DDA4210/AIR6002 Advanced Machine Learning
Lecture 09 Causal Machine Learning

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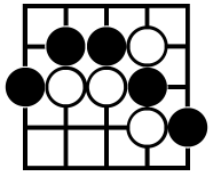
Motivation

Trustworthy ML

AI Tools are Everywhere

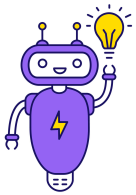
AI/ML Methods/Predictions

AlphaGo → Suggested Moves



OpenAI → Suggested Strategies

GPT-4 → AI Assistants



Review

First Part of This Course:

- Ensemble
- Learning Theory
- GNN
- Generative Models

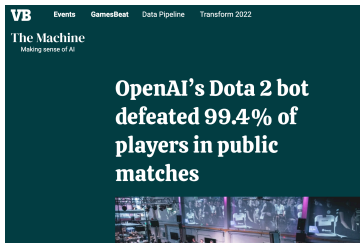
Focus more on a single merit: accuracy

AI Tools Are NOT Always Trustworthy

Blackbox AI Tools/Imperfect Predictions

AlphaGo → Suggested Moves

OpenAI → Suggested Strategies



Defeated by 0.6 % players using adversarial strategies

ChatGPT → AI Assistants

ChatGPT版必应疑似「发疯」，微软紧急限制回答数目，植入广告赚钱提上日程

Image sources: New Bing

A Toy Example

GPT-4 Technical Report

OpenAI*

Abstract

We report the development of GPT-4, a large-scale, multimodal model which can accept image and text inputs and produce text outputs. While less capable than humans in many real-world scenarios, GPT-4 exhibits human-level performance on various professional and academic benchmarks, including passing a simulated bar exam with a score around the top 10% of test takers. GPT-4 is a Transformer-based model pre-trained to predict the next token in a document. The post-training alignment process results in improved performance on measures of factuality and adherence to desired behavior. A core component of this project was developing infrastructure and optimization methods that behave predictably across a wide range of scales. This allowed us to accurately predict some aspects of GPT-4's performance based on models trained with no more than 1/1,000th the compute of GPT-4.

A Toy Example

GPT-4 Technical Report

OpenAI*

Abstract

we used python

A Toy Example

[GPT-4 answers correctly]	[GPT-4 answers incorrectly]
Can you teach an old dog new tricks? Yes, you can teach an old dog new tricks ← choice You can't teach an old dog new tricks No, you can't teach an old dog new tricks	Son of an actor, this American guitarist and rock singer released many songs and albums and toured with his band. His name is "Elvis" what? Perkins Presley ← choice Elvis Presley His name is Elvis Presley

Table 4: Example of GPT-4 giving correct and incorrect responses on TruthfulQA

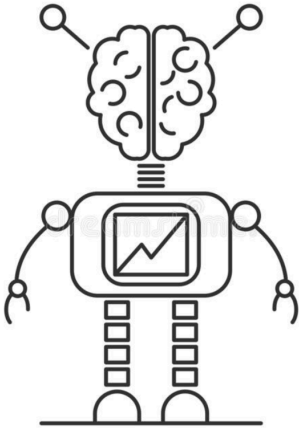
A Toy Example

2 Scope and Limitations of this Technical Report

This report focuses on the capabilities, limitations, and safety properties of GPT-4. GPT-4 is a Transformer-style model [33] pre-trained to predict the next token in a document, using both publicly available data (such as internet data) and data licensed from third-party providers. The model was then fine-tuned using Reinforcement Learning from Human Feedback (RLHF) [34]. Given both the competitive landscape and the safety implications of large-scale models like GPT-4, this report contains no further details about the architecture (including model size), hardware, training compute, dataset construction, training method, or similar.

We are committed to independent auditing of our technologies, and shared some initial steps and ideas in this area in the system card accompanying this release.[2] We plan to make further technical details available to additional third parties who can advise us on how to weigh the competitive and safety considerations above against the scientific value of further transparency.

