

Introduction to Causal Inference and Causal Data Science

Day 4 Part 2: Causal Structure Learning

Oisín Ryan

Department of Data Science and Biostatistics
Julius Center
UMC Utrecht

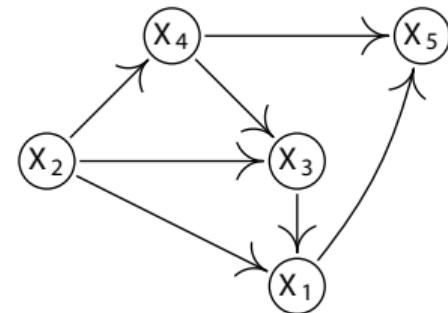
August 7, 2024

Why are DAGs helpful?

DAGs allow us to “read off” all the *paths* by which two variables are **marginally** and **conditionally** (in)dependent

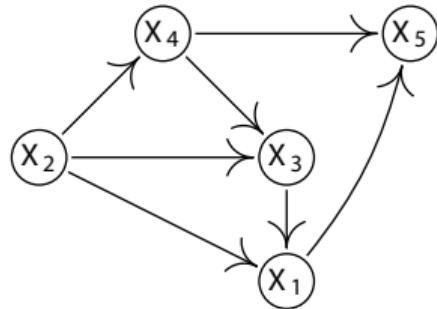
- Formalizes the idea that two variables can be statistically dependent **in a particular way** without one being a *cause* of the other
- d-seperation gives us the explicit rules which govern this: open-paths!

If we want a **statistical dependency** to reflect a **causal dependency** we need to condition on variables such that we *block* uninteresting (non-causal) paths



Days 1 - 3: Causal Reasoning

causal model, e.g. DAG G



infer
→

expectations about
observational data $P(X_1, \dots, X_5)$
& interventions $P_{do}(X_1, \dots, X_5)$

X ₁	X ₂	X ₃	X ₄	X ₅
3.4	-0.3	5.8	-2.1	2.2
1.7	-0.2	7.0	-1.2	0.4
-2.4	-0.1	4.3	-0.7	3.5
2.3	-0.3	5.5	-1.1	-4.4
3.5	-0.2	3.9	-0.9	-3.9
⋮	⋮	⋮	⋮	⋮

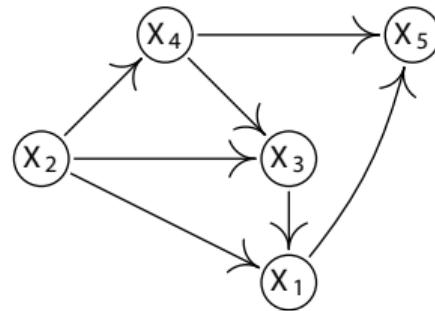
This session: **Causal Learning** (also called: Causal Discovery / Structure Learning)

observational data $P(X_1, \dots, X_5)$

X_1	X_2	X_3	X_4	X_5
3.4	- 0.3	5.8	- 2.1	2.2
1.7	- 0.2	7.0	- 1.2	0.4
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:	:	:	:	:

infer
?

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Causal Learning

Causal Learning is somewhat different from **Statistical Learning**

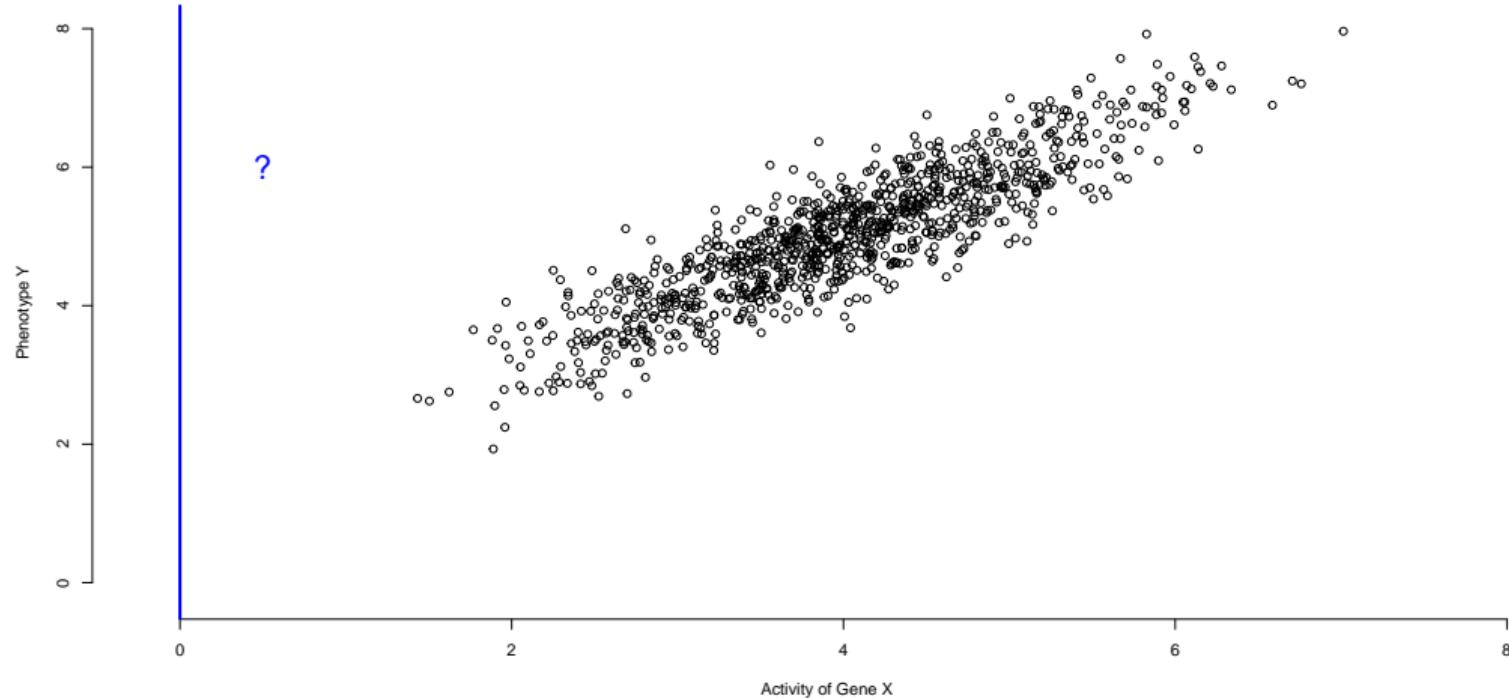
Statistical Learning is concerned with finding a model which minimizes out-of-sample prediction error.

- Using data observed under certain conditions to **learn** a model which enables us to make predictions about what we expect to see in a new data point collected under **exactly those conditions**

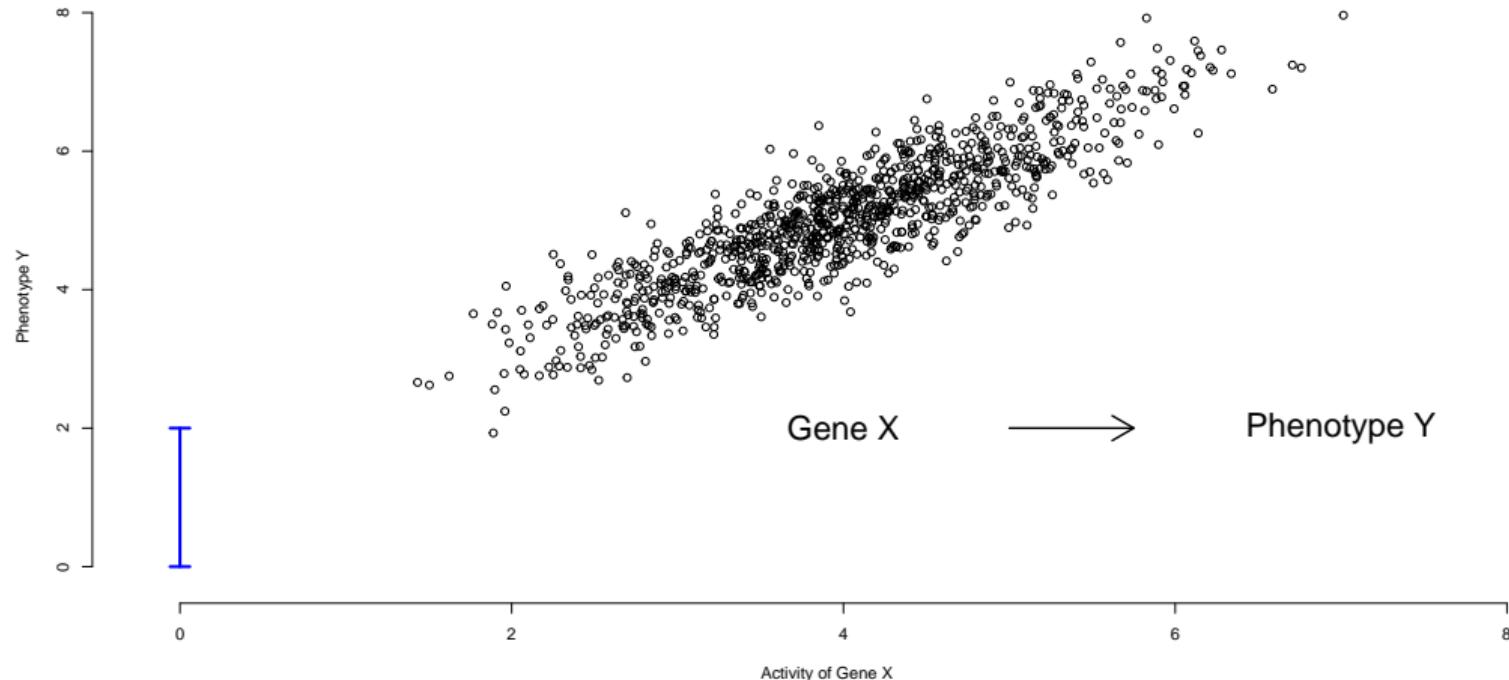
Causal Learning is more general, but harder.

- Using data to **learn** a model which enables predictions about **new** or **different** situations. I.e., using observational data to learn about that says something about the **intervention** setting.

