## Introduction to Causal Inference \& Causal Discovery

## Overview

## Causal inference:

■ Causal graphical models
■ Interventions (the "do" operator)
■ Example: Study of Kidney Stone Treatments
■ Backdoor criterion

- The ladder of causation
- Counterfactuals

Causal discovery:
■ Markov equivalence

- Faithfulness
- Structure identifiability
- Constraint-based methods

■ Score-based methods

## Causal Inference

## Causal graphical models (CGM)

- A causal graphical model (CGM) is a pair $(p, \mathcal{G})$ s.t.
$\square \mathcal{G}$ is a directed acyclic graph (DAG)
- $p \in \mathcal{L}(\mathcal{G})$, i.e. $p$ factorizes according to $\mathcal{G}$.

■ $\mathcal{G}$ describes causal relationships between variables, i.e., how the system reacts to interventions.

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- $\mathcal{G}$ describes causal relationships between variables, i.e., how the system reacts to interventions.


$$
p(S, T, R)=p(S) p(T \mid S) p(R \mid S, T)
$$

## The "do" operator

Throughout, we will assume perfect deterministic interventions.
Definition (The "do" operator)
Given a causal graphical model $(p, \mathcal{G})$,

$$
p\left(x \mid d o\left(x_{k}^{\prime}\right)\right):=\delta\left(x_{k}, x_{k}^{\prime}\right) \prod_{i \neq k} p\left(x_{i} \mid x_{\pi_{i}^{\mathcal{G}}}\right)
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■ Can compute marginals, e.g. $p\left(x_{i} \mid d o\left(x_{k}^{\prime}\right)\right)=\sum_{x_{\backslash \backslash\{i\}}} p\left(x \mid d o\left(x_{k}^{\prime}\right)\right)$

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$■ \ldots$ and conditionals, e.g. $p\left(x_{i} \mid x_{j}, d o\left(x_{k}^{\prime}\right)\right)=\frac{p\left(x_{i}, x_{j} \mid d o\left(x_{k}^{\prime}\right)\right)}{p\left(x_{j} \mid d o\left(x_{k}^{\prime}\right)\right)}$

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■ Remark: $p\left(x_{V \backslash\{k\}} \mid d o\left(x_{k}\right)\right)=\prod_{i \neq k} p\left(x_{i} \mid x_{\pi_{i}^{\mathcal{G}}}\right)$.

## The "do" operator

■ Back to our example

$P(S, R \mid d o(T))=P(S) \underbrace{P(T \mid S)} P(R \mid S, T)$
The decision of taking treatment $T$ does not depend on $S$ anymore

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\mathcal{G}^{\prime}=\left(V, E^{\prime}\right) \quad E^{\prime}=\{(i, j) \in E \mid j \neq k\}
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## Different types of interventions

## Intervening on the treatment $T$

$T=$ Treatment $\in\{A, B\}$
$S=$ Stone size $\in\{$ small, large $\}$
$R=$ Patient recovered $\in\{0,1\}$

Observations

Perfect intervention
Imperfect intervention


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Perfect intervention
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$p(S) \tilde{p}(T) p(R \mid S, T)$

$p(S) \tilde{p}(T \mid S) p(R \mid S, T)$

Definition presented previously is a perfect intervention with $\tilde{p}(T):=\delta\left(T, T^{\prime}\right)$. It is sometimes called a perfect deterministic intervention.

## Why should I care!?! (Kidney Stone Treatment)

$T=$ Treatment $\in\{A, B\}$
$S=$ Stone size $\in\{$ small, large $\}$
$R=$ Patient recovered $\in\{0,1\}$


|  | Overall | Patients with <br> small stones | Patients with <br> large stones |
| :--- | :---: | :---: | :---: |
| Treatment $a:$ <br> Open surgery | $78 \%(273 / 350)$ | $\mathbf{9 3 \%}(81 / 87)$ | $\mathbf{7 3 \%}(192 / 263)$ |
| Treatment $b:$ <br> Percutaneous <br> nephrolithotomy | $\mathbf{8 3 \%}(289 / 350)$ | $87 \%(234 / 270)$ | $69 \%(55 / 80)$ |

(Example taken from Element of Causal Inference by Peters et al. p111)

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Pay attention to these two questions...

1- What is your chance of recovery knowing that the doctor gave you treatment A?

