

CAUSAL INFERENCE AND MACHINE LEARNING

(or a crash course on causality for ML practitioners)

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About this talk

The relationship between causality and artificial intelligence can be seen from two points of view: how causality can help solve some of the current problems of AI and how causal inference can leverage machine learning techniques. In this course we will review the two points of view with special emphasis on examples and practical cases.

01 | **Introduction**
Observational and Interventional
Distributions. Causal Thinking.

02 | **Causal Graphs**
Do Calculus

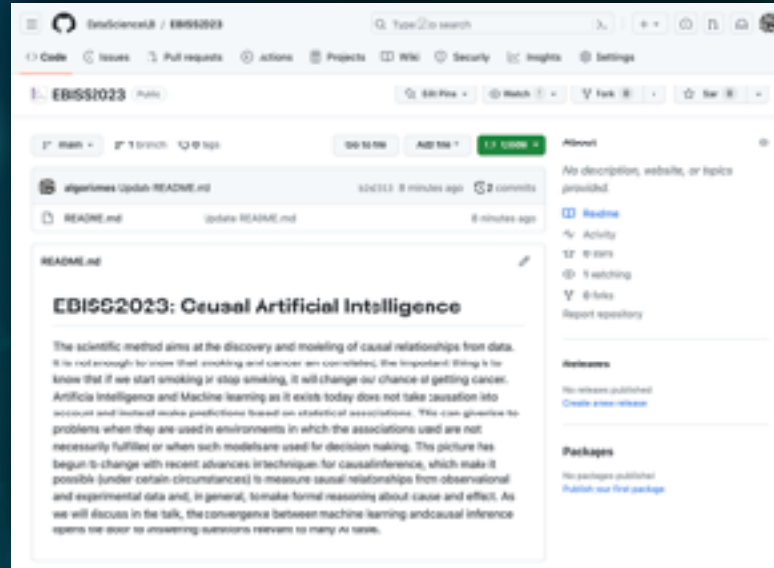
03 | **Estimands**
From Metalearners to Counterfactuals

04 | **Causal Machine Learning**
Supervised and Reinforcement Learning

05 | **Practical Causal Inference**
Example

About the course

The relationship between causality and artificial intelligence can be seen from two points of view: how causality can help solve some of the current problems of AI and how causal inference can leverage machine learning techniques. In this course we will review the two points of view with special emphasis on examples and practical cases.




<https://github.com/DataScienceUB/EBISS2023>

Introduction

Observational and Interventional Distributions.
Causal Thinking.

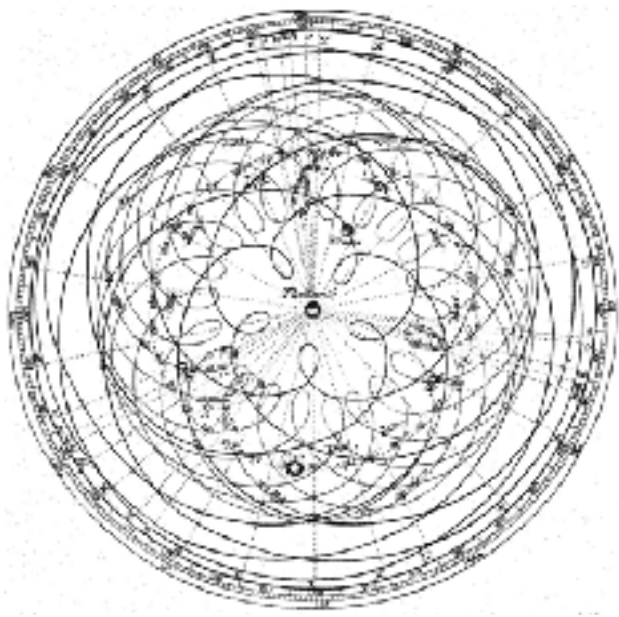
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A night sky filled with stars and the Milky Way galaxy. In the lower-left foreground, the silhouette of a wind turbine is visible, with its central hub illuminated by two red lights. The horizon is a dark, silhouetted line.

Can we predict what we see in the sky?

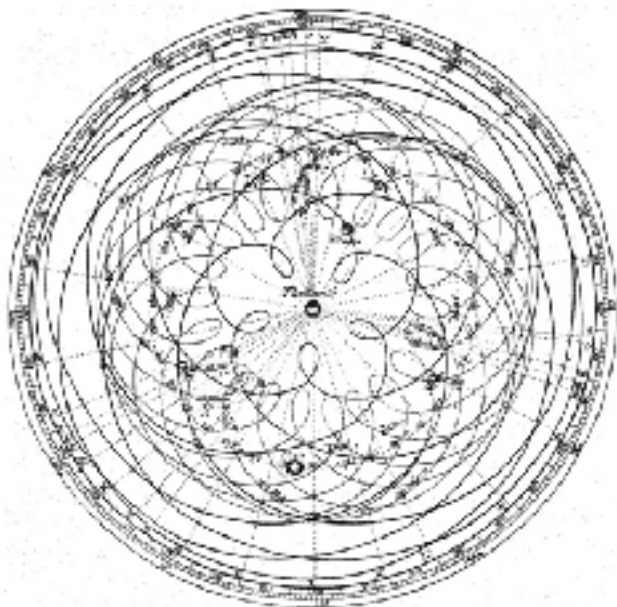
ML Mindset = Gathering data + Building a model

Predicting observations vs predicting interventions



Ptolemaic model (circular orbits, geocentric)
100 AD

Predicting observations vs predicting interventions



Ptolemaic model (circular orbits, geocentric)
100 AD



Copernican model (heliocentric, harmonious = fewer causes)
1543 AD

Predicting observations vs predicting interventions

Ptolomeus and Copernicus build models with **high predictive power**. (Statistical/ML Mindset)



But they both were **“false”!**
(Causal/Scientific Mindset)



Predicting observations vs predicting interventions



- Predictions were not false in the “predictive” (Statistical/ML) sense, but in the “**interventional**” (scientific/causal) sense.
- What about aliens destroying (**intervening**) a planet instantly?

Predicting observations vs predicting interventions

Statistical inference and machine learning models are designed to predict **observations** (observational data) in **stable** environments.

They are based on analyzing data to answer **associative questions**.

Predicting observations vs predicting interventions



the weather
What can I say about Y given
that I have observed X ?
umbrellas

What can I say about X given
that I have observed Y ?

Predicting observations vs predicting interventions



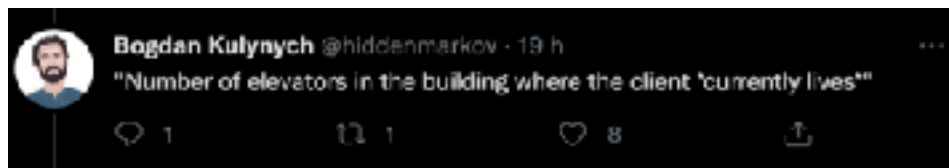
Modern ML models are very good at discovering and using associative structures in (X, Y) for predicting the value of Y in **pure observational settings**.