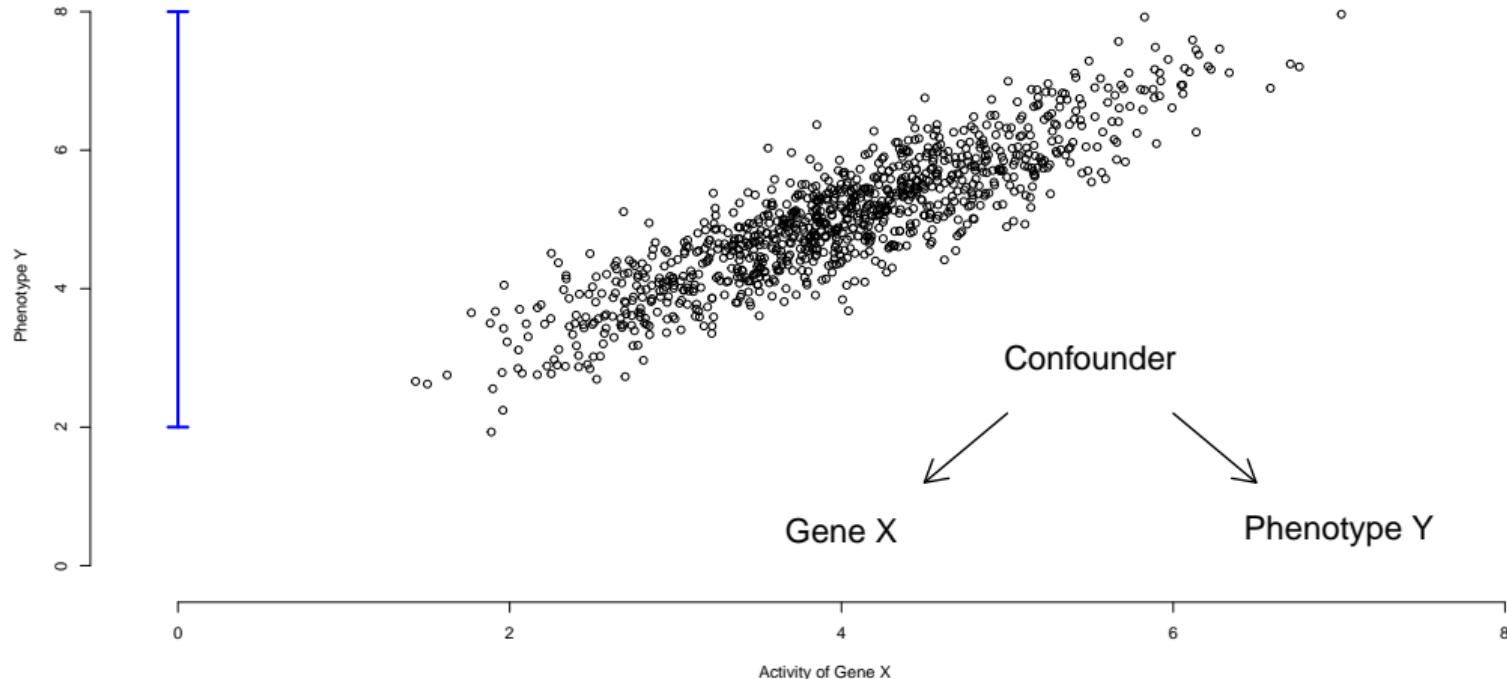
Example Causal vs Statistical Learning



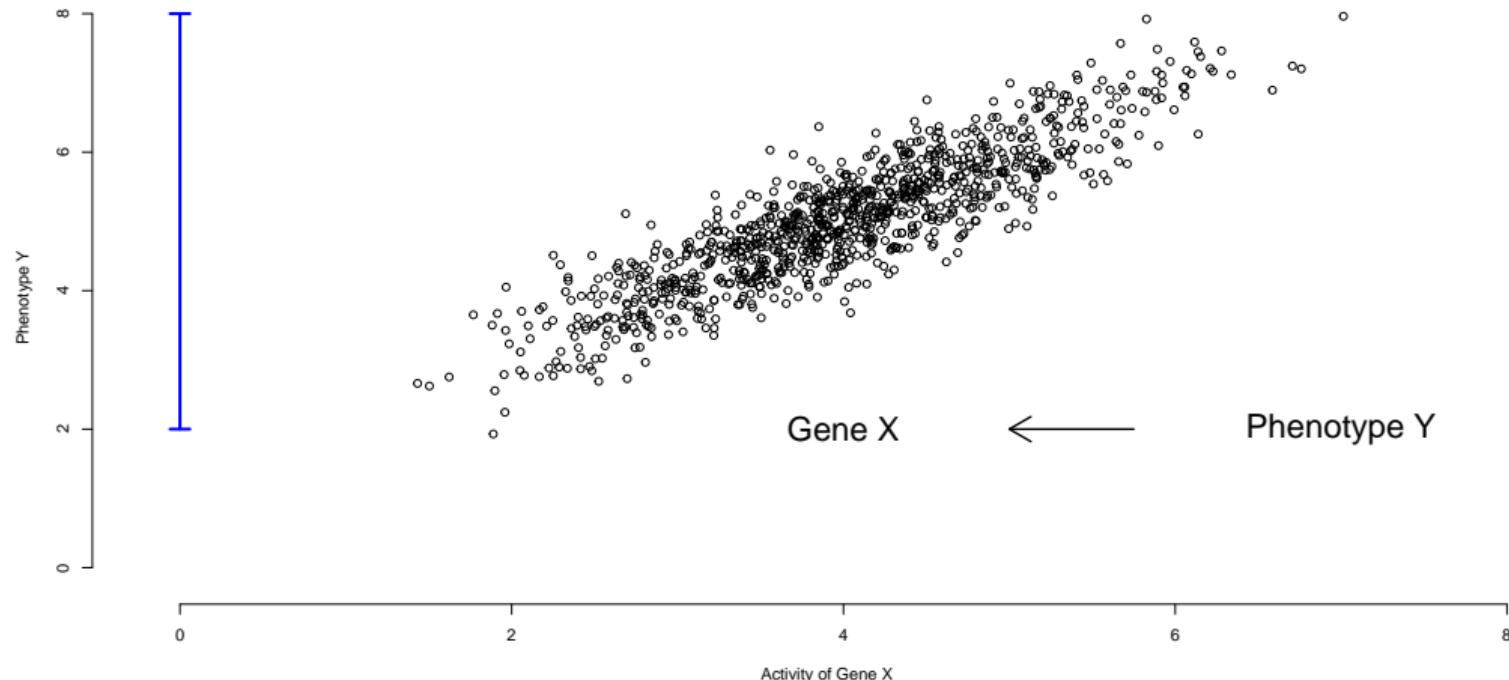
Example Causal vs Statistical Learning



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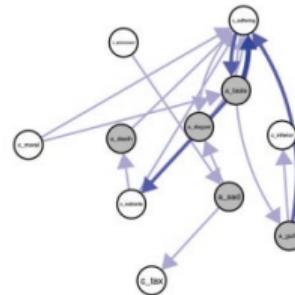
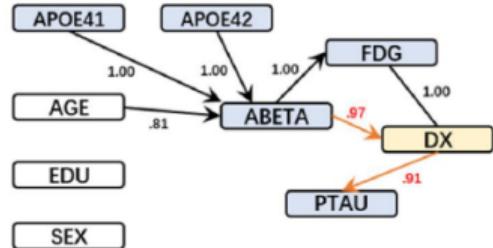
Example Causal vs Statistical Learning

The answer to questions about *intervention effects* depends on the **causal graph**

For that reason, **causal learning** is often focused on recovering the **structure** of the causal graph from data

Challenges and Opportunities with Causal Discovery Algorithms: Application to Alzheimer's Pathophysiology

Xinpeng Shen^{1*}, Sisi Ma¹, Prashanthi Vemuri², Gyorgy Simon^{1*} & the Alzheimer's Disease Neuroimaging Initiative¹



The Search for Causality: A Comparison of Different Techniques for Causal Inference Graphs

Jolanda J. Kossakowski, Lourens J. Waldorp, and Han L. J. van der Maas
Department of Psychology, University of Amsterdam

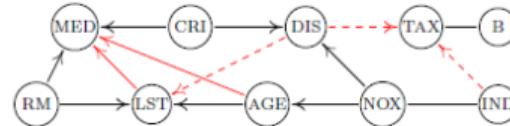
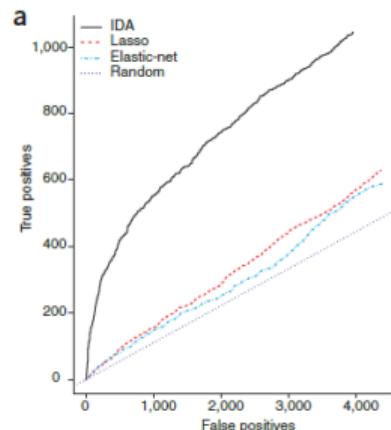


Figure 4: Outcome of the PC algorithm applied to the continuous variables of the Boston Housing Data Set (red lines: $PC_{CI,PERM}$, solid lines: $PC_{KCI-test}$).

Predicting causal effects in large-scale systems from observational data





Toward Causal Representation Learning

This article reviews fundamental concepts of causal inference and relates them to crucial open problems of machine learning, including transfer learning and generalization, thereby assaying how causality can contribute to modern machine learning research.

By BERNHARD SCHÖLKOPF¹⁰, FRANCESCO LOCATELLO¹¹, STEFAN BAUER¹⁰, NAN ROSEMARY KE,
NAL KALCHBRENNER, ANIRUDH GOYAL, AND YOSHUA Bengio¹²

Example Causal vs Statistical Learning

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Causal learning has been applied most notably in fields like **systems biology**, **genetic research**, **neural connectivity** research

- In these fields, predictions about the effects of do-interventions can be (relatively) easily empirically validated, e.g., gene knockout experiments
- But these methods *can* and *have* been applied in other fields.
- Today we learn about the principles behind these causal discovery methods!

Causal Learning: An overview

In this session we will learn about three different strategies for causal discovery.

- ① Using Conditional (In)dependence
- ② Restricting the Structural Causal Model
- ③ Using Different Environments (data from multiple sources)

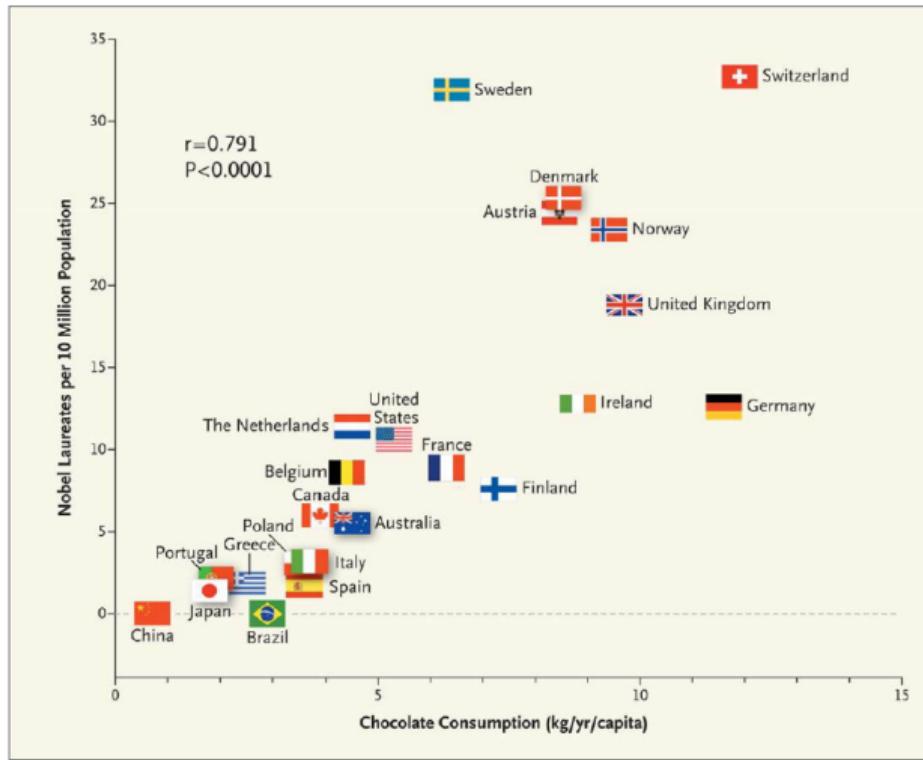
Different ways to exploit relationship between causal models and data: Different assumptions, able to recover different things

Disclaimer: This is by no means a comprehensive review of causal discovery methods. Instead, an introduction to three general strategies that show up in many developments.