2- What is your chance of recovery if you decide to take treatment $\mathbf{A}$ ?
(In both cases, assume you don't know the size of your stone)

## Why should I care!?! (Kidney Stone Treatment)

$T=$ Treatment $\in\{A, B\}$
$Z=$ Stone size $\in\{$ small, large $\}$
$R=$ Patient recovered $\in\{0,1\}$


What is your chance of recovery knowing that the doctor gave you treatment A?
■ Compute $P(R=1 \mid T=A)$ ! (we know how to do that: D )
■ Knowing that your doctor gave you treatment A tells you that you probably have a large kidney stone $\ldots P(S=\operatorname{large} \mid T=A)=0.75$

■ ... which reduces your chance of recovery
$P(R=1 \mid T=A, S=$ large $)=0.73<0.93=P(R=1 \mid T=A, S=$ small $)$

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What is your chance of recovery if you decide to take treatment $A$ ?

- $P(R=1 \mid d o(T=A))$

■ Your really don't know anything about your kidney stone

## Why should I care!?! (Kidney Stone Treatment)

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P(S, R \mid d o(T))=P(S) \underbrace{P(T \mid S)} P(R \mid S, T)
$$

The decision of taking treatment $T$ does not depend on $S$ anymore

Then simply marginalize as usual:

$$
\begin{aligned}
P(R=1 \mid d o(T=A)) & =\sum_{S} P(R=1, S \mid d o(T=A)) \\
& =\sum_{S} P(R=1 \mid S, T=A) P(S)=0,832
\end{aligned}
$$

## Why should I care!?! (Kidney Stone Treatment)

$T=$ Treatment $\in\{A, B\}$
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$R=$ Patient recovered $\in\{0,1\}$


What is your chance of recovery knowing that the doctor gave you treatment A?

$$
P(R=1 \mid T=A)=0,78 \quad P(R=1 \mid T=B)=\mathbf{0 , 8 3}
$$

What is your chance of recovery if you decide to take treatment A?

$$
P(R=1 \mid d o(T=A))=\mathbf{0 , 8 3 2}
$$

$$
P(R=1 \mid d o(T=B))=0,782
$$

## Why should I care!?! (Kidney Stone Treatment)

- What just happened? We showed
$\underbrace{P(R=1 \mid \operatorname{do(T=A))}}_{\text {Never observed data from } p(T, S, R \mid \text { do(T=A) })}=\underbrace{\sum_{S} P(R=1 \mid S, T=A) P(S)}_{\text {...Yet I can estimate the query, since there is no "do" here :D }}$


## Why should I care!?! (Kidney Stone Treatment)

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■ Formally, this means $p(R=1 \mid d o(T=A))$ is identifiable from $p(R, T, S)$ and $\mathcal{G}$ (our computations critically relied on the causal graph).

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■ Formally, this means $p(R=1 \mid d o(T=A))$ is identifiable from $p(R, T, S)$ and $\mathcal{G}$ (our computations critically relied on the causal graph).

■ Turns out what we just did is an instance of the backdoor criterion...

## Backdoor criterion

## Theorem (Backdoor criterion)

$p\left(x_{i} \mid d o\left(x_{k}\right)\right)=\sum_{x_{S}} p\left(x_{i} \mid x_{k}, x_{S}\right) p\left(x_{S}\right)$ if
$11 S$ contains no descendants of $x_{k}$, and
2 S blocks all paths from $x_{i}$ to $x_{k}$ entering $x_{k}$ from "the backdoor", i.e. such that $x_{k} \leftarrow \ldots x_{i}$

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Say we want to compute $p(y \mid d o(x))$ :


Left path: Only backdoor path. Blocked by $S=\{K\}$. Right path: Why we cannot include a descendant of $X$ in $S$.

## Backdoor criterion

Can all identifiable queries $p\left(x_{i} \mid d o\left(x_{k}\right)\right)$ be expressed with the backdoor criterion?

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Answer: No!

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Answer: No!


■ Since $U$ is unobserved, we cannot apply the backdoor criterion...

- Turns out we can nevertheless identify $p(y \mid d o(x))$ from $p(X, Z, Y)$ using the front-door criterion. Look it up!


## Do-calculus

- Do-calculus is a set of three rules that can be applied to transform an interventional query (including a "do") into an observational expression (without any "do").

■ Not enough time to present them...

- All identifiable queries can be found by a subsequent application of these rules, i.e. the rules are complete.