Trustworthy Methods Connect AI to Physical Worlds



Outlook

Second Part of This Course:

- **Causal Learning** (This lecture)
- Differential Privacy and Federated Learning
- Fairness in ML
- Explainable AI (XAI)

Focus on more attributes: **causality**, **privacy**, **fairness,** and **interpretability**

This Lecture:

Introduction to Causal Learning

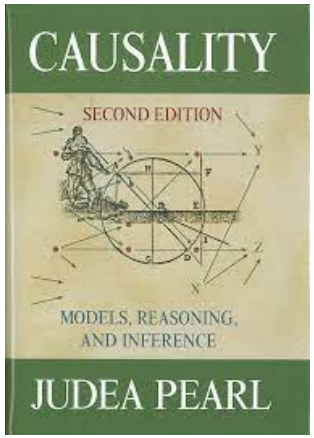
Outline

- Examples — Simpson's Paradox
- Causal inference — Backdoor Adjustment — ~~Formal Definitions~~
- Causal discovery — Nonlinear ICA — ~~The PC Algorithm~~
- Disentanglement — Identifiable VAE

Outline

- Causal inference
- Causal discovery
- Disentanglement

Many online resources and talks

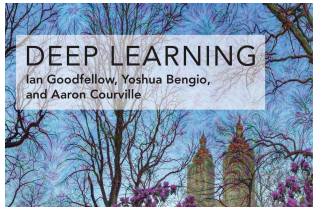


Introduction to Causal Inference

from a Machine Learning Perspective

Brady Neal

December 17, 2020



TOWARDS CAUSAL REPRESENTATION LEARNING:

AN AI & DEEP LEARNING PERSPECTIVE ON CAUSALITY

YOSHUA BENGIO

Causal learning is a full course in many schools

We will only cover selective topics

Part I

Causal Inference

Part I.1

Simpson's paradox and Examples

Motivating example: Simpson's paradox

Simpson's paradox: COVID-29

New Virus 

Treatment T: A (0) or B (1)

Condition C: Mild (0) or Severe (1)

Outcome Y: Happy (0) or Unhappy (1)

Motivating example: Simpson's paradox

Simpson's paradox: COVID-29

New Virus 

Treatment T: A (0) or B (1)

Condition C: Mild (0) or Severe (1)

Outcome Y: Survive (0) or Not (1)

Mortality Rate Table

Treatment	Total
A	16% (240/1500)
B	19% (105/550)

$\mathbb{E}[Y|T]$

Simpson's paradox: Mortality Rate Table

Mortality Rate Table

Treatment	Total
A	**16%** (240/1500)
B	19% (105/550)

$\mathbb{E}[Y|T]$

Simpson's paradox: Mortality Rate Table

Mortality Rate Table

Treatment	Condition: Mild	Condition: Severe	Total
A	15% (210/1400)	30% (30/100)	**16%** (240/1500)
B	**10%** (5/50)	**20%** (100/500)	19% (105/550)
	$\mathbb{E}[Y\|T, C = 0]$	$\mathbb{E}[Y\|T, C = 1]$	$\mathbb{E}[Y\|T]$

Simpson's paradox: Mortality Rate Table

Mortality Rate Table Statistics/Data

Treatment	Condition: Mild	Condition: Severe	Condition: Total
A	15% (210/1400)	30% (30/100)	16% (240/1500)
B	10% (5/50)	20% (100/500)	19% (105/550)
	$\mathbb{E}[Y\|T, C=0]$	$\mathbb{E}[Y\|T, C=1]$	$\mathbb{E}[Y\|T]$

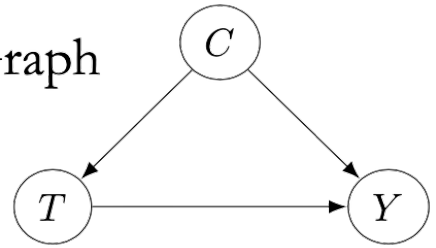
$$\frac{1400}{1500}(0.15) + \frac{100}{1500}(0.30) = 0.16$$

$$\frac{50}{550}(0.10) + \frac{500}{550}(0.20) = 0.19$$

Which treatment should you choose?