But predictive models can be accurate without being “correct” in **interventional settings**.

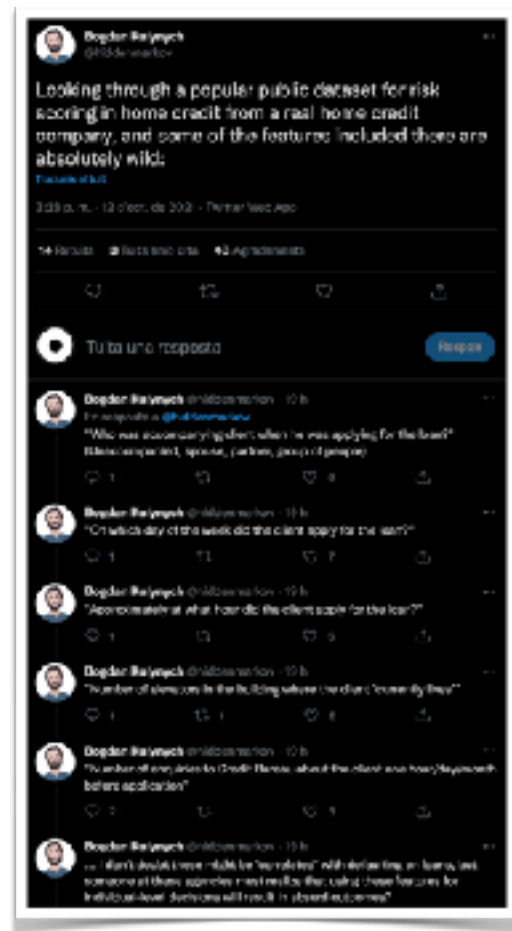
AI sucks...
or how CI can help ML

AI sucks...

AI based **high stake decisions**
(risk scoring in home credit)



Use of spurious correlations.



AI sucks...

Image classification



(A) **Cow: 0.99**, Pasture: 0.99, Grass: 0.99, No Person: 0.98, Mammal: 0.98



(B) No Person: 0.99, Water: 0.98, Beach: 0.97, Outdoors: 0.97, Seashore: 0.97



(C) No Person: 0.97, **Mammal: 0.96**, Water: 0.94, Beach: 0.94, Two: 0.94

Use of spurious correlations.

AI sucks...

Spoiler:

A **spurious correlation** is a correlation that **results** from a **non-causal path**.

$$P(Y | X) - P(Y | do(X))$$

AI sucks...

- We want to minimize the **Empirical Risk**.
- We want to maximize **robustness** against changes in data distribution.
- We want to maximize **robustness** against adversarial attacks.
- We want to be able of **explaining** my predictions to different stakeholders.
- We want to measure and mitigate harmful biases (**discrimination**).
- We want to use predictions to support a **decision** that may influence the outcome they aim to predict (performative predictions).
- Etc.

AI sucks...

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All these considerations involve causal thinking.

Causal Data Science

Causal Data Science

OBSERVATIONAL DATASET (passive observation of the world)

	Sex	Race	Height	Income	Marital Status	Years of Educ.	Liberal-ness
R1001	M	1	70	50	1	12	1.73
R1002	M	2	72	100	2	20	4.53
R1003	F	1	55	250	1	16	2.99
R1004	M	2	65	20	2	16	1.13
R1005	F	1	60	10	3	12	3.81
R1006	M	1	68	30	1	9	4.76
R1007	F	5	66	25	2	21	2.01
R1008	F	4	61	43	1	18	1.27
R1009	M	1	69	67	1	12	3.25

Let's consider some different features in this dataset, (X, Y, Z) .

Which can of questions can we answer from this dataset?

Causal Data Science

X Y Z

	Sex	Race	Height	Income	Marital Status	Years of Educ.	Liberal-ness
R1001	M	1	70	50	1	12	1.73
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R1009	M	1	69	67	1	12	3.25

Causal Data Science

Q1: Which is the *expected income* Y that would have been observed if an individual had $X = x$ and $Z = z$?

Association (or prediction) is using data to map some features of the world (the inputs) to other features of the world (the outputs) based on the observed $p(X, Y, Z)$. For example, $\mathbb{E}(Y | X, Z)$.

All we need to do prediction is a dataset sampled from $p(X, Y, Z)$ and some inference tools (statistical inference & machine learning).

Causal Data Science

Q1: Which is the *expected income* Y that would have been observed if an individual had $X = x$ and $Z = z$?

Mapping observed inputs to observed outputs is a **natural candidate for automated data analysis** because this task only requires

- 1) a large **dataset** with inputs and outputs, 2) an **algorithm** that establishes a mapping between inputs and outputs, and 3) a metric to assess the performance of the mapping, often based on a gold standard.

Causal Data Science

Causal effect of Race on Income

Q2: Estimate the **mean income** Y that would have been observed if all individuals had ($X = 1$) vs. if they had ($X \neq 1$).

Causal Inference is using data to **predict certain features of the world if the world had been different in some aspect**. We cannot get these data by passive observation of the world! The world was real only in a way!

Causal Data Science

Causal effect of Race on Income

Q2: Estimate the **mean income** Y that would have been observed if all individuals had ($X = 1$) vs. if they had ($X \neq 1$).

Answers to causal questions cannot be derived exclusively from $p(X, Y, Z)$. Answering a causal question (yes, sometimes is possible!) typically requires a combination of data, analytics, and **expert causal knowledge**.

Causal Data Science

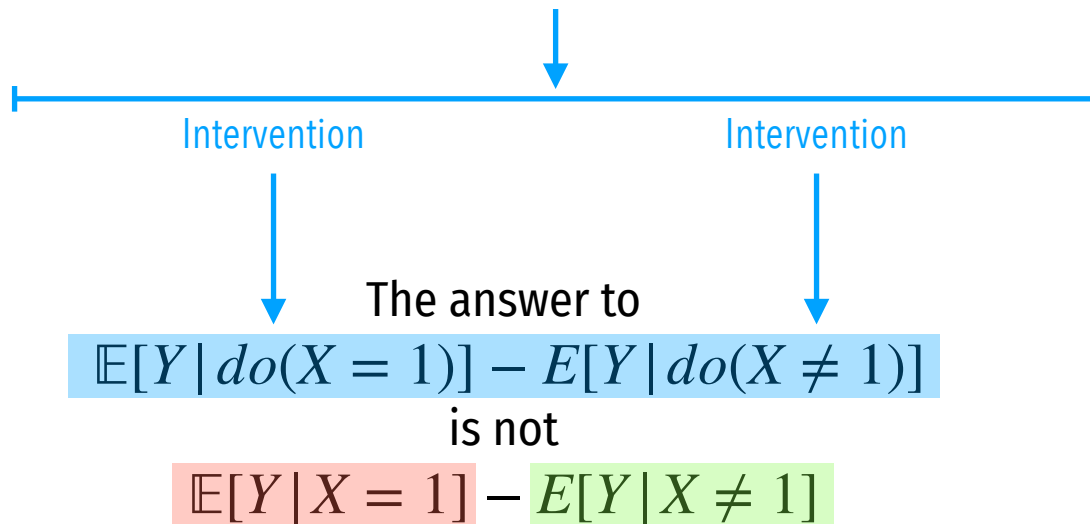
	Sex	Race	Height	Income	Marital Status	Years of Educ.	Liberalness
R11001	M	1	70	50	1	12	1.73
R11002	M	2	72	100	2	20	1.53
R11003	F	1	55	250	1	16	2.99
R11004	M	2	65	30	2	16	1.13
R11005	F	1	60	10	3	12	1.81
R11006	M	1	68	30	1	9	1.76
R11007	F	2	66	25	2	21	2.11
R11008	F	1	61	45	1	18	1.27
R11009	M	1	69	60	1	12	1.25