Causal Discovery using Conditional (In)Dependence

Fundamentals of Dependence and Causality

Well-known problem of causal discovery: Correlation does not imply causation



F. H. Messerli: Chocolate Consumption, Cognitive Function, and Nobel Laureates, N Engl J Med 2012

Fundamentals of Dependence and Causality

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Reichenbach's Common Cause Principle

If $X \not\perp\!\!\!\perp Y$ then either:

- $X \rightarrow \dots \rightarrow Y$
- $X \leftarrow \dots \leftarrow Y$
- X and Y share a common cause
- A combination of the above

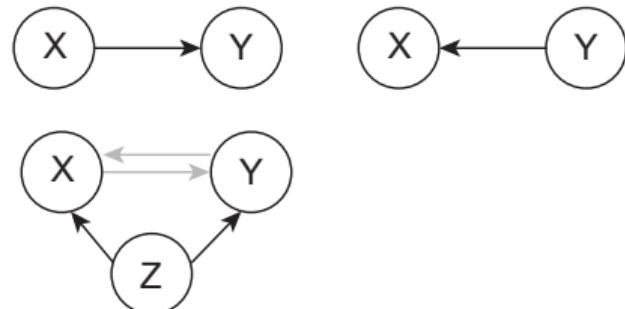
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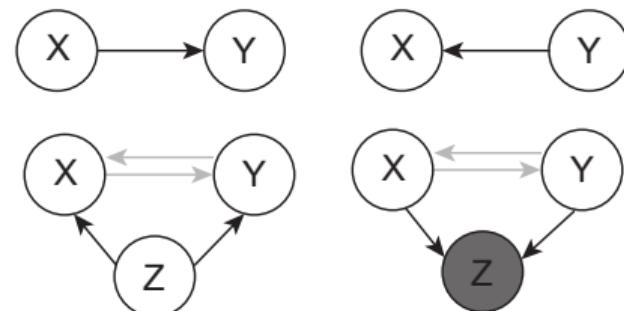
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Or: we have unknowingly conditioned on a collider Z

- i.e. $X \not\perp\!\!\!\perp Y$ is actually $X \not\perp\!\!\!\perp Y|Z$
- In practice - selection bias



Causal Discovery using Conditional Independence

Basic Idea:

- ① Find all conditional independence relations present in the data
- ② Draw the DAG in which all (and only) those independences follow from d-seperation rules

Known as **Constraint-Based** (related to **Score-Based**) methods

Assume:

- **Sufficiency:** No unobserved common causes (for now)
- No selection bias (no conditioning on unobserved colliders)
- **Faithfulness:** We'll explain that in a few slides time!

Example 1: CI-based discovery

We gather a very large dataset containing three variables: A , B and C

We choose an appropriate test for independence and find:

$$A \perp\!\!\!\perp C$$

$$A \not\perp\!\!\!\perp C | B$$

All other combinations of variables are dependent (e.g. $A \not\perp\!\!\!\perp B$, and $B \not\perp\!\!\!\perp C | A$)

What is the data-generating DAG?

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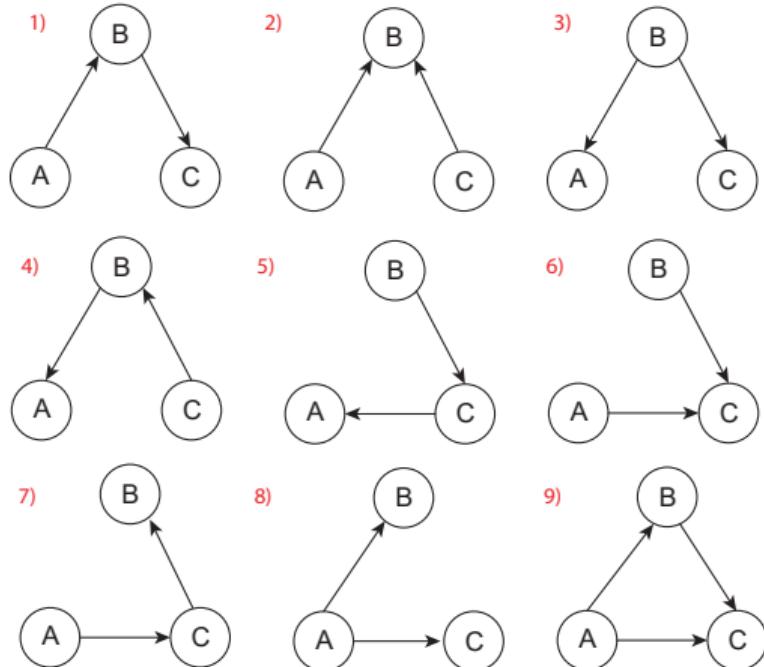
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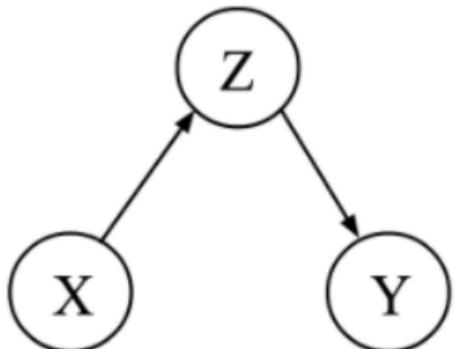
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Chain

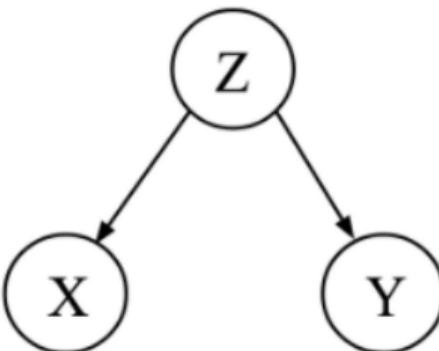


X: Smoking
Z: Tar
Y: Cancer

$$X \not\perp\!\!\!\perp Y$$

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Fork

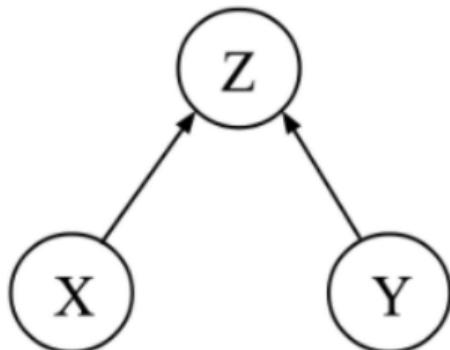


X: Storks
Z: Environment
Y: Babies

$$X \not\perp\!\!\!\perp Y$$

$$X \perp\!\!\!\perp Y \mid Z$$

Collider



X: Attractiveness
Z: Being Single
Y: Intelligence

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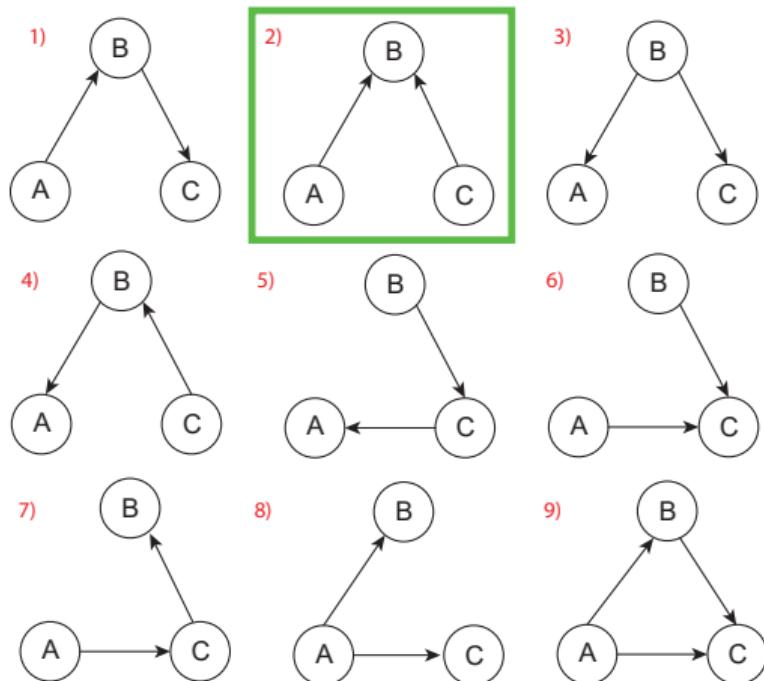
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Example 2: CI-based discovery

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What is the data-generating DAG?

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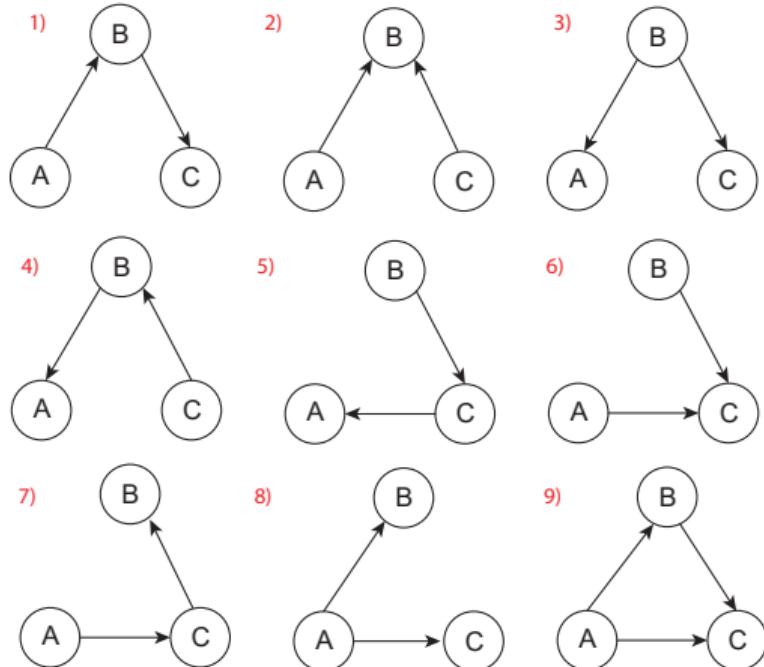
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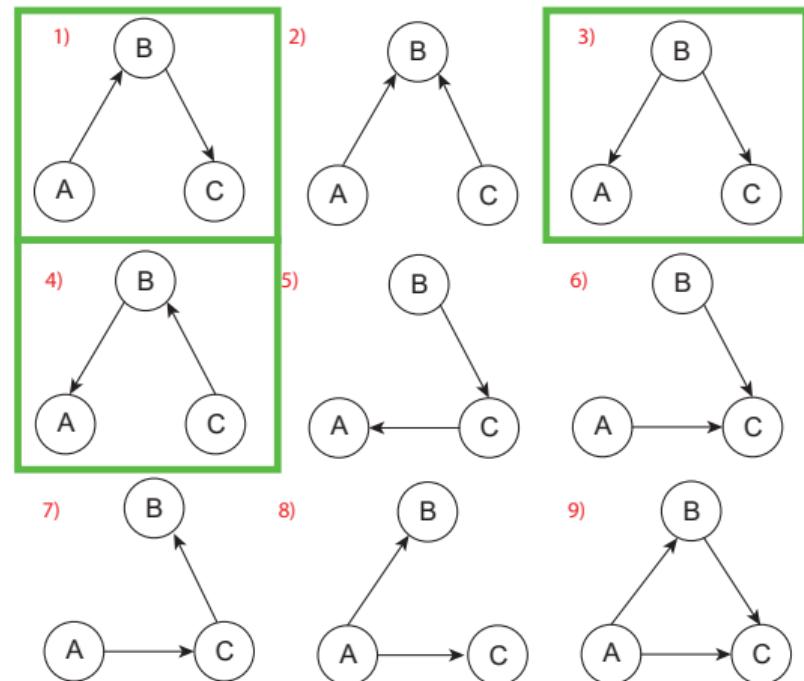
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Basics of CI-based discovery

In the general case, we usually cannot **uniquely** identify the DAG based only on patterns of statistical independence and dependence.

