and the same v-structures.

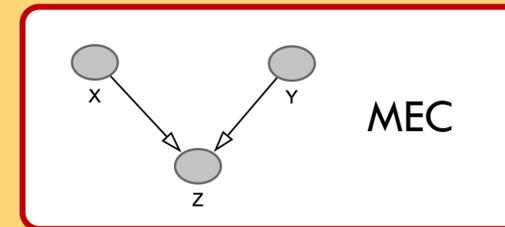
### Intuition

Constraint-based methods face **Observational Equivalence**: multiple DAGs can satisfy the same set of independence statements.

We have already seen that chains and forks share the same independence statements.



This is not the case for v-structures!



# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED



## Markov equivalence class (MEC):

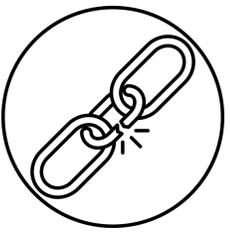
A set of DAGs that have the same skeleton and the same v-structures.

A MEC can be represented through a **CPDAG** (Complete Partially Directed Graph):

→ **Directed Edges:** These are invariant across the entire MEC. We are certain about this causal direction (often found via v-structures). → in every member of the MEC.

— **Undirected Edges:** These represent reversible relations. The data is consistent with arrows in either direction.  
→ in some members of the MEC; ← in some others.

**No edge:** not adjacent in any member of the MEC.

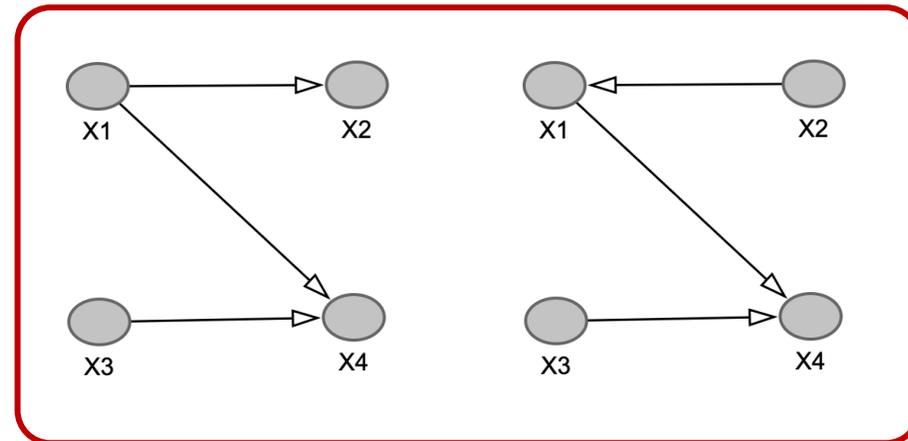
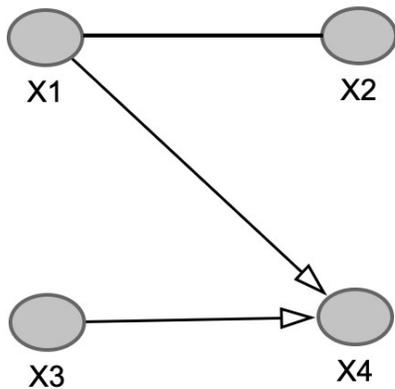


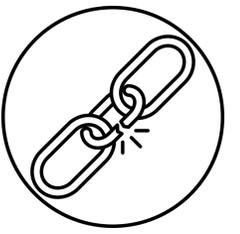
# CAUSAL DISCOVERY METHODS — CONSTRAINT-BASED

## Markov equivalence class (MEC):

A set of DAGs that have the same skeleton and the same v-structures.

Example: how many DAGs in this MEC?





# THE PC ALGORITHM

The PC algorithm, named after Peter Spirtes and Clark Glymour<sup>1</sup>, is a classical and still widely used constraint-based causal discovery method. Its output is a CPDAG. It assumes: Markov condition, Faithfulness and causal sufficiency.