Simpson's paradox: scenario 1

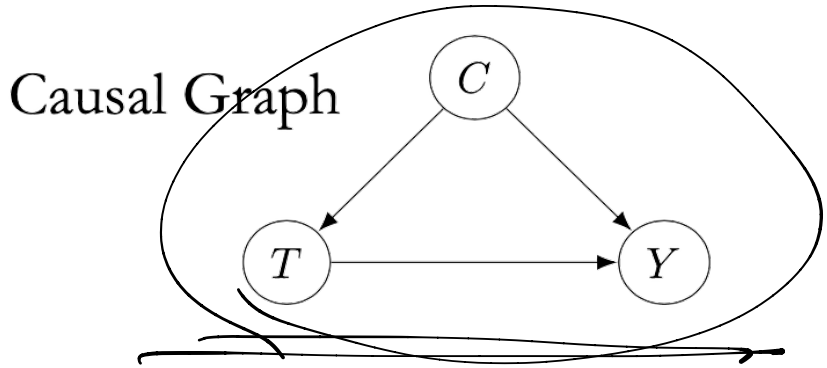
Causal Graph



Which treatment is better?

		Condition: Mild	Condition: Severe	Condition: Total
Treatment	A	15% (210/1400)	30% (30/100)	**16%** (240/1500)
	B	**10%** (5/50)	**20%** (100/500)	19% (105/550)

Simpson's paradox: scenario 1 (treatment B)



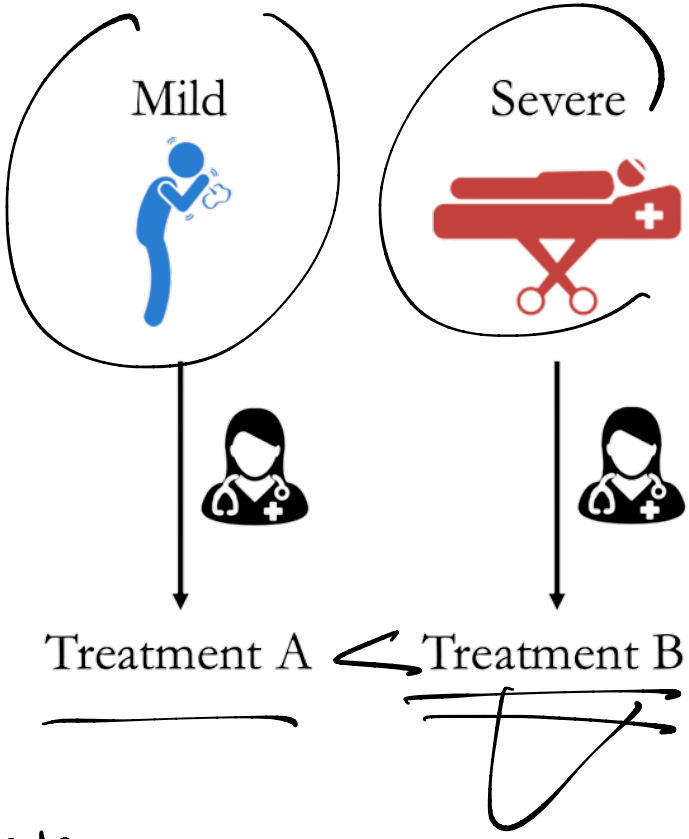
Condition

Treatment	Mild	Severe	Total
A	15% (210/1400)	30% (30/100)	**16%** (240/1500)
B	**10%** (5/50)	**20%** (100/500)	19% (105/550)