We already know this from d-seperation rules, since they tell us that different DAGs can yield the same statistical dependencies

Markov Equivalence:

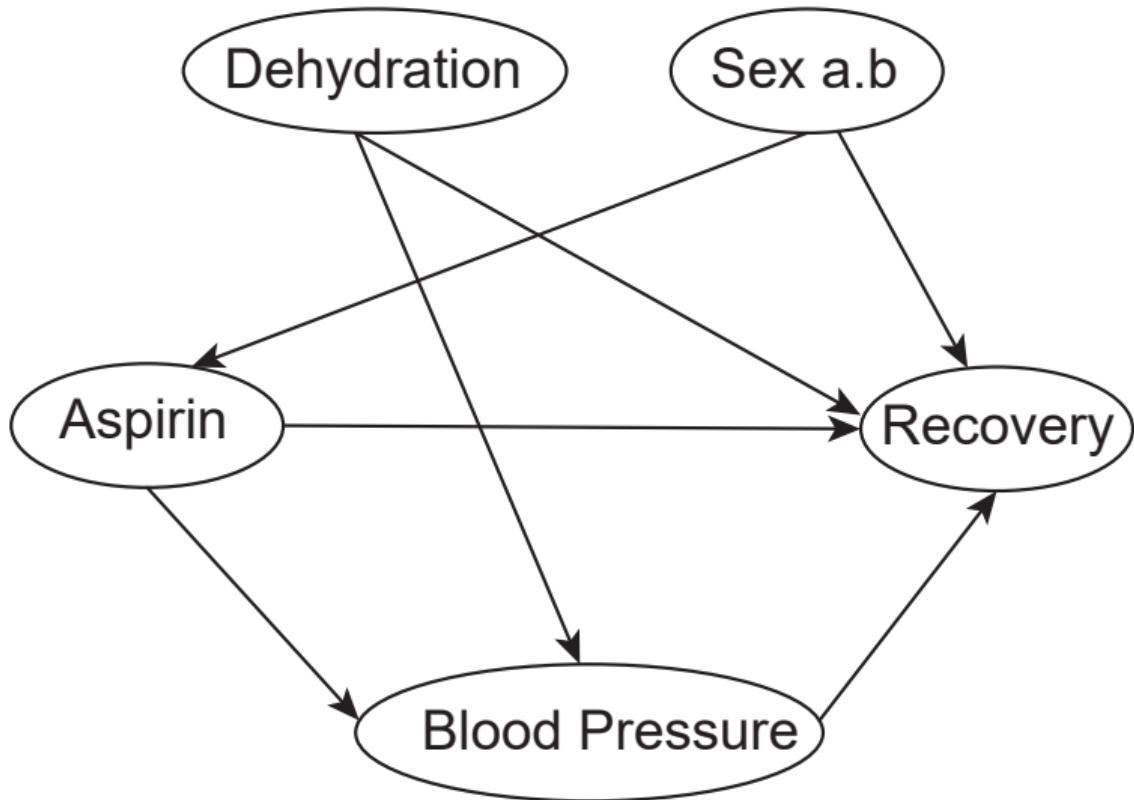
Two DAGs are *Markov Equivalent* if they satisfy the same d-seperation statements, and so the same set of (conditional) (in)dependence relations

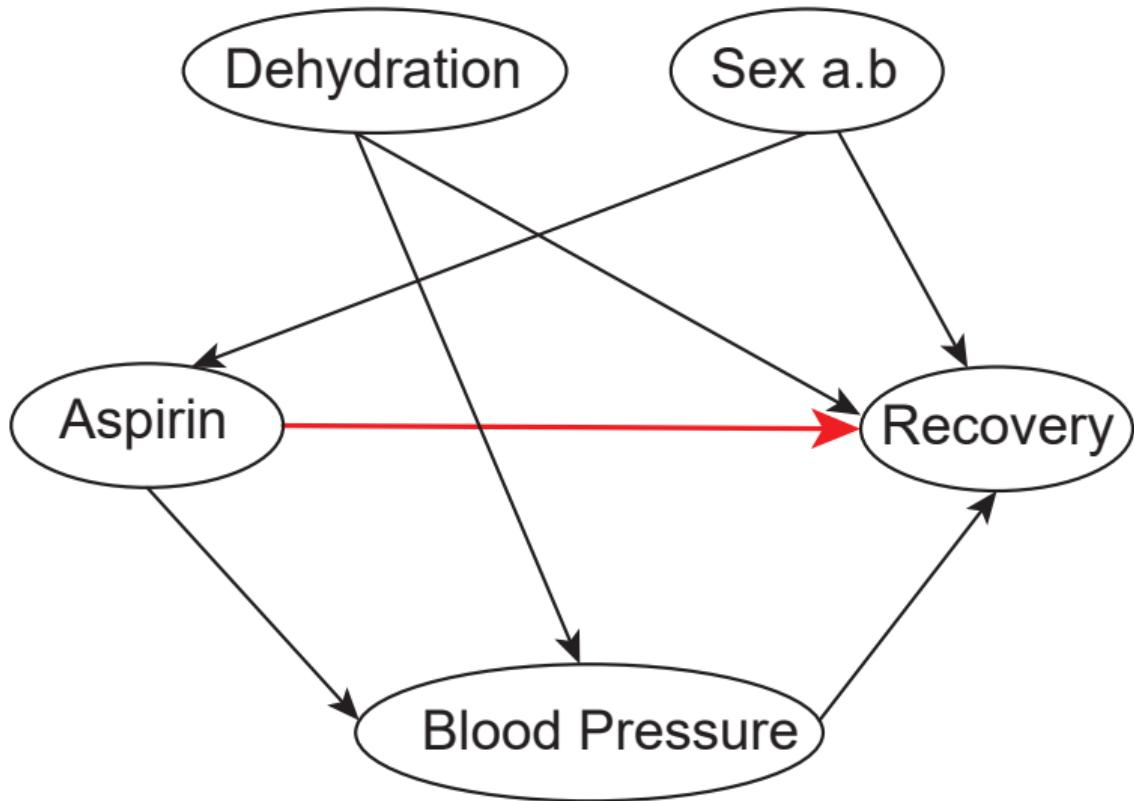
Basics of CI-based discovery

But we can learn **something** about the underlying DAG!

Implications of d-seperation:

- ① If two variables share a *direct causal path* $X \rightarrow Y$ OR $X \leftarrow Y$, then you can **never** block that path by conditioning on other variables!
 - If two variables are dependent **no matter what we condition on**, they share a direct causal link **of some direction**





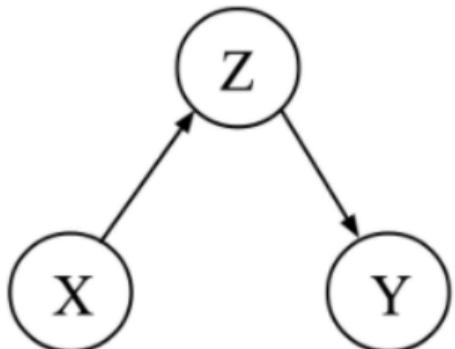
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- ② Colliders imply a different pattern of dependencies than chains and forks

Chain

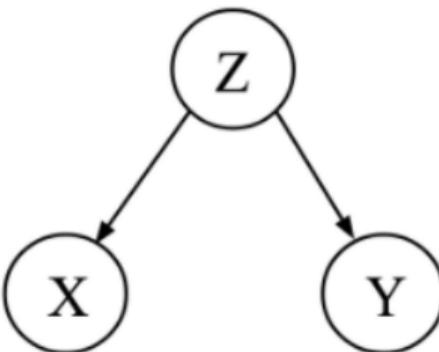


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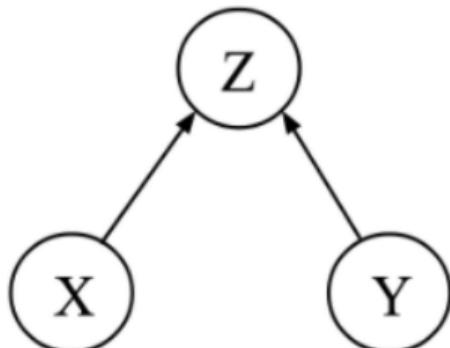


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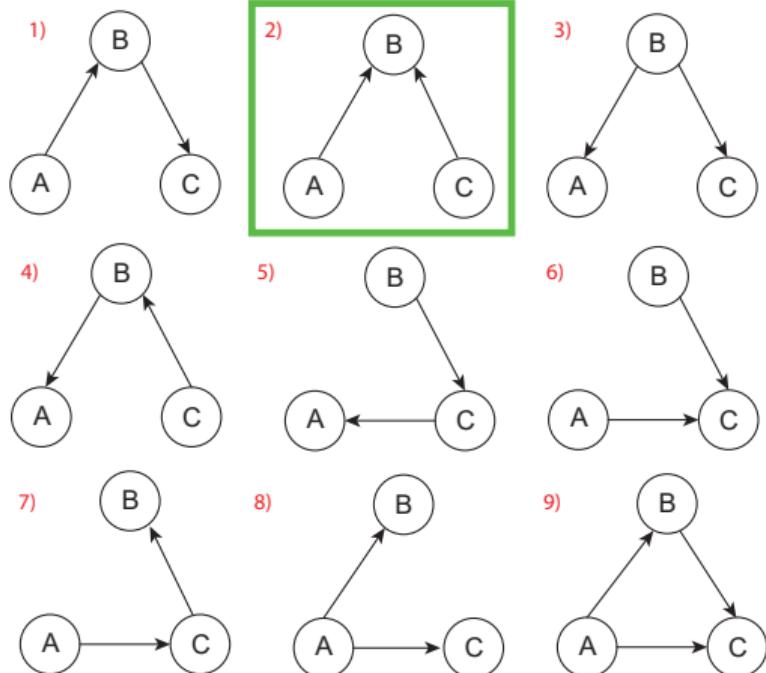
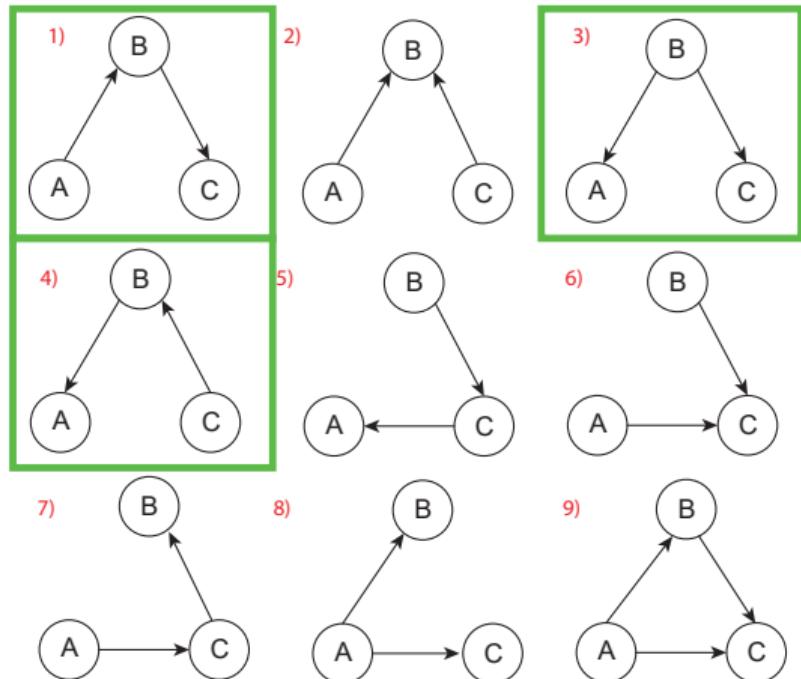
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$A \perp\!\!\!\perp C$  $A \perp\!\!\!\perp C | B$ 

The basics of CI-based discovery

CI-based methods can discover:

A Which variables share a direct causal link and which variables don't

- This is known as the *skeleton* of a DAG
- If $X \rightarrow Y$ or $X \leftarrow Y$, then X and Y *will never be statistically independent* (marginally or conditionally).