$$\mathbb{E}[Y | do(X = 1)] - \mathbb{E}[Y | do(X \neq 1)]?$$

Causal effect of Race on Income

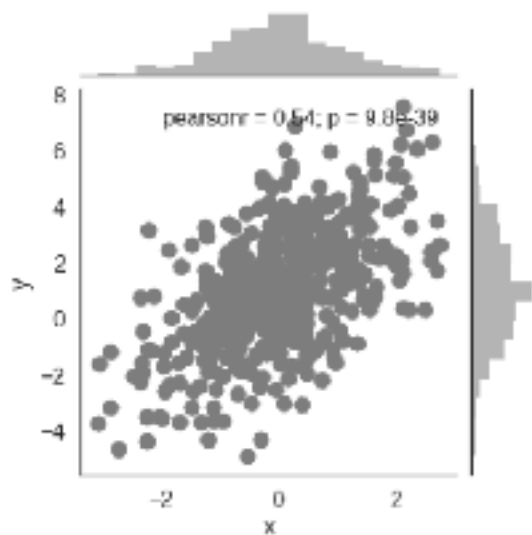
Causal Data Science

Causal effect of Race on Income



Causal Data Science

In order to understand what is $p(Y | do(X = x))$, let's suppose I have observed $p(X, Y)$.



This is all we need to compute $p(Y | X)$. We can give an answer to any associational question.

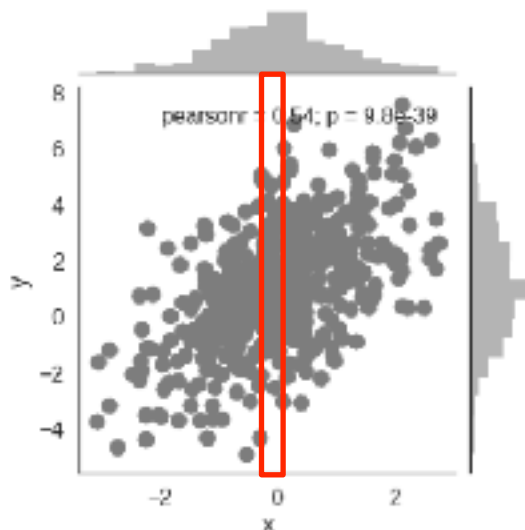
For example:

- What is the expected value of Y if we observe $X = 0$, $\mathbb{E}(Y | X = 0)$? (**Regression**)
- What is the expected MAX/MIN/MEDIAN value of Y if we observe $X = 0$? (**Quantile regression**)
- Etc.

Causal Data Science

- What is the expected value of Y if we observe $X = 0$, $\mathbb{E}(Y | X = 0)$? (**Regression**)

$$p(Y | X = 0)$$



<https://www.inference.vc/causal-inference-2-illustrating-interventions-in-a-toy-example/>

Causal Data Science

OBS

$$p(Y | X)$$

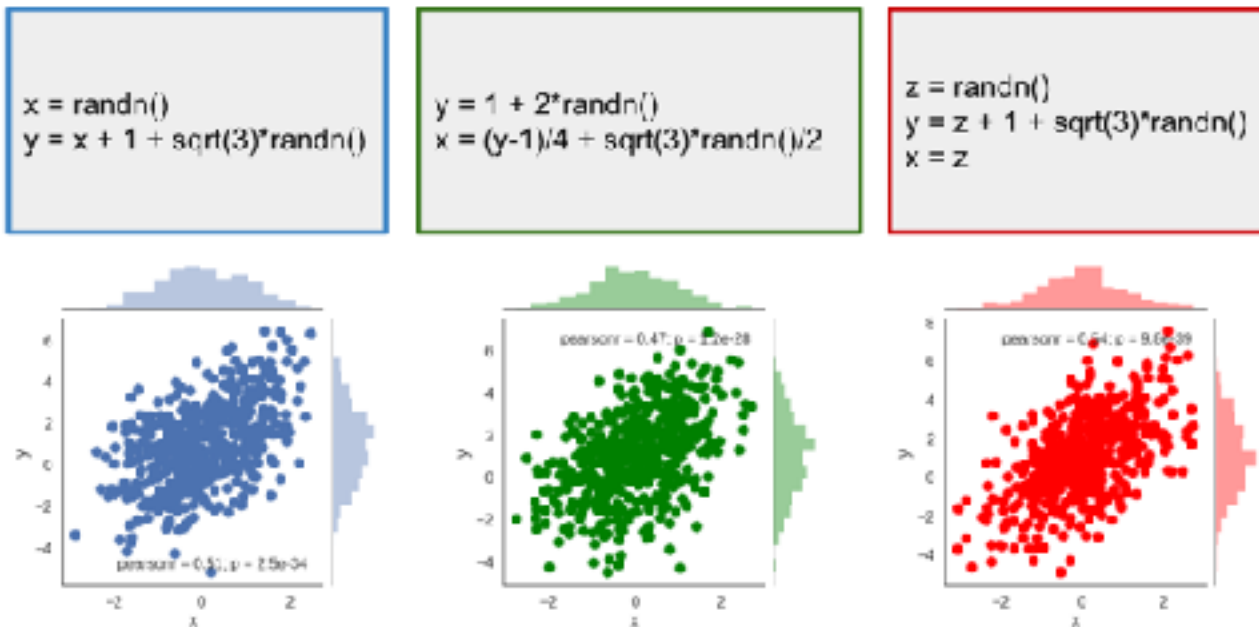
INT

$$p(Y | do(X = x))$$

OBS and INT are not generally the same!
Let's consider three generative models
corresponding to the same $p(X, Y)$

Causal Data Science

Generative Models



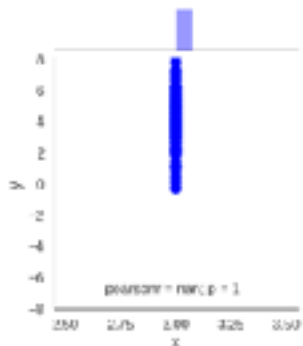
Based on the joint distribution the three scripts are indistinguishable.