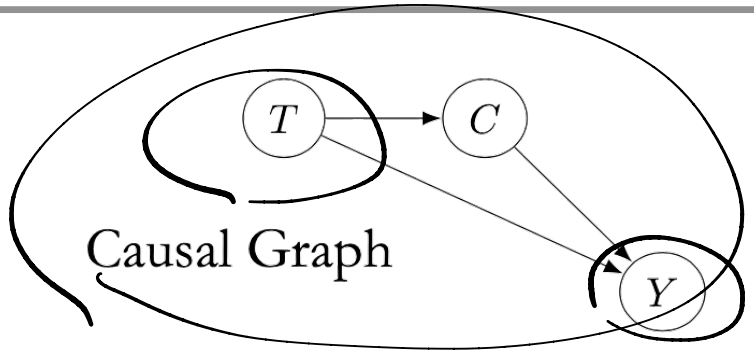
1400 >> 100

500 >> 50

Data



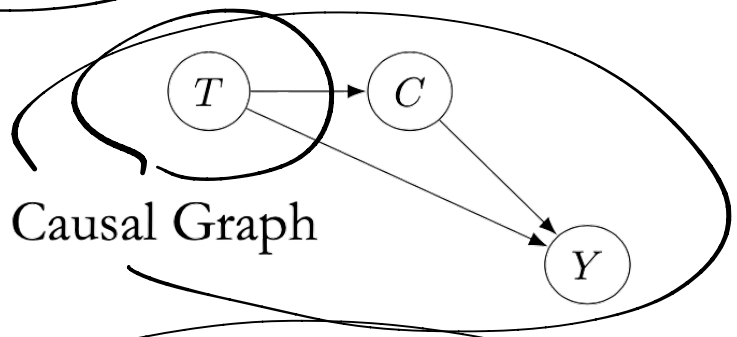
Simpson's paradox: scenario II



Which treatment is better?

		Condition: Mild	Condition: Severe	Condition: Total
Treatment	A	15% (210/1400)	30% (30/100)	**16%** (240/1500)
	B	**10%** (5/50)	**20%** (100/500)	19% (105/550)

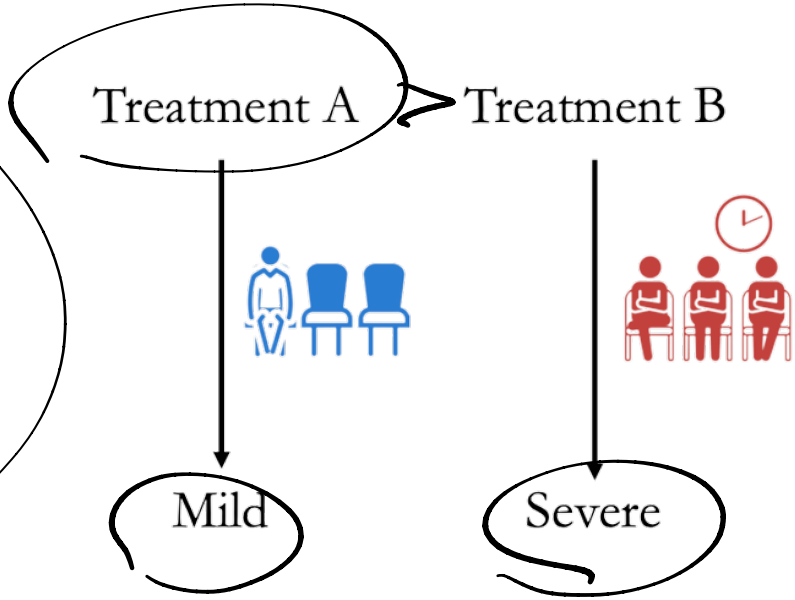
Simpson's paradox: scenario II (treatment A)