B If there's a collider, we can detect the direction of causal arrows, **as long as** the two "cause" variables don't also cause each other

- Also known as an "immorality" - two parent nodes who share a child but are not "married" (!!!)
- **If everything is dependent on everything - very little can be learned!**

In general, outside of (immoral) colliders, we can't determine the direction of the causal arrow

Assumptions for CI-based discovery

Global Markov Condition:

P is Markov w.r.t G if

$$X \text{ and } Y \text{ are d-separated by } S \implies X \perp\!\!\!\perp Y \mid S$$

Faithfulness:

P satisfies faithfulness w.r.t G if

$$X \perp\!\!\!\perp Y \mid S \implies X \text{ and } Y \text{ are d-separated by } S$$

Essentially: Paths never “perfectly cancel out”

Statistical (conditional) Independence \implies causal independence (d-separation)

Violations of Faithfulness

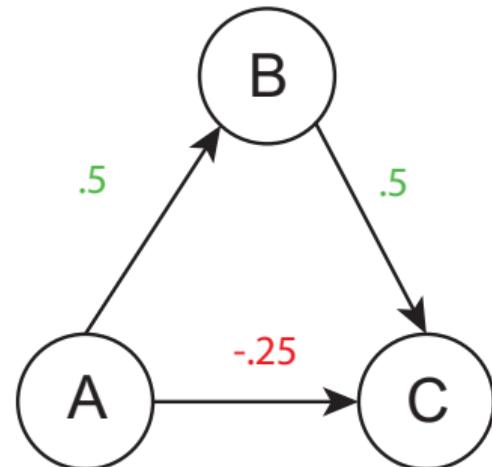
$$A := \epsilon_A$$

$$B := .5A + \epsilon_B$$

$$C := -.25A + .5B + \epsilon_C$$

where

- $\epsilon_A, \epsilon_B, \epsilon_C$ are iid, $\sim \mathcal{N}(0, 1)$



$$\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \mathcal{N} \left[\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & .5 & 0 \\ .5 & 1.25 & .5 \\ 0 & .5 & 1.25 \end{pmatrix} \right]$$

Violations of Faithfulness

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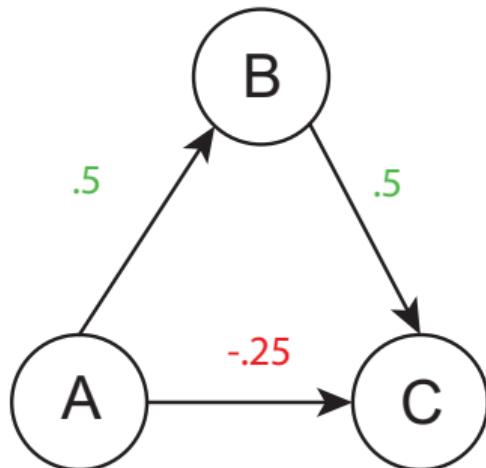
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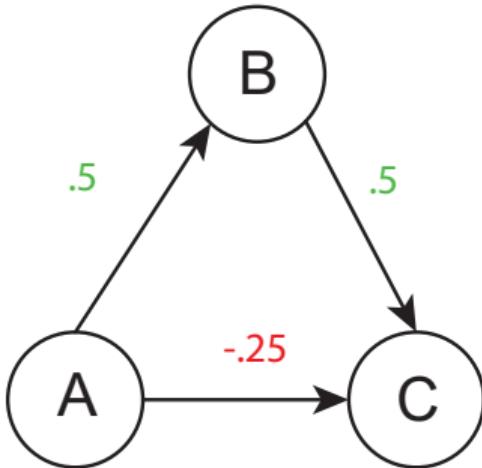
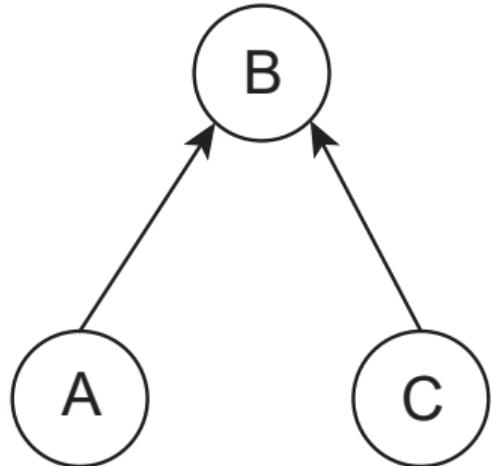
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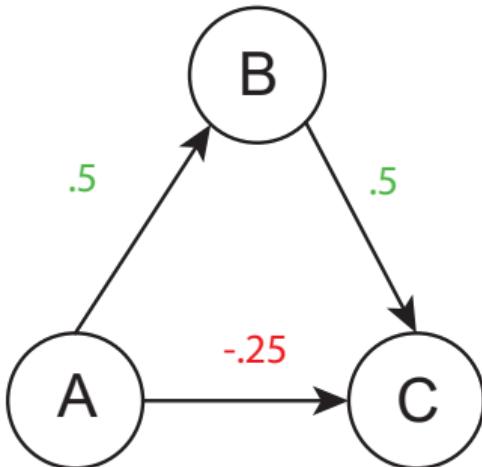
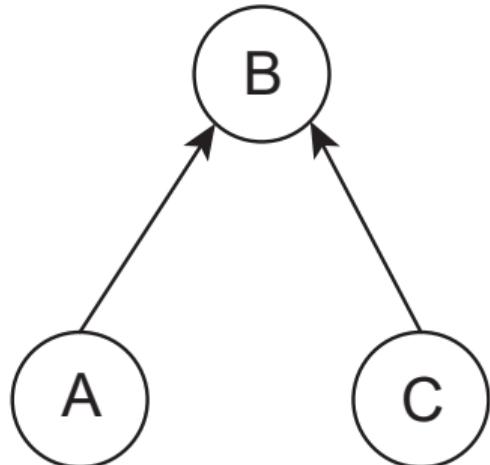


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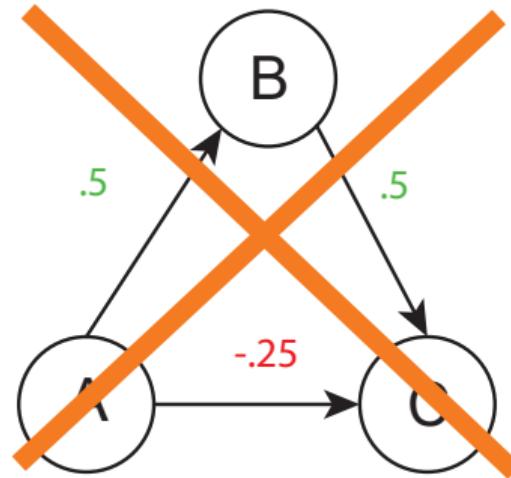
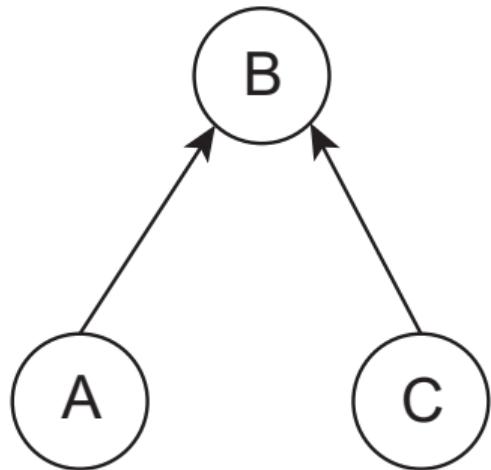


$$A \perp\!\!\!\perp C$$

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Assume Faithfulness

Violations of Faithfulness



$$A \perp\!\!\!\perp C$$
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The basics of CI-based discovery

Typically CI-based methods cannot *uniquely* identify the underlying DAG from observational data. Instead they can identify a *Markov Equivalence set*

Markov Equivalence:

Two DAGs are *Markov Equivalent* if they satisfy the same d-seperation statements, and so the same set of (conditional) (in)dependence relations

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- A They have the same skeleton
- B They have the same immoralities

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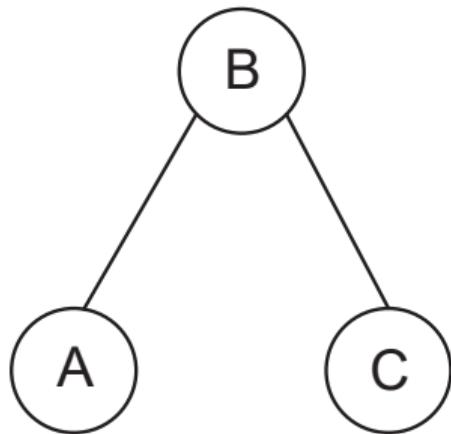
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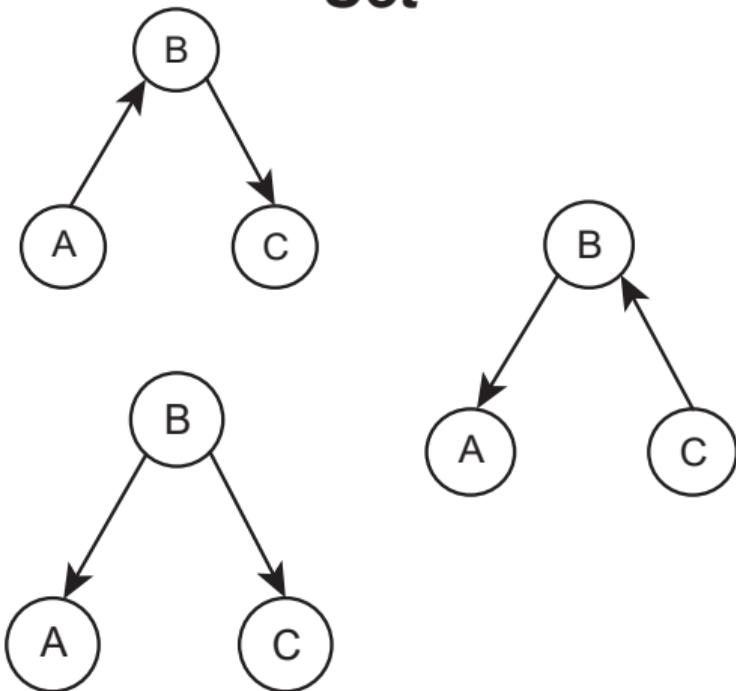
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Represented by a Complete Partially-Oriented Directed Acyclic Graph (**CPDAG**)