<https://www.inference.vc/causal-inference-2-illustrating-interventions-in-a-toy-example/>

Causal Data Science

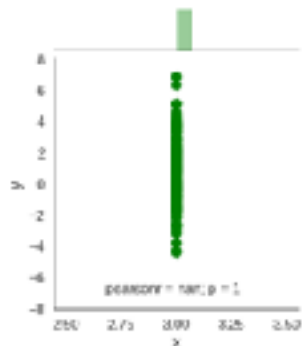
Intervention $p(Y | do(X = 3))$

```
x = randn()
x = 3
y = x + 1 + sqrt(3)*randn()
x = 3
```



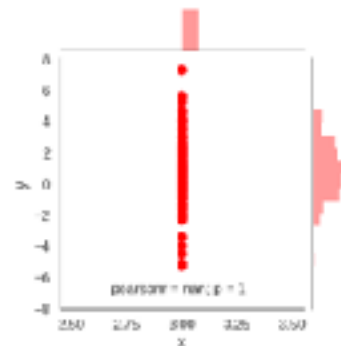
$p(Y | do(X = 3))$

```
y = 1 + 2*randn()
x = 3
x = (y-1)/4 + sqrt(3)*randn()/2
x = 3
```



$p(Y | do(X = 3))$

```
z = randn()
x = 3
x = z
x = 3
y = z + 1 + sqrt(3)*randn()
x = 3
```



$p(Y | do(X = 3))$

The joint distribution of data $p(X, Y, Z)$ alone is insufficient to predict behavior under interventions.

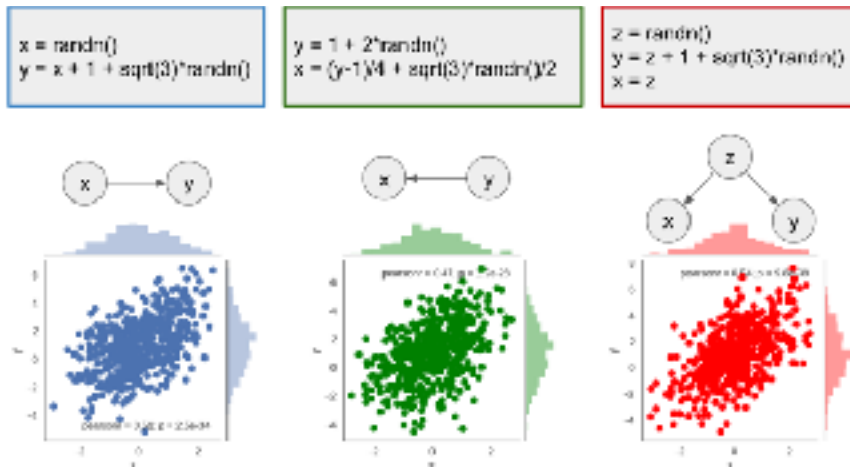
<https://www.inference.vc/causal-inference-2-illustrating-interventions-in-a-toy-example/>

Causal Data Science

Generative Models

An intervention can be understood as a **modification of the generative model of the data, producing a different probability distribution:**

$$p(\text{do}(X = 3), Y, Z)$$



Directed Acyclic Graphs (DAG).

No assumptions about the exact form of the functional relationships are needed. The only requirement is that causal relationships are **acyclic**.

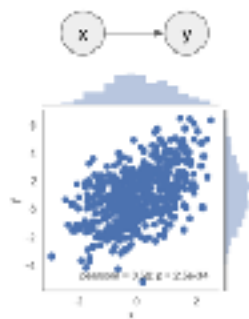
Causal Data Science

Generative Models

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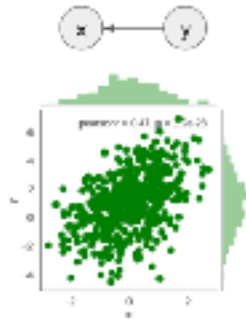
$p(\text{do}(X = 3), Y, Z)$

```
x = randn()
y = x + 1 + sqrt(3)*randn()
```



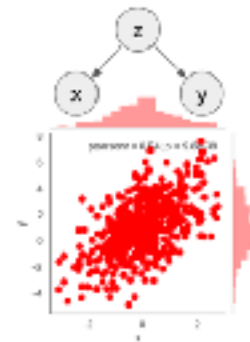
X is the cause of Y

```
y = 1 + 2*randn()
x = (y-1)/4 + sqrt(3)*randn()/2
```



Y is the cause of X

```
z = randn()
y = z + 1 + sqrt(3)*randn()
x = z
```



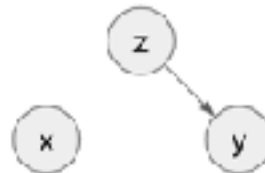
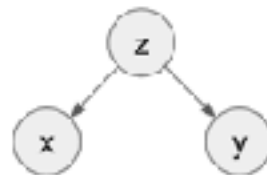
X and Y are not causally related (but they are associated!)

<https://www.inference.vc/causal-inference-2-illustrating-interventions-in-a-toy-example/>

Causal Data Science

What is an intervention?

Graphically, to **simulate the effect of an intervention**, you **mutilate** the graph by removing all edges that point into the variable on which the intervention is applied, in this case x .



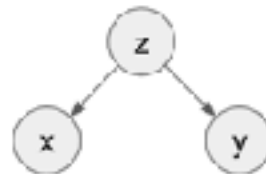
$$P(Y | do(X = x)) = P(Y | X = x)$$

$$P(Y | do(X = x)) = P(Y)$$

$$P(Y | do(X = x)) = P(Y)$$

Causal Data Science

What is an intervention?



$$P(Y | do(X = x)) = P(Y | X = x)$$

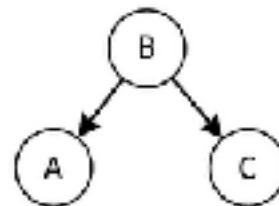
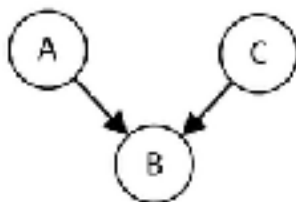
$$P(Y | do(X = x)) = P(Y)$$

$$P(Y | do(X = x)) = P(Y)$$

Just by looking at the causal diagram, we are now **able to predict** how the scripts are going to behave under the intervention $X = 3$.

Causal Data Science

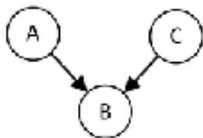
- The primary language for modeling causal mechanisms and expressing our assumptions is the **language of causal graphs**.



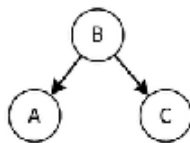
- Causal graphs encode our domain knowledge about the causal mechanisms underlying a system or phenomenon under study.
- Causal graphs are assumed to be **acyclic**. This is why they are called **DAGs (Directed Acyclic Graphs)**.