Step 1 – Skeleton discovery

Start – complete undirected graph

Test for (conditional) independence with an increased cardinality of the conditioning set to remove edges.

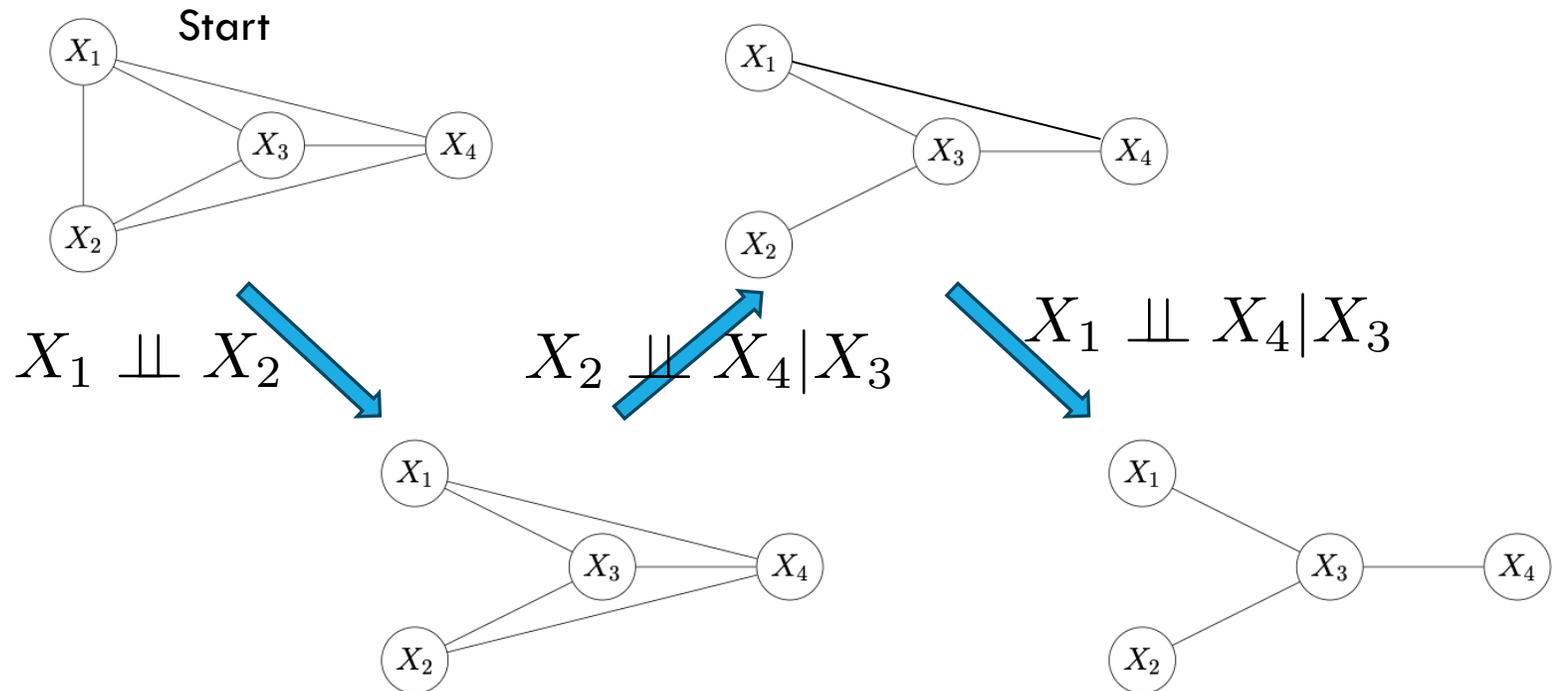
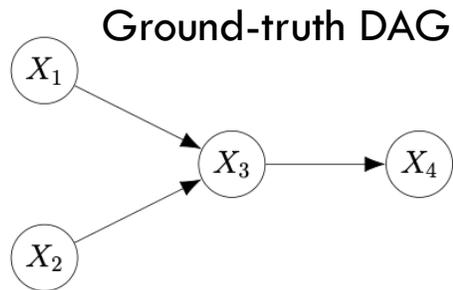