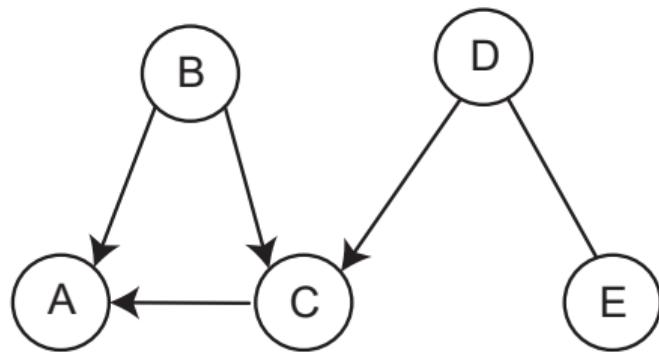
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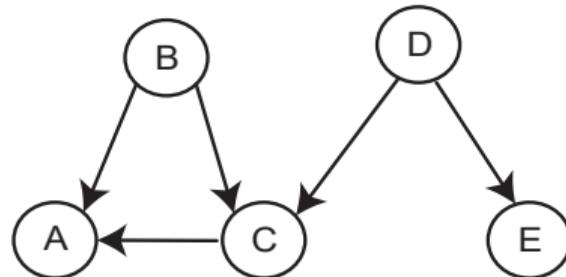
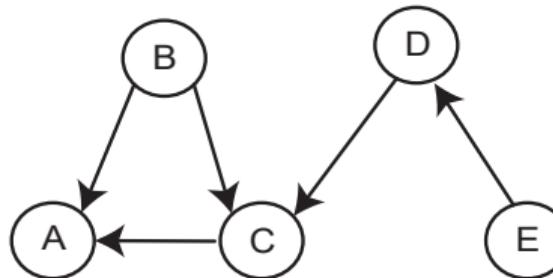
Markov-Equivalence Set



CPDAG



Markov-Equivalence Set



In Practice

Original approaches: PC algorithm, FCI algorithm (Spirtes et al. 2000)

- Don't need to test all independences, but can do a quicker "search"
- Extensions exist that deal with violations of *sufficiency*
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 - In a given sample : Type I and II errors
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 - In a given sample : Type I and II errors
 - Faithfulness \neq No false negatives!
- CI testing easy if linear + Gaussian (partial correlation / regression) or discrete (cross-tables)
 - Can be difficult in other cases (Shah & Peters, 2020)
 - Non-parametric methods exist but require large sample size

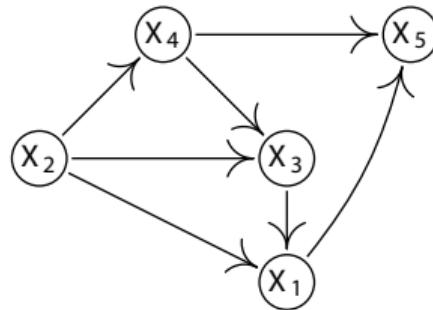
Causal Discovery with Conditional Independence: In a Nutshell

observational data $P(X_1, \dots, X_5)$

X_1	X_2	X_3	X_4	X_5
3.4	-0.3	5.8	-2.1	2.2
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-2.4	-0.1	4.3	-0.7	3.5
2.3	-0.3	5.5	-1.1	-4.4
3.5	-0.2	3.9	-0.9	-3.9
:	:	:	:	:

infer
?

causal model, e.g. DAG G



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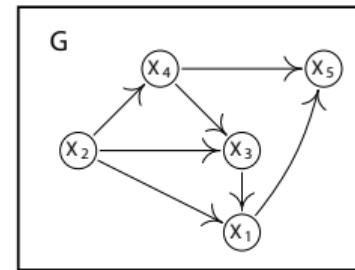
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:	:	:	:	:

independence tests



$$\begin{aligned}X_5 &\perp\!\!\!\perp X_2 | X_1 X_3 X_4 \\X_3 &\perp\!\!\!\perp X_5 | X_1 X_2 X_4 \\&\vdots \\X_1 &\not\perp\!\!\!\perp X_2 | X_3 X_4\end{aligned}$$

Faithfulness
Markov Cond.



Causal Discovery with Conditional Independence: In a Nutshell

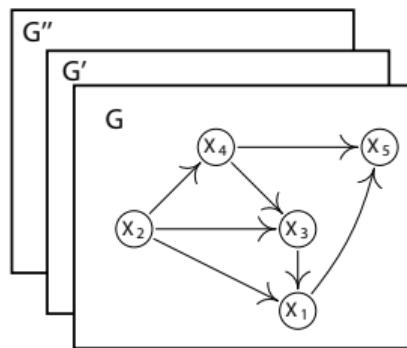
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Faithfulness
Markov Cond.



Restricted Causal Models

Restricted SCMs

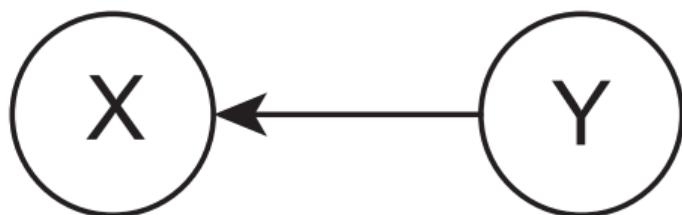
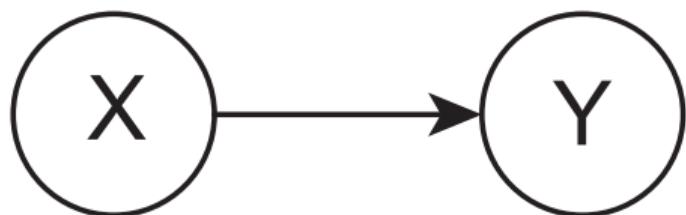
Recall: SCMs are in principle non-parametric - relationships can take any form, and the errors can have any distribution

In some special cases we can “buy” an ability to learn the causal structure if we are willing to make more assumptions about the **types of relationships** and/or **distribution of the noise term** in the SCM

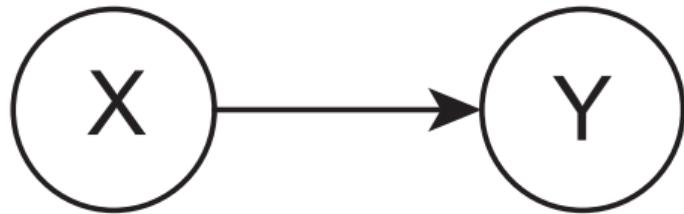
Examples so far: $Y := BX + \epsilon$, where ϵ is Gaussian, $\epsilon \sim N(0, \sigma^2)$

- This is a special type of model called a **linear model** with **additive Gaussian noise**
- Recall: In an SCM, the *noise variable* is independent of the cause variable. $\epsilon \perp\!\!\!\perp X$
- As we have seen: In general, many different causal models of this form that are **statistically equivalent**

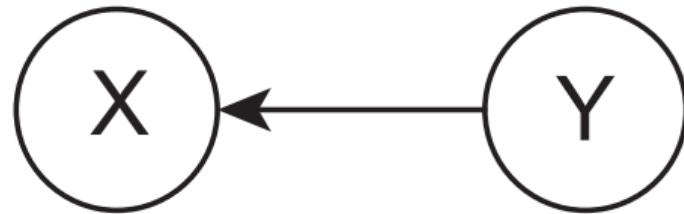
Bivariate SCMs



Bivariate SCMs



$$Y := B_X X + \epsilon_Y \quad \epsilon_Y \sim \mathcal{N}(0, \sigma_Y^2)$$



$$X := B_Y Y + \epsilon_X \quad \epsilon_X \sim \mathcal{N}(0, \sigma_X^2)$$

Bivariate SCMs: Linear with Gaussian Additive Noise



$$Y := BX + \epsilon_Y \quad \epsilon_Y \sim \mathcal{N}(0, \sigma_Y^2)$$

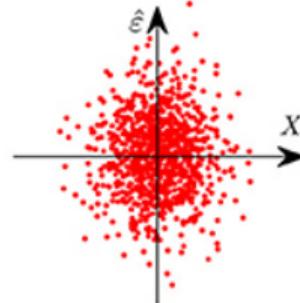
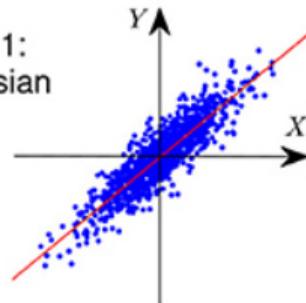
Bivariate SCMs: Linear with Gaussian Additive Noise



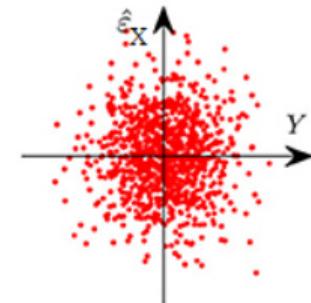
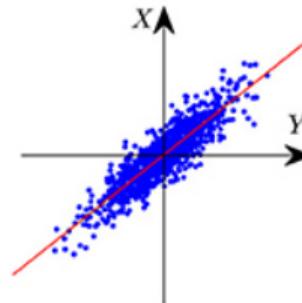
$$Y := BX + \epsilon_Y \quad \epsilon_Y \sim \mathcal{N}(0, \sigma_Y^2)$$

Regression of Y given X : $Y = bX + \epsilon$

Case 1:
Gaussian



Regression of X given Y : $X = b_Y Y + \epsilon_X$



Restricted SCMs

If we are dealing with a **bivariate system** with **linear relationships** and **Gaussian noise**, we can never distinguish if $X \rightarrow Y$ or $Y \rightarrow X$.

- In the true model we know that the cause variable is independent of the error, $\epsilon_Y \perp\!\!\!\perp X$
- But in this situation, when we fit a statistical model in the **wrong** causal direction, we still get errors which are independent of the predictor, $\epsilon_X \perp\!\!\!\perp Y$

Restricted SCMs

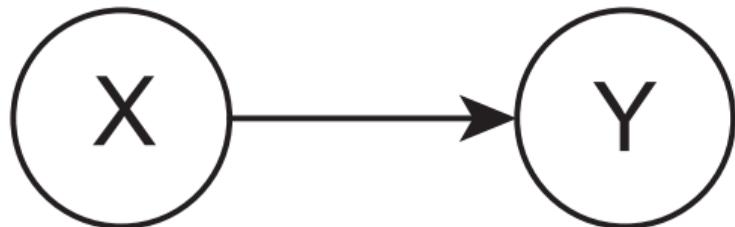
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But causal models **are** statistically distinguishable if we are willing to assume the SCM is **either**:

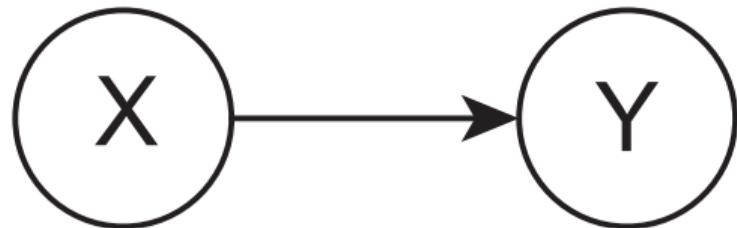
- A Linear Model with **Non-Gaussian** Additive Noise
- B **Non-Linear** Model with Gaussian Additive Noise

Bivariate SCMs: Linear with non-Gaussian Additive Noise



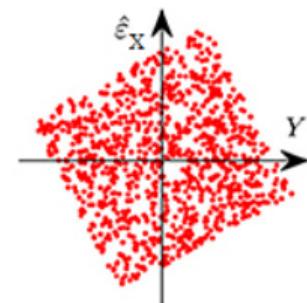
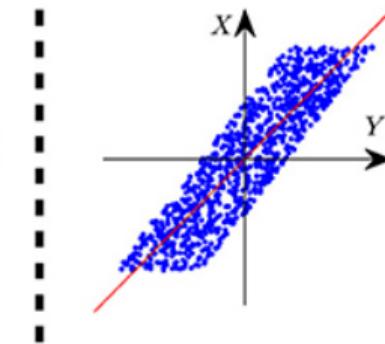
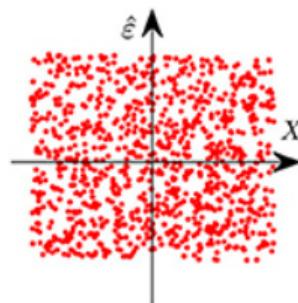
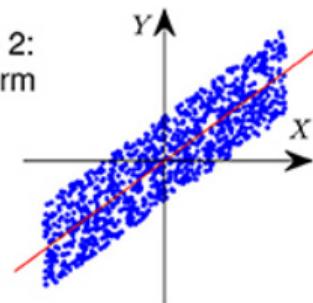
$$Y := BX + \epsilon_Y \quad \epsilon_Y \sim U(lb, ub)$$

Bivariate SCMs: Linear with non-Gaussian Additive Noise



$$Y := BX + \epsilon_Y \quad \epsilon_Y \sim U(lb, ub)$$

Case 2:
Uniform



Bivariate SCMS: Linear with non-Gaussian Additive Noise

We assume an underlying SCM where the *noise variable* is independent of the cause variables.