Causal Data Science

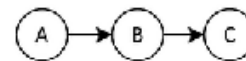
- Fundamentally, a causal graph describes a **non-parametric data-generating process** over its nodes.
- By specifying independence and dependence between the nodes, the graph constrains relationship between generated variables corresponding to those nodes.



B is a **collider** for A and C
A and B create an **inverted fork** to B
A and C are independent



B is a **confounder**
B creates a **fork** to A and C
A and C are not independent.
A and C are independent
conditional on B



B forms a **chain** from A to C
A and C are conditionally
independent given B

Causality Theory

A DAG provides enough extra-data information
(in terms of conditional independences)
to answer many causal queries,
even with the data generating process hidden.

Causal Thinking

Basic Concepts: Causal Effect

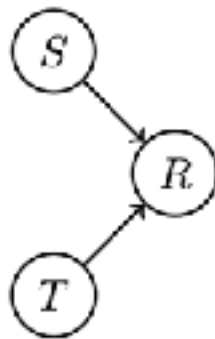
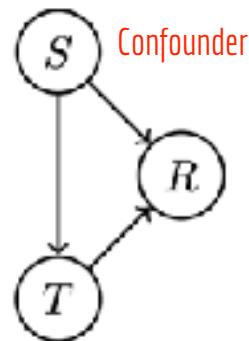
- The **average treatment/causal effect** (ATE) of T on R :

$$\mathbb{E}[R \mid do(T = 1)] - \mathbb{E}[R \mid do(T = 0)]$$

- The **conditional average treatment/causal effect** (CATE):

$$\mathbb{E}[R \mid do(T = 1), S] - \mathbb{E}[R \mid do(T = 0), S]$$

Symptoms, Treatment, Recovery

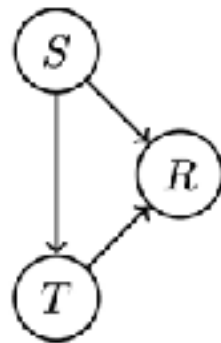


Intervened graph
 $do(T = t)$

Basic Concepts: Counterfactual

- **Counterfactuals**: hypothetical result that an intervention may have on an individual for whom we have already observed a different *factual* outcome.
 - Counterfactuals allow us to mix factual information with alternative scenarios.
 - Explainability and Fairness applications.
- Given a certain patient with symptoms s , who was not given a treatment and didn't recover, **would they have recovered had we given them the treatment?**
- The **individual treatment/causal effect** (ITE):

$$\mathbb{E}[R_i | do(T_i = 1)] - E[R_i | do(T_i = 0)]$$



Causal Thinking Process

1. Asking a causal/counterfactual query (ATE, CATE, ITE,...)
2. Gathering knowledge from experts
3. Building a DAG
4. **Identifying** the causal query
5. Gathering data.
6. Computing and estimand/building a SCM
7. Answering the causal/counterfactual query

Asking a causal query

Salary Dataset

→ Variables:

- **Gender.**
- **Department.**
- **Benefits.**
- **Seniority.**
- **Salary.**
- **Termination.**

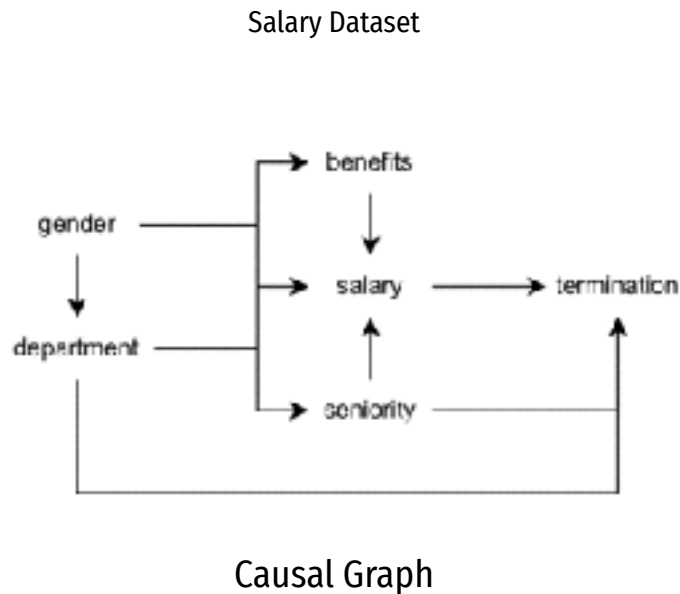
→ Possible interesting queries:

- $\mathbb{E}[S \mid do(G = male)] - \mathbb{E}[S \mid do(G = female)]:$
ATE of gender (binary) on salary.
- $\mathbb{E}[S_i^* \mid do(G_i^* = male), G_i = female, S_i = s]:$
given a particular woman i with salary s , **counterfactual** salary when male.

Gathering knowledge and data

→ We need to find the corresponding causal graph.

- Causal Discovery algorithms.
- Domain Experts.
- Experiments.



Identifying a causal query

There are two ways to measure the **causal relationship** between two variables, S and G :

1. The easiest way is an **intervention** in the real world: You **randomly** force G to have different values and you measure S .

This is what we do in Randomized Clinical Trial (RCT) or in an A/B Test.

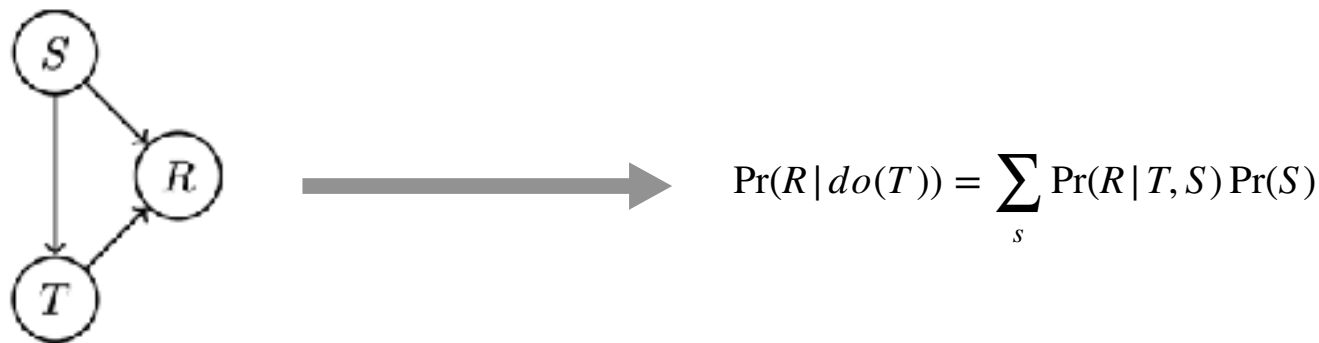
This is not always feasible (because of **practical, ethical** or **economical** reasons)

Identifying a causal query



2. If the query is **identifiable** we can compute an estimand.

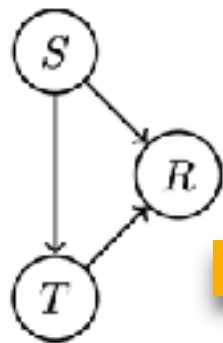
For example, in this case, **do-calculus** allows us to massage $p(S, R, T)$ until we can express $p(R | do(T))$ in terms of various marginals, conditionals and expectations under $p(S, R, T)$.