# THE PC ALGORITHM

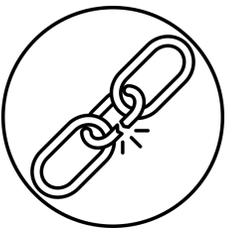
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## Step 1 – Skeleton discovery

### Example



1. P.Spirtes, C.N.Glymour. Causation, prediction, and search. MIT press, 2000.

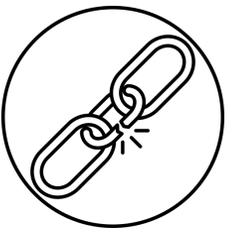


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Step 2 – v-structure discovery

Orient as a v-structure each triple of nodes  $(X, Z, Y)$  such that  $X, Z$  and  $Y, Z$  are adjacent in the discovered skeleton, but  $X, Y$  are independent (without conditioning).

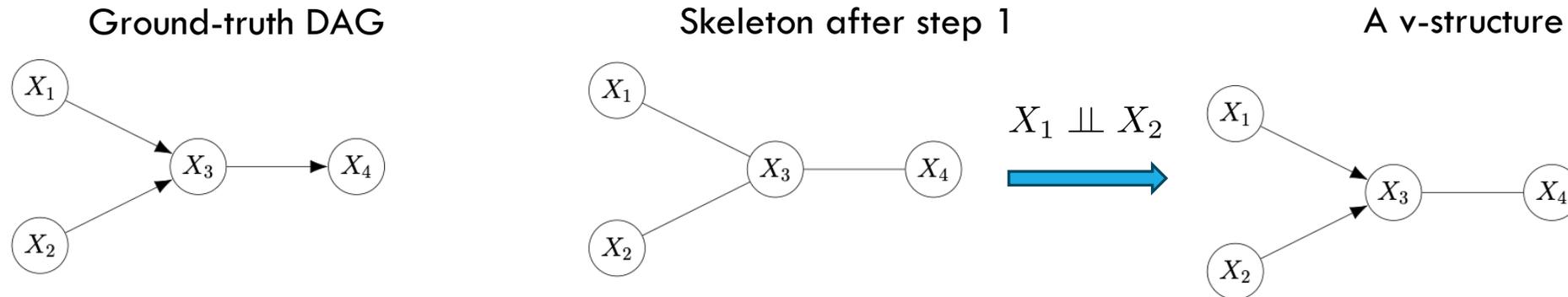


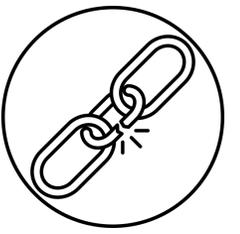
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Step 2 – v-structure discovery

## Example



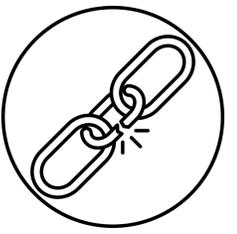


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Step 3 – orientation propagation

$X \rightarrow Z - Y$ , and  $X, Y$  are not adjacent  $\Rightarrow X \rightarrow Z \rightarrow Y$