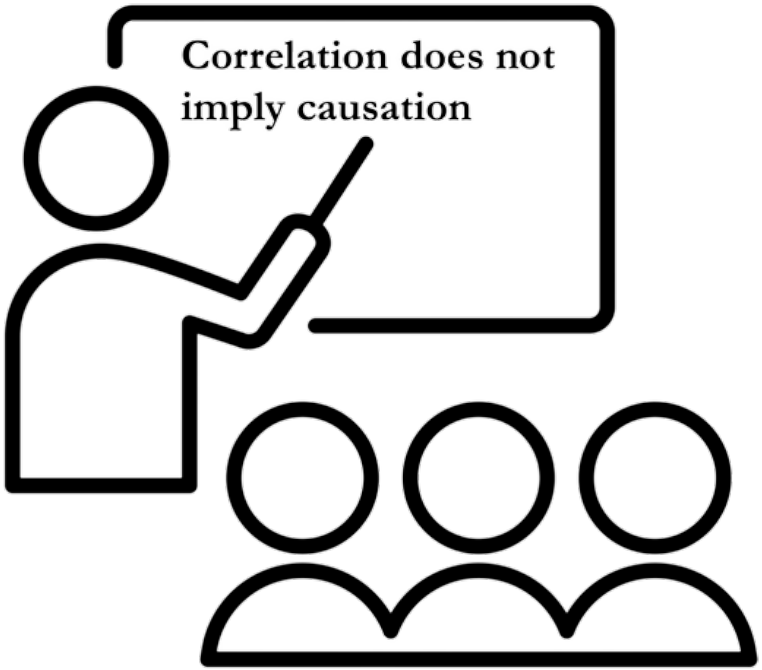
Causal Graph

Which treatment is better?

Treatment	Condition: Mild	Condition: Severe	Condition: Total
A	15% (210/1400)	30% (30/100)	**16%** (240/1500)
B	**10%** (5/50)	**20%** (100/500)	19% (105/550)

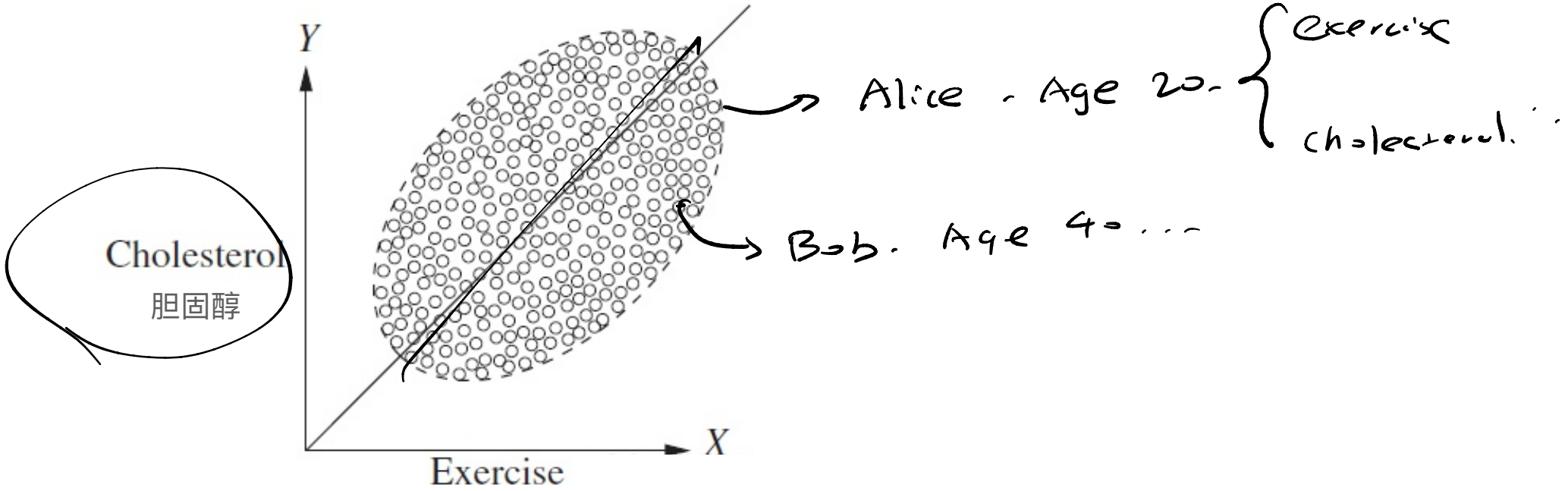


What do we learn from the simpson's paradox?