Identifying a causal query

2. If the query is **identifiable** we can compute an estimand.

For example, in this case, **do-calculus** allows us to massage $p(S, R, T)$ until we can express $p(R \mid do(T))$ in terms of various marginals, conditionals and expectations under $p(S, R, T)$.



It only depends on the causal graph!

$$\Pr(R \mid do(T)) = \sum_s \Pr(R \mid T, S) \Pr(S)$$

Identifying the causal query

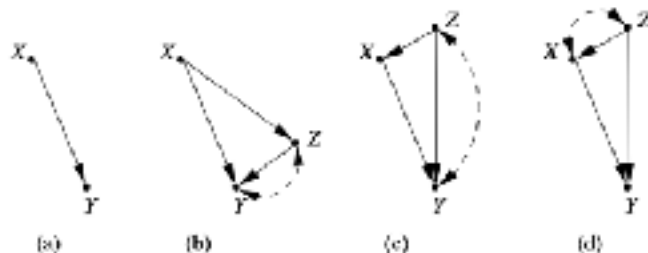
- Causal query \mathcal{Q} , e.g., $\mathcal{Q} := \mathbb{E}[S \mid do(G = male)] - \mathbb{E}[S \mid do(G = female)]$.
 - It contains interventional terms, so we can't use the dataset directly.
 - **Identification**: transform every interventional term into an expression using only observational terms \Rightarrow **estimand**.
 - There are **automated algorithms** that do this work for us.

Identifying the causal query

Salary Dataset

Given a causal query for a certain DAG, we say it is **identifiable** if we can derive an statistical estimand (**only using observational terms**) for this query using the rules of **do-calculus**.

The **do-calculus** is an axiomatic system for replacing probability formulas containing the *do* operator with ordinary conditional probabilities. It consists of three axiom schemas that provide **graphical criteria** for when certain substitutions may be made.



Causal graphs where $F(y|do(x))$ is identifiable

Source: Complete Identification Methods for Causal Inference, PhD Thesis, University of California. I.Shpitzer

Dashed lines correspond to **unobserved confounders**, associations produced by unobserved variables.

Identifying the causal query

The screenshot shows the GitHub repository page for 'causaleffect' by user 'pedemonte96'. The repository is public and has 3 watchers, 10 stars, and 3 forks. The main branch is 'main'. The repository contains a table of files and folders with their commit history. The right sidebar shows the 'About' section, which describes the package as a Python package to compute conditional and non-conditional causal effects. It also shows the 'Releases' section with a single release 'v0.0.2' and the 'Packages' section, which is currently empty.

File/Folder	Description	Commit Date
pedemonte96 Create CONTRIBUTING.md		3 months ago
.github/ISSUE_TEMPLATE	Update issue templates	3 months ago
causaleffect	improved version c-separation	4 months ago
documentation	improved documentation	4 months ago
examples	fixed example and added documentation	4 months ago
images	updated README	4 months ago
tests	add all tests	3 months ago
.gitignore	causal effect add	4 months ago
CODE_OF_CONDUCT.md	Create CODE_OF_CONDUCT.md	3 months ago
CONTRIBUTING.md	Create CONTRIBUTING.md	3 months ago
LICENSE	Create LICENSE	3 months ago
README.md	removed sysair dependency	4 months ago
pyproject.toml	build done	4 months ago
requirements.txt	removed sysair dependency	4 months ago
setup.py	Update setup.py	3 months ago

About
Python package to compute conditional and non-conditional causal effects.
Roadmap
MIT License

Releases
v0.0.2 (Latest)
on 17 Jan
+ 1 release

Packages
No packages published
Publish your first package

Languages
Python 100%

Identifying the causal query

```
import causalEffect

G = causalEffect.createGraph(['X<->Y', 'Z->Y', 'X->Z', 'W->Z', 'W->X'])
causalEffect.plotGraph[G]
```

```
P = causalEffect.EE(['Y'], ['X'], G)
P.prettyLatex()
```

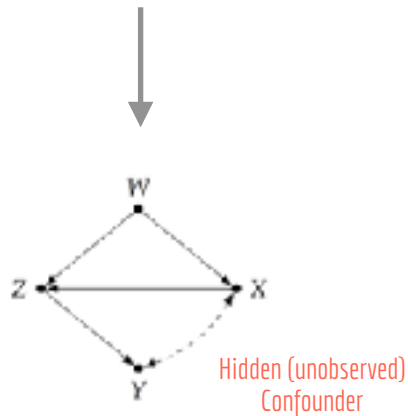
The code above computes the causal effect, and returns a string encoding the distribution in LaTeX notation:

```
"1sum_w, z)P(w,P(z|w, x))P(x|1sum_x)P(y|w, x, z)P(z|w, x)"
```

This string, in LaTeX, is

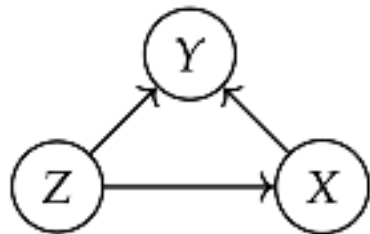
$$\sum_{w,z} P(w)P(z|w, x) \left(\sum_x P(x|w)P(y|w, x, z) \right)$$

$p(X, W, Z, Y)$



Building a causal model

- Once we have an estimand, we need to build **models** to use it for our estimation.
 - $\mathcal{Q} := \mathbb{E}[Y \mid do(X = x)] = \mathbb{E}_Z[\mathbb{E}_{Y|x,Z}[Y]]$.
 - We need to model the $f(x, Z) := \mathbb{E}_{Y|x,Z}[Y]$ term.
 - If Y is binary, with a ML classifier.
 - If Y is continuous, with a ML regressor.



Answering the query

→ Now that we have our ML model, we can follow the **estimand** formula:

$$\rightarrow \mathcal{Q} := \mathbb{E}[Y \mid do(X = x)] = \mathbb{E}_Z[\mathbb{E}_{Y|x,Z}[Y]].$$

→ The \mathbb{E}_Z expectation can be estimated by averaging dataset samples:

$$\mathcal{Q} = \mathbb{E}_Z[\mathbb{E}_{Y|x,Z}[Y]] \approx \frac{1}{n} \sum_{i=1..N} f(x, z_i).$$

Answering the query

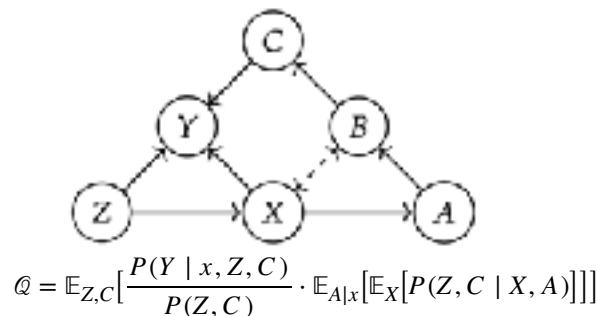
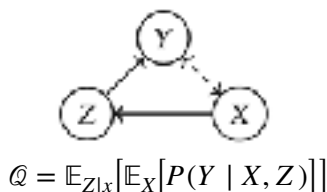
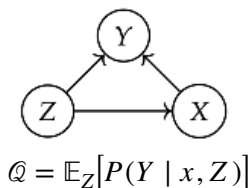
→ The **estimand-based** approach:

1. Derive an **estimand** for our graph & query.
2. Train ML **models** for the terms we need to compute.
3. Follow the estimand formula to obtain an **estimation**.