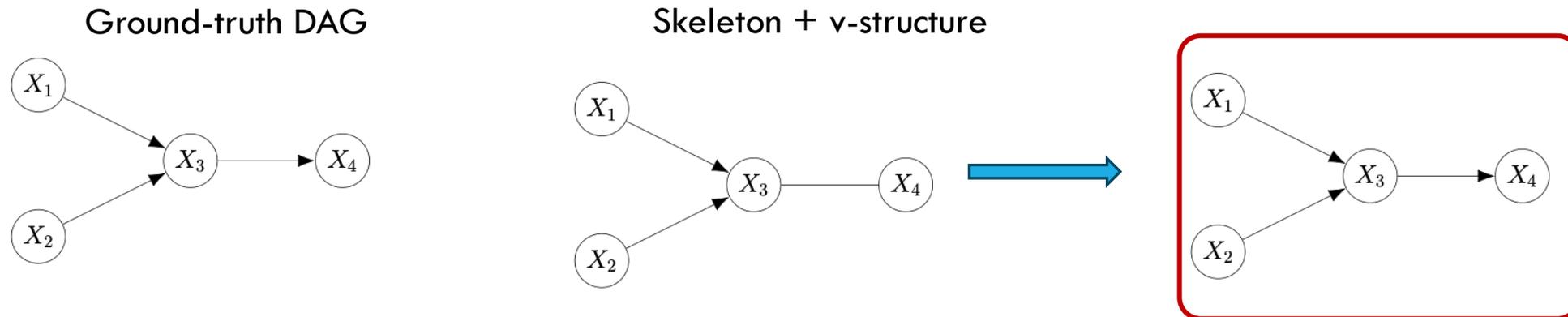


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Step 3 – orientation propagation

## Example





# THE FCI ALGORITHM

The FCI<sup>1</sup> algorithm (Fast Causal Inference) extends the PC algorithm allowing for the presence of latent variables, i.e. variables which are not observed but play a role in the generating process of the observed variables. It assumes: Markov condition, Faithfulness, BUT NOT causal sufficiency.

**Note:** Suppose we are observing samples from the observable variables in the set  $\mathbf{O}$ , which have been actually generated by the interplay of variables in  $\mathbf{V} = \{\mathbf{O}, \mathbf{L}\}$ ,  $\mathbf{L}$  being latent/unobserved. We could marginalize out all latent variables. BUT, DAGs are not closed under marginalization so **in the presence of latent variables, the causal process over measured  $\mathbf{O}$  variables is not necessarily a DAG!**

How to visualize the conditional independencies among the observed variables  $\mathbf{O}$  only for DAGs with *observed and latent variables*? How can we represent (independence) equivalence classes over  $\mathbf{O}$ ?



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## Partial Ancestral Graph (PAG):

Edge	Meaning
Directed $X \rightarrow Y$	$X$ is an <i>ancestor</i> of $Y$ , and there <i>may</i> further be unobserved confounding between the two
Bidirected $X \longleftrightarrow Y$	<i>unobs confounding</i> between $X$ and $Y$ , but <i>no</i> causal ancestral relationship in either direction
Possibly bidirected edge $X \circ \rightarrow Y$	either $X \rightarrow Y$ or $X \longleftrightarrow Y$
Undetermined edge $X \circ \text{---} \circ Y$	no info about the relationship between $X$ and $Y$ . Either $X \rightarrow Y$ , $X \leftarrow Y$ or $X \leftrightarrow Y$ .



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**Note:** PAGs are the equivalence classes of MAGs (Maximal Ancestral Graphs)