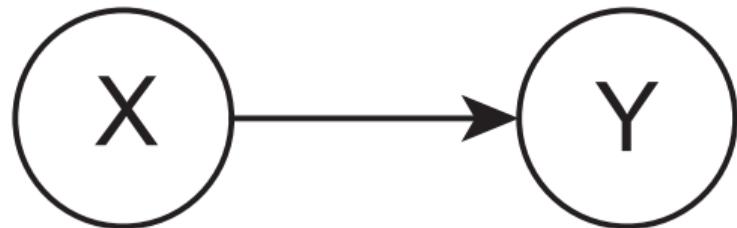
$$Y := BX + \epsilon_Y$$
$$\epsilon_Y \perp\!\!\!\perp X$$

If we fit a model with the “wrong” causal direction, the *noise* of that regression model will not be independent of the predictors

$$X = B_Y Y + \epsilon_X$$
$$\epsilon_X \not\perp\!\!\!\perp Y$$

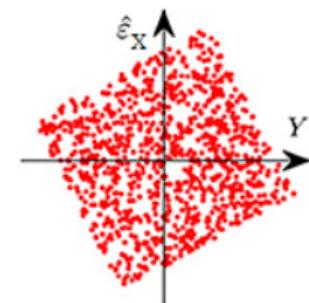
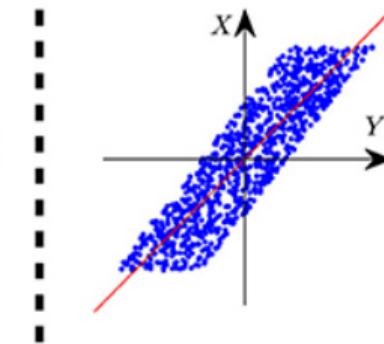
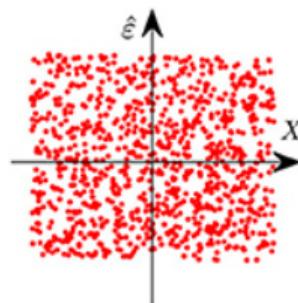
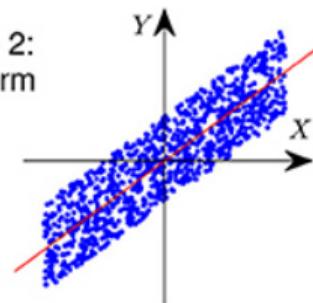
This only works for non-Gaussian noise, but there it allows us to identify the direction of the causal arrow!

Bivariate SCMS: Linear with non-Gaussian Additive Noise

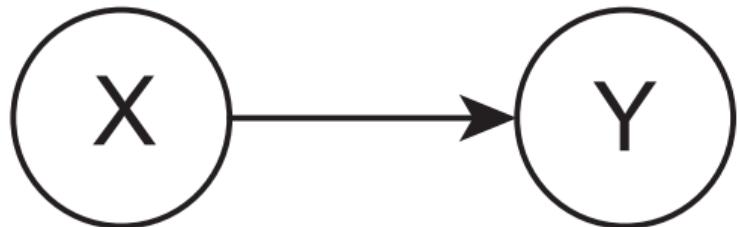


$$Y := BX + \epsilon_Y \quad \epsilon_Y \sim U(lb, ub)$$

Case 2:
Uniform

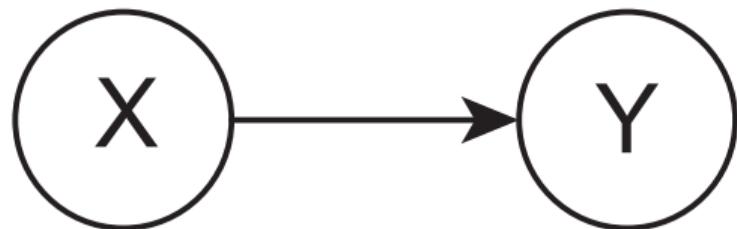


Bivariate SCMS: Non-Linear with Gaussian Additive Noise

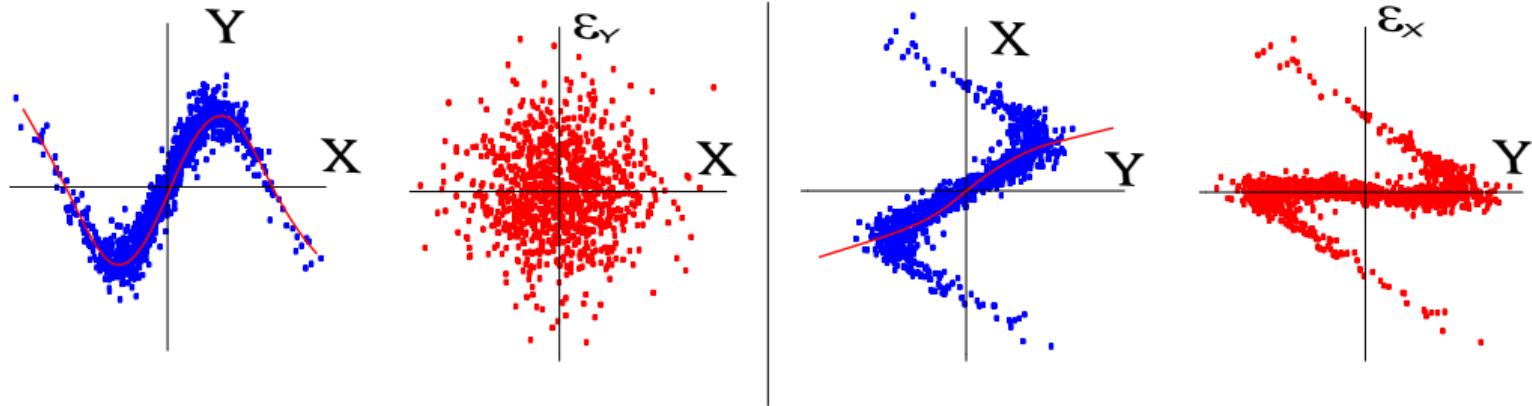


$$Y := \sin(X) + \epsilon_Y \quad \epsilon_Y \sim \mathcal{N}(0, \sigma^2)$$

Bivariate SCMS: Non-Linear with Gaussian Additive Noise



$$Y := \sin(X) + \epsilon_Y \quad \epsilon_Y \sim \mathcal{N}(0, \sigma^2)$$



Bivariate SCMS: Non-Linear with Gaussian Additive Noise

We assume an underlying SCM

$$\begin{aligned} Y &:= f(X) + \epsilon_Y \\ \epsilon_Y &\perp\!\!\!\perp X \end{aligned}$$

If $f(X)$ is *non-linear* (e.g. $\sin(X)$, X^p , e^X), there is **no equivalent statistical model** that satisfies

$$\begin{aligned} X &:= g(Y) + \epsilon_X \\ \epsilon_X &\perp\!\!\!\perp Y \end{aligned}$$

If we fit a model in the wrong causal direction, we will find $\epsilon_X \not\perp\!\!\!\perp Y$ We can test this by fitting non-linear models in both ‘directions’ and testing for independence of errors!

Summary

Linear Non-Gaussian:

- LiNGAM algorithm (Shimizu et al. 2006)
- Extends this idea to the multivariate case
- Can uniquely identify multivariate DAGs!

Disadvantages:

- Need sufficiency (some extensions)
- How common are these systems?
- Degree of non-normality?

Summary

Linear Non-Gaussian:

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- Extends this idea to the multivariate case
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Disadvantages:

- Need sufficiency (some extensions)
- How common are these systems?
- Degree of non-normality?

Non-Linear Gaussian:

- Mooij et al (2016)
- Use non-parametric/smoothing methods
- If we know the noise distribution, can choose best fitting model
- Works well in bivariate case with no confounding

Disadvantages:

- Again, sufficiency needed
- Difficult to scale to multivariate case

Restricted Causal Models: In a Nutshell

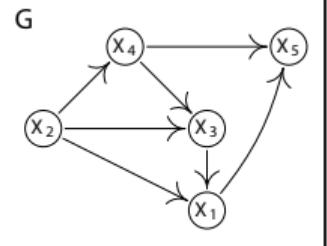
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:	:	:	:	:

Assumptions about SCM
Non-Linear / Non-Gaussian

Search for stat.
model in which

Noise(X)
 $\perp\!\!\!\perp$
Parents (X)



Invariant Causal Prediction

So far we looked at methods for causal discovery that work with a **single observational dataset**

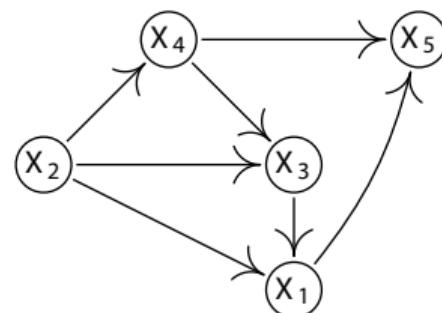
What if we have a mix of **observational** and **experimental** data? Can we do something different?