## The ladder of causation

## You now know about the first two steps of Pearl's "ladder of causation".

| Level <br> (Symbol) | Typical <br> Activity | Typical Questions | Examples |
| :--- | :--- | :--- | :--- |
| 1. Association <br> $P(y \mid x)$ | Seeing | What is? <br> How would seeing $X$ <br> change my belief in $Y$ ? | What does a symptom tell me about <br> a disease? <br> What does a survey tell us about the <br> election results? |
| 2. Intervention <br> $P(y \mid d o(x), z)$ | Doing <br> Intervening | What if? <br> What if $I$ do $X ?$ | What if I take aspirin, will my <br> headache be cured? <br> What if we ban cigarettes? |
| 3. Counterfactuals <br> $P\left(y_{x} \mid x^{\prime}, y^{\prime}\right)$ | Imagining, <br> Retrospection | Why? <br> Was it $X$ that caused $Y ?$ <br> What if $I$ had acted <br> differently? | Was it the aspirin that stopped my <br> headache? <br> Would Kennedy be alive had Os- <br> wald not shot him? <br> What if $I$ had not been smoking the <br> past 2 years? |

Fig. 1. The Causal Hierarchy. Questions at level $i$ can only be answered if information from level $i$ or higher is available.
Taken from "The Seven Tools of Causal Inference with Reflections on Machine Learning" by Judea Pearl

## Counterfactual

You need structural causal models (SCM). Let $\mathcal{G}$ be a DAG:

$$
\begin{align*}
& X_{1}:=f_{1}\left(X_{\pi_{1}^{\mathfrak{G}}}\right)+N_{1}  \tag{1}\\
& X_{2}:=f_{2}\left(X_{\pi_{2}^{\mathfrak{G}}}\right)+N_{2}  \tag{2}\\
& \ldots  \tag{3}\\
& X_{d}:=f_{d}\left(X_{\pi_{d}^{\mathfrak{G}}}\right)+N_{d}
\end{align*}
$$

■ This induces an observational distribution

■ Can define interventions as well

■ Can define counterfactual statements (not possible with a causal graphical model). See Section 6.4 in ECI.

## Causal Discovery

## Markov Equivalence

■ Recall: A Directed Graphical Model encodes the Conditional Independence of a distribution.

■ Multiple DAGs may encode the same Conditional Independence statements.


■ Two DAGs encoding the same Conditional Independence statements are called Markov Equivalent.

## Markov Equivalence

## Theorem (Verma \& Pearl, 1991)

Two DAGs $G_{1}$ and $G_{2}$ are Markov Equivalent if and only if they have the same skeleton and the same $v$-structures.

$G_{1}$

$G_{2}$

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CPDAG

Markov Equivalence Classes can be represented as a Completed Partially Directed Acyclic Graph (CPDAG).

## Faithfulness

## Global Markov Property

$A \& B$ are d-separated given $C$ in $\mathcal{G}$
$X_{A} \Perp X_{B} \mid X_{C}$

## Faithfulness

## Global Markov Property



## Faithfulness

## Global Markov Property



## Exercise: Violation of Faithfulness



$$
\begin{aligned}
& X:=N_{X} \\
& Y:=X+N_{Y} \\
& Z:=X-Y+N_{Z} \\
& \text { with } N_{X}, N_{Y}, N_{Z} \stackrel{i i d}{\sim} \mathcal{N}\left(0, \sigma^{2}\right)
\end{aligned}
$$

$p(X, Y, Z)$ is a Multivariate Normal distribution, where the only conditional independence statements are: $X \Perp Z$ and $X \not \Perp Z \mid Y$.

## Faithfulness

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## Structure


$p(X, Y, Z)$ is a Multivariate Normal distribution, where the only conditional independence statements are: $X \Perp Z$ and $X \not \Perp Z \mid Y$.

## Structure Identifiability

## Theorem

Assume that $p$ is faithful wrt. $\mathcal{G}^{0}$. The Markov Equivalence class of $\mathcal{G}^{0}$, represented by its CPDAG, is identifiable from $p$.

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■ Only the Markov Equivalence class is identifiable from observations, not an individual graph. Two Markov Equivalent graphs may lead to different causal conclusions!

or


■ Under different assumptions, an individual DAG may be identifiable

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- Additive Noise Model (ANM): $X_{j}:=f_{j}\left(X_{\mathrm{Pa}_{j}}\right)+N_{j}, N_{j} \stackrel{i i d}{\sim} \mathcal{N}\left(0, \sigma^{2}\right)$, where $f_{j}$ are nonlinear.


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■ Using interventional data (i.e. data resulting from controlled experiments).