Answering the query

→ However, depending on the graph, even the same query results in different estimands.

→ $P(Y \mid do(X = x))$:



Example

From “Causal Inference in AI Education: A Primer”

Example 3.1. AdBot Consider an online advertising agent attempting to maximizing clickthroughs, with $X \in \{0, 1\}$ representing two ads, $Y \in \{0, 1\}$ whether or not it was clicked upon, and $Z \in \{0, 1\}$ the sex of the viewer. A marketing team collects the following data on purchases following ads shown to focus groups to be used by AdBot:

	Ad 0	Ad 1
Male	108/120 (90%)	340/400 (85%)
Female	266/380 (70%)	65/100 (65%)
Total	374/500 (75%)	405/500 (81%)

Table 1. Clickthroughs in the AdBot setting striated by the ad shown to participants in a focus group, and the sex of the viewer.

If the sex of a viewer is not know, which ad is the best choice?

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Simpson's paradox

	Ad 0	Ad 1
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Table 1. Clickthroughs in the AdBot setting striated by the ad shown to participants in a focus group, and the sex of the viewer.

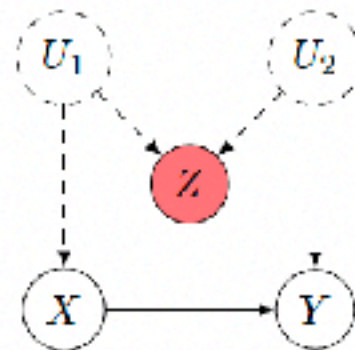
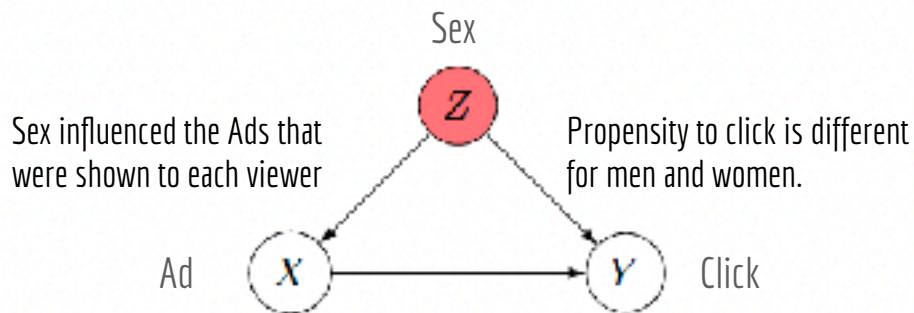
If the sex of a viewer is not know, which ad is the best choice?

Example

From “Causal Inference in AI Education: A Primer”

If the sex of a viewer is not known, which ad is the best choice?

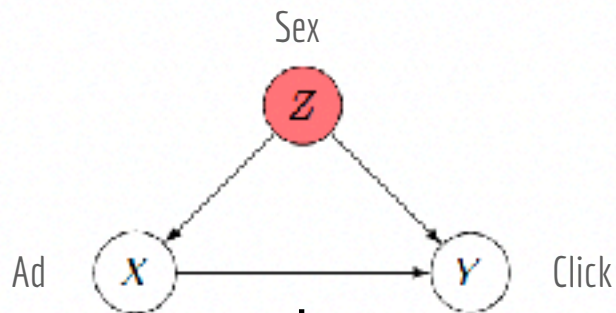
These are two different causal stories:



Relevant question: $p(Y | \text{do}(X_0)) > p(Y | \text{do}(X_1))$?

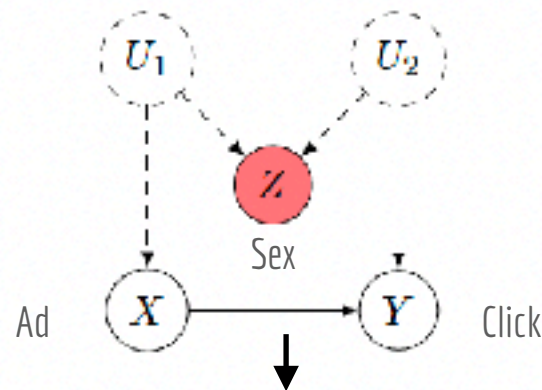
Example

From “Causal Inference in AI Education: A Primer”



```
1 G = causaleffect.createGraph(['X->Y', 'Z->Y', 'Z->X'])  
2 P = causaleffect.ID(['Y'], ['X'], G)
```

$$p(Y|\text{do}(X)) = \sum_Z P(Y|X,Z)P(Z)$$



```
1 G = causaleffect.createGraph(['U1->X', 'U2->Z', 'Z->X', 'Z->Y', 'X->Y'])  
2 P = causaleffect.ID(['Y'], ['X'], G)  
3 P.printLatex()
```

$$p(Y|\text{do}(X)) = P(Y|X)$$

Example

From “Causal Inference in AI Education: A Primer”

Example 3.1. AdBot Consider an online advertising agent attempting to maximizing clickthroughs, with $X \in \{0, 1\}$ representing two ads, $Y \in \{0, 1\}$ whether or not it was clicked upon, and $Z \in \{0, 1\}$ the sex of the viewer. A marketing team collects the following data on purchases following ads shown to focus groups to be used by AdBot:

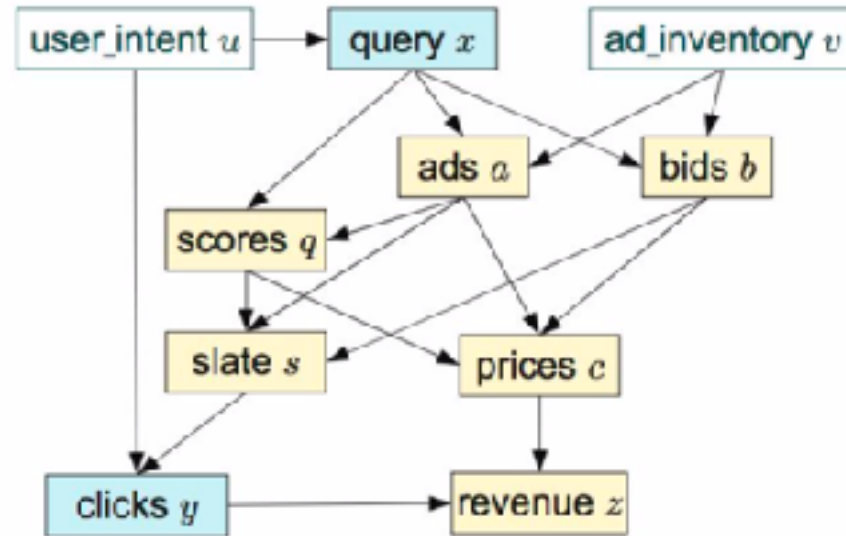
If (a) is our explanation of the data, then AdBot should display Ad0.