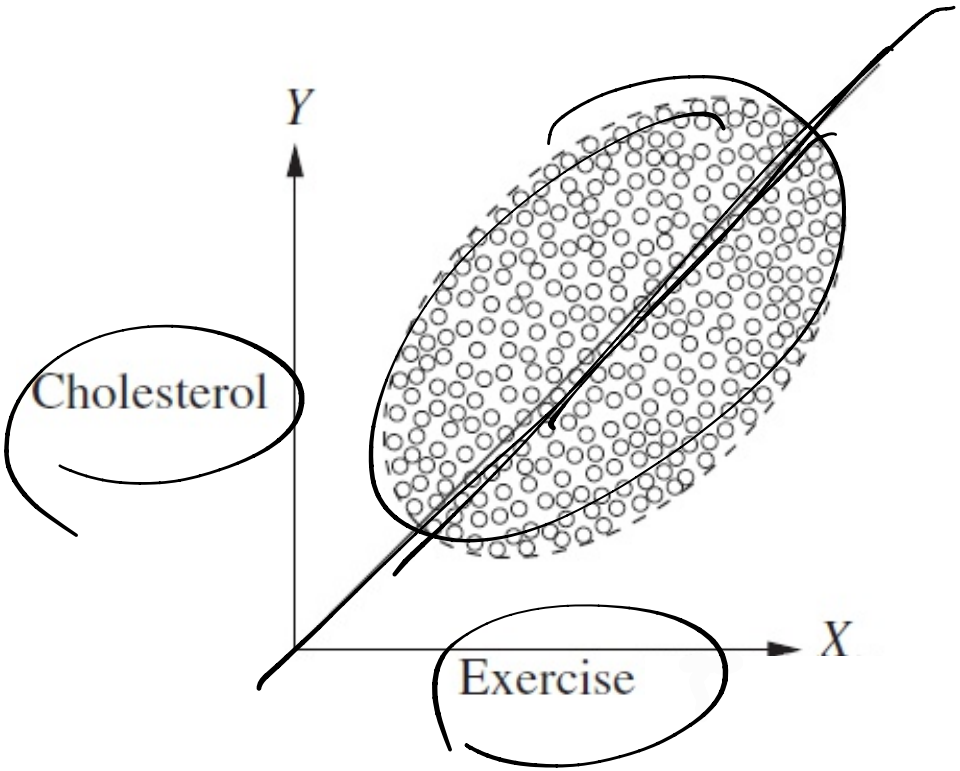
What do we learn from the simpson's paradox?

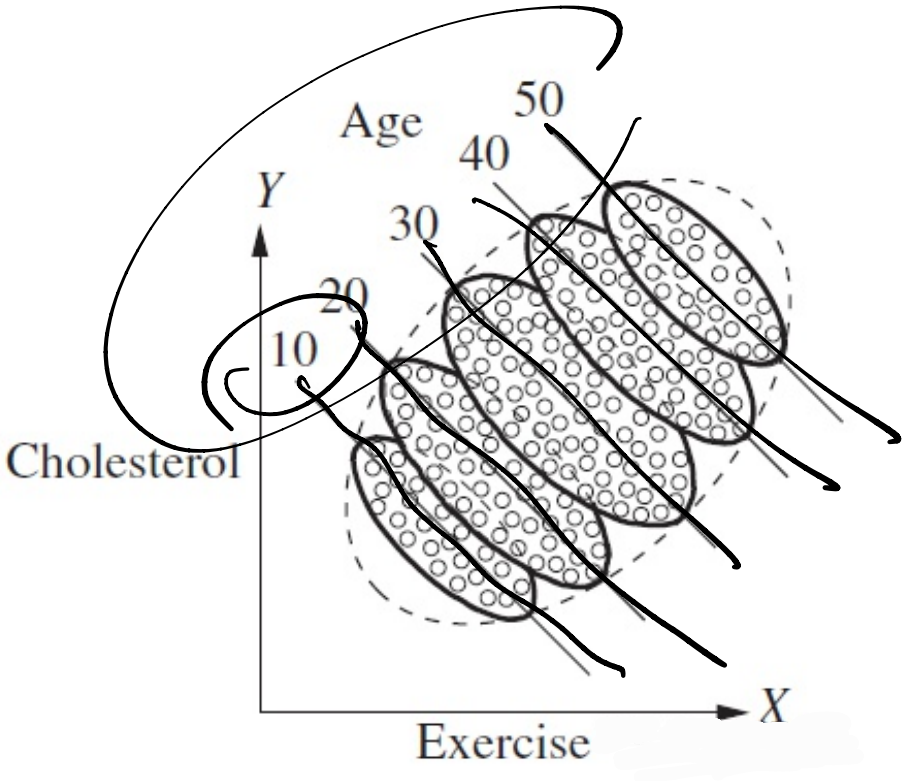
More examples



What do we learn from the simpson's paradox?