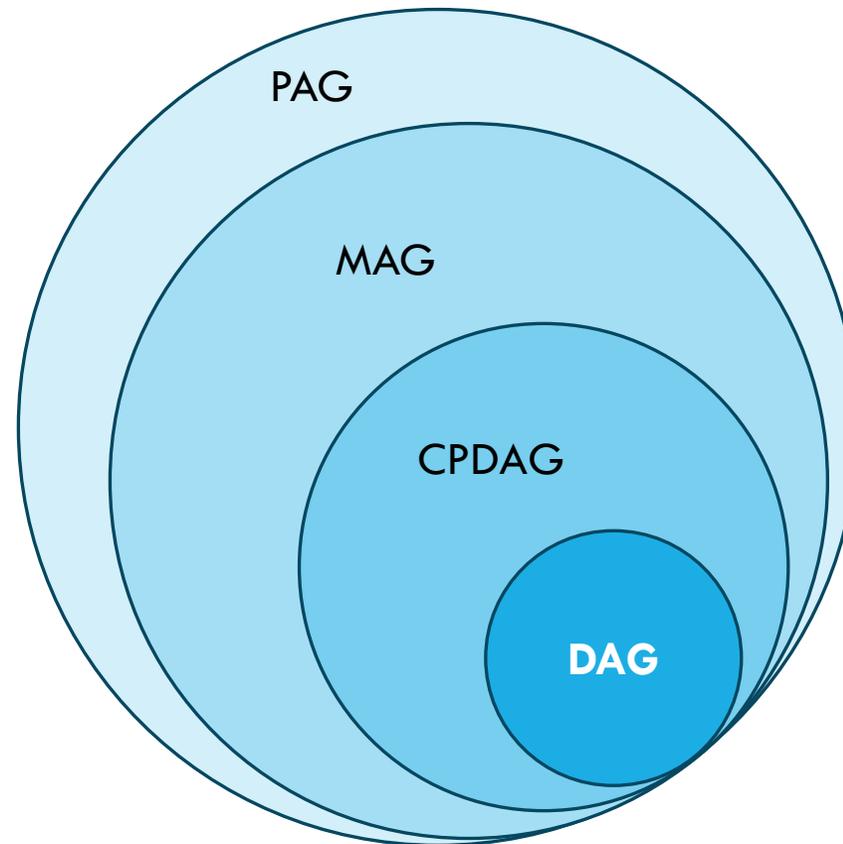
## A MAG

- may contain two kinds of edges:
  - directed edges ( $X \rightarrow Y$ )
  - bi-directed edges ( $X \leftrightarrow Y$ ), which means *no directed* path from  $X$  to  $Y$
- has no directed cycles
- is maximal: no edge can be added without changing the independence model



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FCI works similarly to PC (same steps), but:

1. Instead of reasoning in terms of independence, it reasons in terms of paths and d-separation (ancestors/descendants rather than parents/children).
2. The rules for edge orientation are more theoretically and technically elaborate, but the principle remains similar.

# IMPLEMENTATION AND PACKAGES

- Several implementations of PC, FCI, and other causal discovery methods are available, both in R and Python  
→ we will use the Python package causal-learn (intuitive and easy to use).

The image shows the documentation page for the 'causal-learn' Python package. On the left is a dark blue sidebar with a search bar and navigation links. The main content area is white with a blue header. It features a 'Welcome to causal-learn's documentation!' heading, a brief description of the package, and a note about its active development status with a link to the GitHub repository.

- Another widely used tool is Tetrad, which can also provide a graphical user interface (GUI).

The image displays four columns representing different ways to use Tetrad. Each column has an icon at the top and a text block below. The first column shows a screenshot of the GUI application. The second column features a blue snake coiled around a white cup of soup. The third column shows the R logo with a yellow snake. The fourth column shows a blue square with a white right-pointing arrow and a minus sign.

Option	Icon	Description
Tetrad GUI Application	Screenshot of the Tetrad GUI	The Tetrad Application is a desktop Java application that creates, simulates data from, estimates, tests, predicts with, and searches for causal and statistical models. The Application aims to provide sophisticated methods in a uniform drag-and-drop interface requiring no programming knowledge to navigate.
Tetrad in Python	Blue snake around a cup of soup	The Python interface (py-tetrad) is a Python tool that gives Python users direct access to the entire Tetrad library.
Tetrad in R	R logo with a yellow snake	The R interface (rpy-tetrad) is a tool giving R users access to a wide swath of the Tetrad library.
Command Line Tetrad	Blue square with arrow and minus sign	The Command Line tool (Causal Command) gives users access to all algorithms in the Tetrad library via the command line.