If (b) is our explanation of the data, then AdBot should display Ad1.

	Ad 0	Ad 1
Male	108/120 (90%)	340/400 (85%)
Female	266/380 (70%)	65/100 (65%)
Total	374/500 (75%)	405/500 (81%)

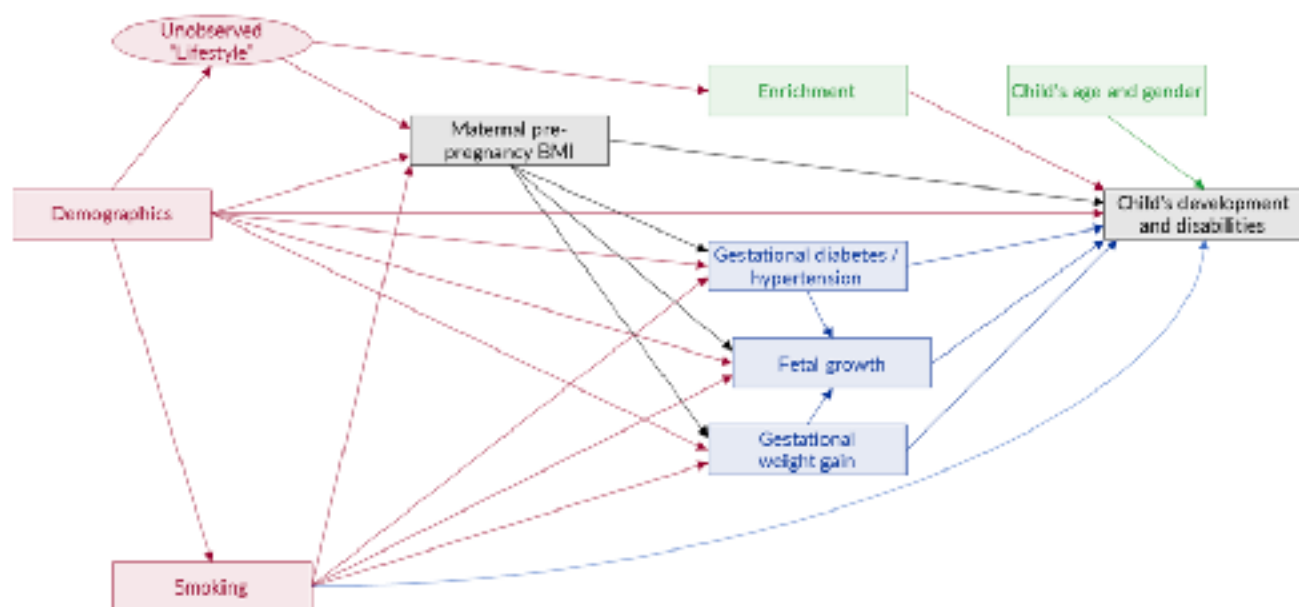
$$\left[\begin{array}{l} p(Y | \text{do}(X)) = \sum_z P(Y | X, Z)P(Z) \\ p(Y | \text{do}(X)) = P(Y | X) \end{array} \right.$$

Example



Bottou, Léon, et al. "Counterfactual reasoning and learning systems: the example of computational advertising." *The Journal of Machine Learning Research* 14.1 (2013): 3207-3260.

Example



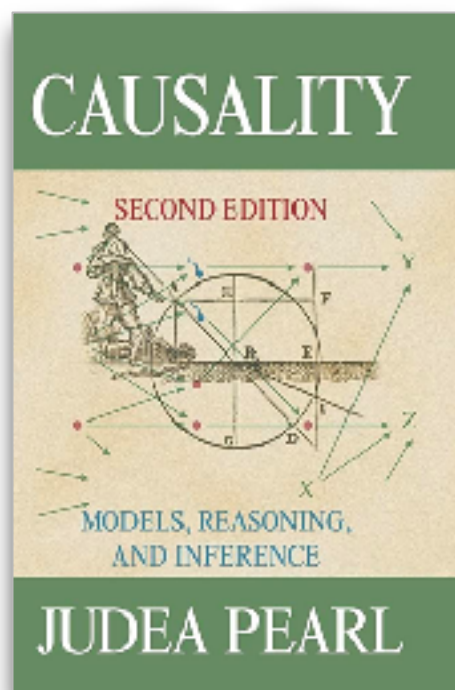
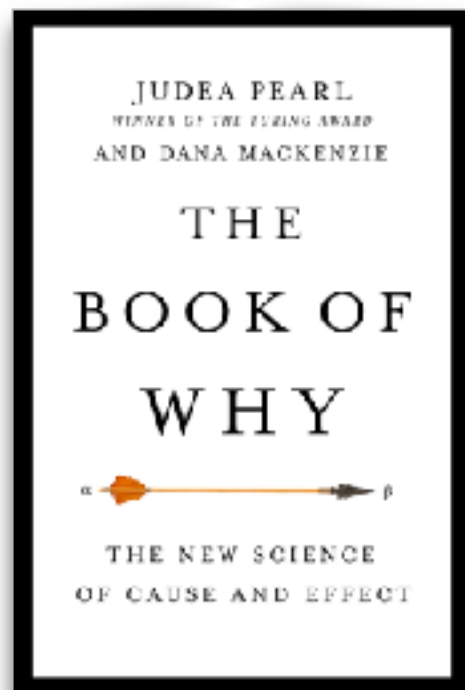
ADAPTED FROM: Hinkle SN, Sharma AJ, Kim SY, Schieve LA. Maternal prepregnancy weight status and associations with children's development and disabilities at kindergarten. *Int J Obes (Lond)*. 2013;37(10):1344-51. DOI: 10.1038/ijo.2013.128 (Figure 1). Freely available at: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4407562>

Example



REPRODUCED UNDER CC-BY 4.0 LICENSE FROM: [Vandij, Offedal B, Krog NH, et al. Road traffic noise and registry-based use of sleep medication. *Environ Health*. 2017;16(1):110. DOI: 10.1186/s12910-017-0330-5 (Figure S1). Freely available at <https://www.doi.org/10.1186/s12910-017-0330-5>

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Which causal inference book you should read

Flowchart

<https://www.bradynear.com/which-causal-inference-book>