This is the idea behind causal discovery using *Invariant Causal Prediction*

Invariant Causal Prediction

Basic Idea:

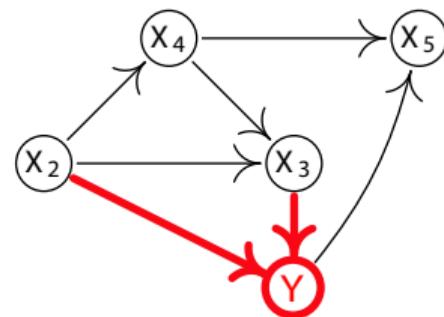
- ① There is some unknown causal graph, but we only care about learning **the direct causes** of one *target variable* Y
- ② We have data drawn from different *environments*
 - Here: A mix of observational and intervention data
 - Interventions act on variables other than Y
- ③ We identify the direct causes of Y by looking for those conditional **dependencies** that are *invariant* (remain the same) across environments



Invariant Causal Prediction (ICP)

Basic Idea:

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 - Here: A mix of observational and intervention data
 - Interventions act on variables other than Y
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ICP: Key Assumption

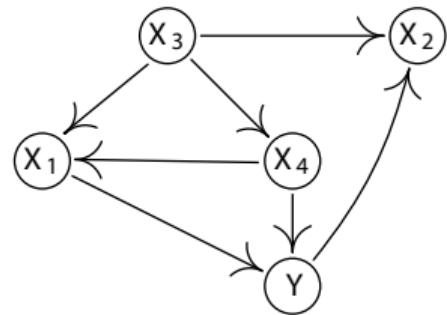
Modularity and Localized Interventions:

We assume that it is possible to intervene on a variable without fundamentally changing how it relates to other variables

- We can change $p(X)$ without changing $p(Y | X)$
- We can change one cause-effect mechanism without changing the others

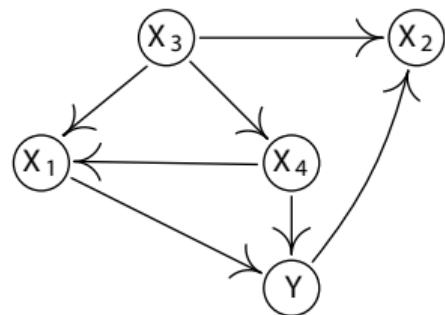
Example

Observational Data



Example

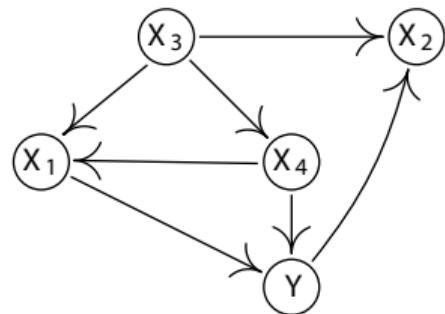
Observational Data



What **open paths** make up the statistical dependency $\text{cor}(Y, X_1 | X_4)$?

Example

Observational Data

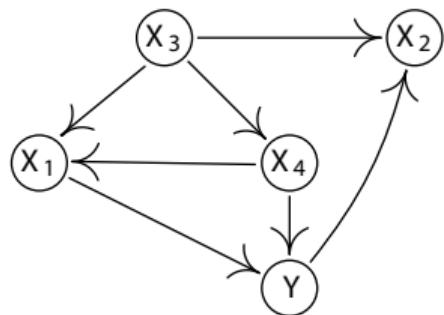


What **open paths** make up the statistical dependency $\text{cor}(Y, X_1 | X_4)$?

- $X_1 \rightarrow Y$

Example

Observational Data



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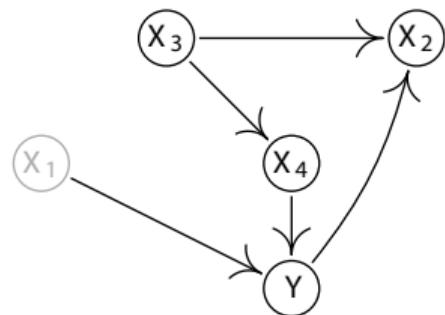
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What **open paths** make up the statistical dependency $\text{cor}(Y, X_3)$?

- $X_3 \rightarrow X_4 \rightarrow Y$
- $X_3 \rightarrow X_1 \rightarrow Y$
- $X_3 \rightarrow X_4 \rightarrow X_1 \rightarrow Y$

Example

Intervention Data: e.g. $do(X_1)$

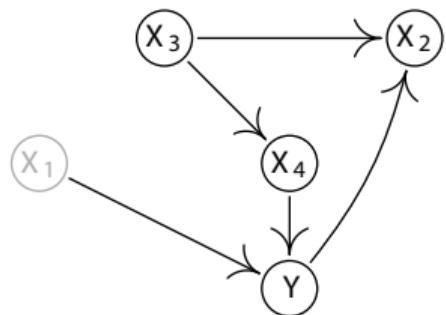


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Example

Intervention Data: e.g. $do(X_1)$



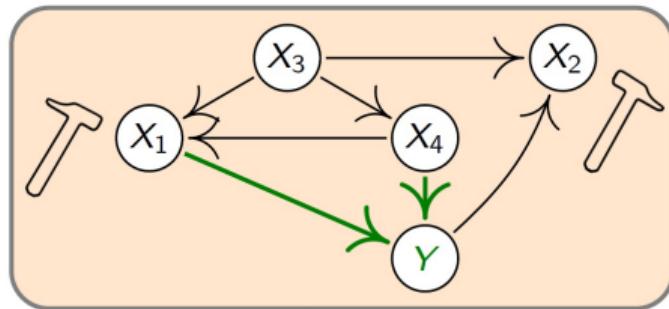
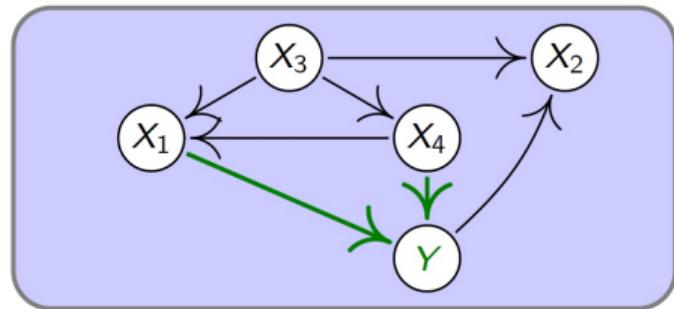
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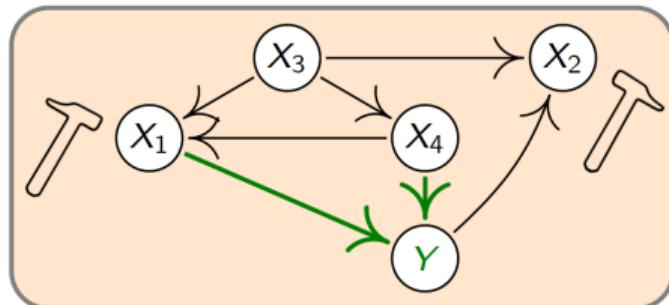
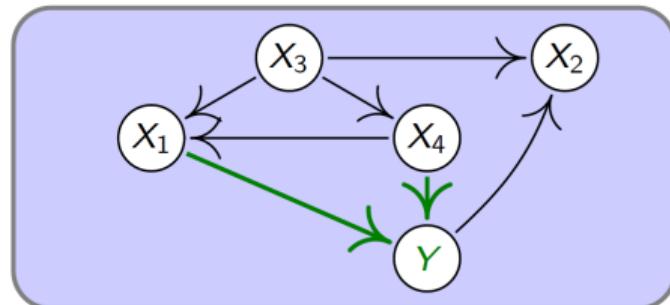
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Fundamental assumption: $X_1, X_4 \rightarrow Y$ is invariant under interventions.



cf. modularity, autonomy, Haavelmo 1944, Aldrich 1989, Pearl 2009, ...

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cf. modularity, autonomy, Haavelmo 1944, Aldrich 1989, Pearl 2009, ...

Key idea: Use and data and search for invariant models.

set	\emptyset	$\{1\}$	$\{2\}$	$\{3\}$	\dots	$\{1, 4\}$	$\{2, 4\}$	\dots	$\{1, 3, 4\}$
invariance	X	X	X	X	\dots	✓	X	\dots	✓

$$\hat{S} := \bigcap_{S \text{ invariant}} S = \{1, 4\}$$

ICP in Practice

Invariant Causal Prediction (Peters, Buhlmann, Meinshausen, 2016)

- Can be used even when it is not known what variables are intervened on or what interventions are applied (“fat hand interventions”)
- Basic idea can be extended to other “environments” - non-descendants and time
- Can also be extended to learning the full graph, with some caveats
- Extended/Generalized to non-linear case

Disadvantages:

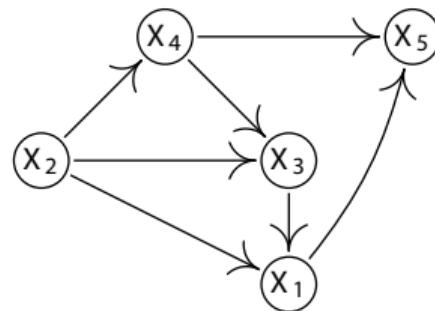
- Sufficiency (again, some extensions)
- (Subset of) environments where interventions do not act directly on Y
- **Need different environments:** The more environments the better!

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:	:	:	:	:

infer
?

causal model, e.g. DAG G



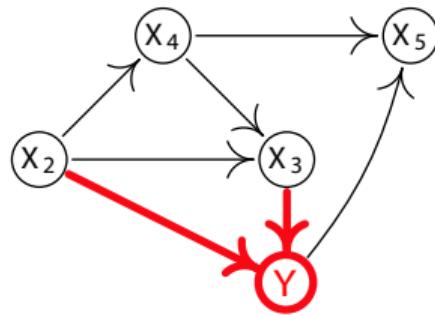
In a Nutshell: ICP

observational data $P(X_1, \dots, X_5)$
& intervention data $P_{\text{do}}(X_1, \dots, X_5)$

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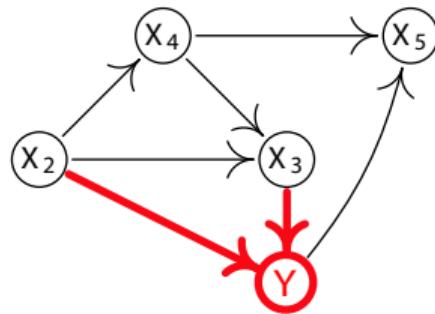
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:	:	:	:	:

Modularity
→
Interventions
Not on Y

causal model, e.g. DAG G



Causal Learning: An overview

Can we infer causal structure from data?

Short answer:

- It's difficult
- There is usually more than one SCM that generates the same observational data

Long answer:

- Yes, or at least, we can learn *something* about the causal structure
- But only under certain conditions - if we are willing to make certain assumptions about the causal system
- Note: This is a limitation of all science - no free lunch!

Summary

In this lecture we learned about three different strategies for causal discovery.

① Using Conditional (In)dependence

- “Flipping” the story of last week: Going from estimated conditional and marginal (in)dependence to the DAG structure
- Generally: Not able to *uniquely identify* the DAG, but instead a set of possible DAGs (Markov Equivalence Set)

Summary

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1 Using Conditional (In)dependence

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2 Restricting the Structural Causal Model

- If we know something about *how exactly* variables look like and/or relate to one another, we can use that to identify the causal model!
- Specifically: Linear but Non-Gaussian or Non-linear models - succeed in getting a single underlying DAG

Summary

In this lecture we learned about three different strategies for causal discovery.

① Using Conditional (In)dependence

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③ Using Invariance and Data from Different Environments

- ICP: Look for predictive relationships that stay the same in different settings (observational/interventional)
- Works if we care about causes of a single variable, and we don't intervene on that variable

Summary

There are different ways to exploit relationship between causal models and data to recover the causal model itself: Different assumptions, able to recover different things

- Many extensions and combinations of these methods also exist, and different strategies are possible

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- So problems of stat. learning also apply, e.g. sample size and data quality
- “Garbage in \rightarrow garbage out”

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- So problems of stat. learning also apply, e.g. sample size and data quality
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No free lunch principle

- All discovery algorithms rely on assumptions about the underlying causal process
- Assumptions/Knowledge in \rightarrow Knowledge Out

Extra References

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- Credit some slides: Jonas Peeters Causal Discovery workshop

ICP Rationale

Let $X \rightarrow Y$ and let $pa(Y)$ denote all other **direct causes** of Y . **Modularity** implies that: $p(Y | X, pa(Y))$ remains the same no matter whether we have:

- Observational data
- Data where we intervene on X
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Invariant Causal Prediction: Only conditional dependence relationships (i.e. *predictions*) that reflect direct cause-effect relationships (i.e. *causal*) will remain the same (i.e. *invariant*) across different **environments**