## Causal Structure Learning (Causal Discovery)

|  | $\mathrm{X}_{1}$ | $\mathrm{X}_{2}$ | $\mathrm{X}_{3}$ |
| :---: | :---: | :---: | :---: |
| sample 1 | 1.2 | 2.6 | 0.2 |
| sample 2 | 2.3 | 5.4 | 0.5 |
| ... |  | ... |  |
| sample n | 0.9 | 1.9 | 0.1 |


| Intervention \#1 |  | $\mathrm{X}_{1} \quad \mathrm{X}_{2}$ | $\mathrm{X}_{3}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| sam\| | Interventio | ion \#2 $\mathrm{X}_{1}$ | $\mathrm{X}_{2}$ | $\mathrm{X}_{3}$ |  |
| sam\| | sample ${ }^{\text {I }}$ | Intervention \#3 | $\mathrm{X}_{1}$ | $\mathrm{X}_{2}$ | $\mathrm{X}_{3}$ |
|  | sample | sample 1 | 1.2 | 2.6 | 0.2 |
| sam\| | ... | sample 2 | 2.3 | 5.4 | 0.5 |
|  | sample | ... |  | $\ldots$ |  |
|  |  | sample n | 0.9 | 1.9 | 0.1 |



How to recover the (CP)DAG using a dataset $\mathcal{D}$ ?

## Constraint-based methods

## Step 1: Identify the skeleton

For each pair of nodes $X \& Y$, and
$\mathbf{A} \subseteq \mathbf{V} \backslash\{X, Y\}$, test if $X \Perp_{\mathcal{D}} Y \mid \mathbf{A}$.
If there is no set $\mathbf{A}$ s.t. $X \Perp_{\mathcal{D}} Y \mid \mathbf{A}$, then add an edge $X-Y$.


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Step 2: Identify the $v$-structures
For each structure $X-Z-Y$ with no edge between $X \& Y$, orient $X \rightarrow Z \leftarrow Y$ iff $Z \notin \mathbf{A}$, where $\mathbf{A}$ is such that $X \Perp_{\mathcal{D}} Y \mid \mathbf{A}$.


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IC Algorithm

## Constraint-based methods

## Step 2': Additional orientations

Use Meek's orientation rules to
orient some of the remaining edges.

$\Downarrow$

$\Downarrow$

$\Downarrow$


Rule 1


Rule 2


Rule 3

$\Downarrow$


Rule 4

## Score-based methods

- Idea: treat the problem of learning the structure of the DAG as a model selection problem

```
\mp@subsup{max}{\mathcal{G}\in\textrm{DAG}}{\operatorname{score}(\mathcal{G}|\mathcal{D})}\mathbf{})
\mathcal{G}\in\textrm{DAG}
```

Recall: choices of scores

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Recall: choices of scores
■ Likelihood score:

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\operatorname{score}_{L}(\mathcal{G} \mid \mathcal{D})=\log p\left(\mathcal{D} \mid \hat{\theta}_{\mathcal{G}}^{\mathrm{MLE}}, \mathcal{G}\right)
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■ Bayesian score:

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\operatorname{score}_{\mathcal{B}}(\mathcal{G} \mid \mathcal{D})=\log p(\mathcal{D} \mid \mathcal{G})+\log p(\mathcal{G})
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■ Bayesian score:

$$
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■ Bayesian Information Criterion (BIC):

$$
\operatorname{score}_{\text {BIC }}(\mathcal{G} \mid \mathcal{D})=\log p\left(\mathcal{D} \mid \hat{\theta}_{\mathcal{G}}^{\mathrm{MLE}}, \mathcal{G}\right)-\frac{\log N}{2} \operatorname{Dim}[\mathcal{G}]
$$

## Score-based methods

```
max }\operatorname{score}(\mathcal{G}|\mathcal{D}
\mathcal{G}\in\textrm{DAG}
```

- How to search over the space of DAGs?
- The number of DAGs over $n$ nodes is super-exponential in $n: 2^{\Theta\left(n^{2}\right)}$.


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The number of DAGs over $n$ nodes is super-exponential in $n: 2^{\Theta\left(n^{2}\right)}$.

## Theorem

Let $G_{\leq d}=\{\mathcal{G}$ a $D A G \mid$ every node has at most d parents $\}$. Finding a $D A G$ in $G_{\leq d}$ that maximizes a score is NP-hard for $d \geq 2$.

## Score-based methods

```
max }\operatorname{score}(\mathcal{G}|\mathcal{D}
G\inDAG
```

■ How to search over the space of DAGs?

■ The number of DAGs over $n$ nodes is super-exponential in $n: 2^{\Theta\left(n^{2}\right)}$.

## Theorem

Let $G_{\leq d}=\{\mathcal{G}$ a $D A G \mid$ every node has at most d parents $\}$. Finding a DAG in $G_{\leq d}$ that maximizes a score is NP-hard for $d \geq 2$.

■ Heuristic solutions:
■ Greedy algorithms: Hill climbing, GES

- Genetic algorithms

■ Constrained continuous optimization: NOTEARS, Gran-DAG, DCDI, etc...