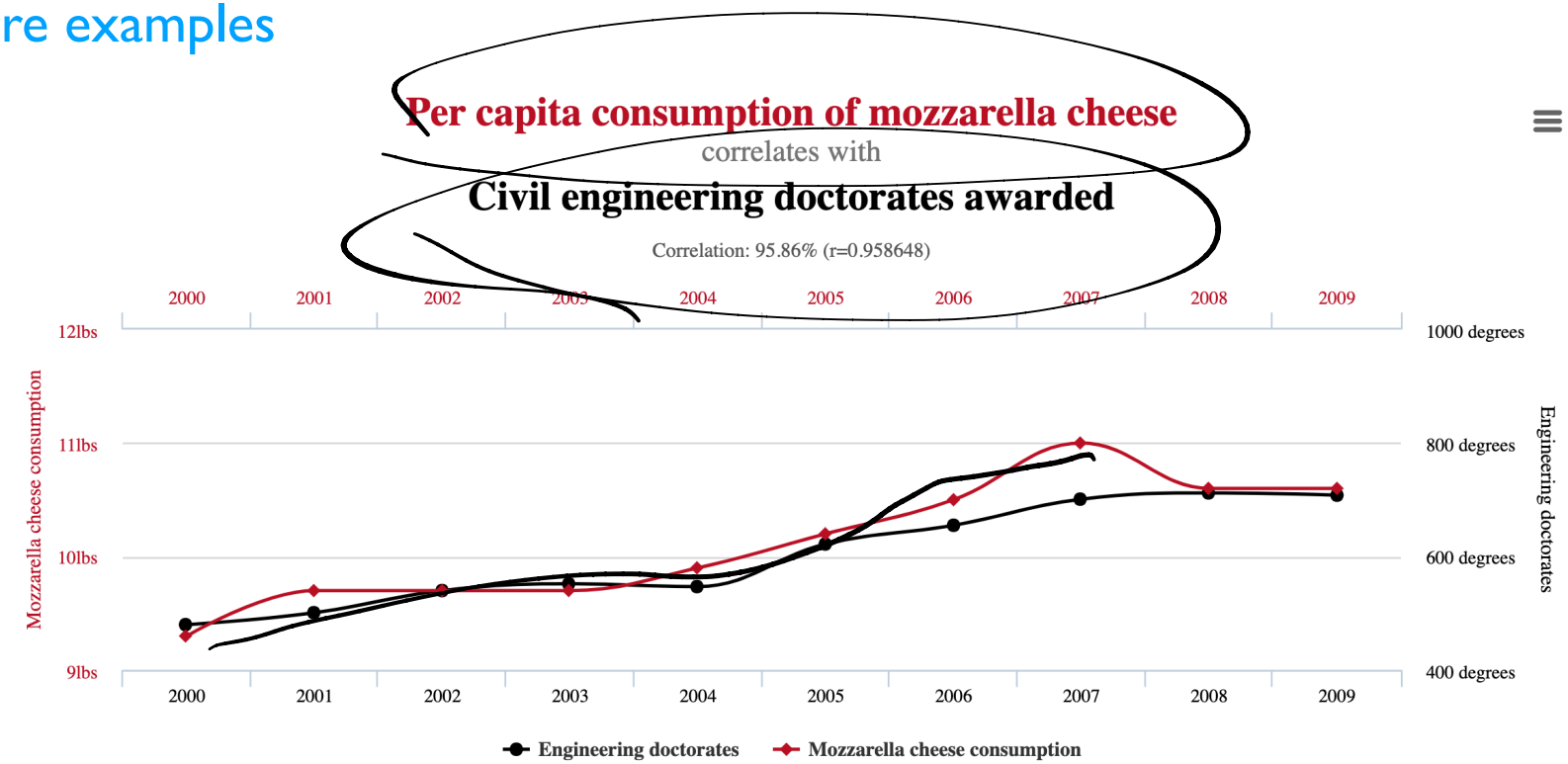
More examples





What do we learn from the simpson's paradox?

More examples



Source: https://www.tylervigen.com/spurious-correlations

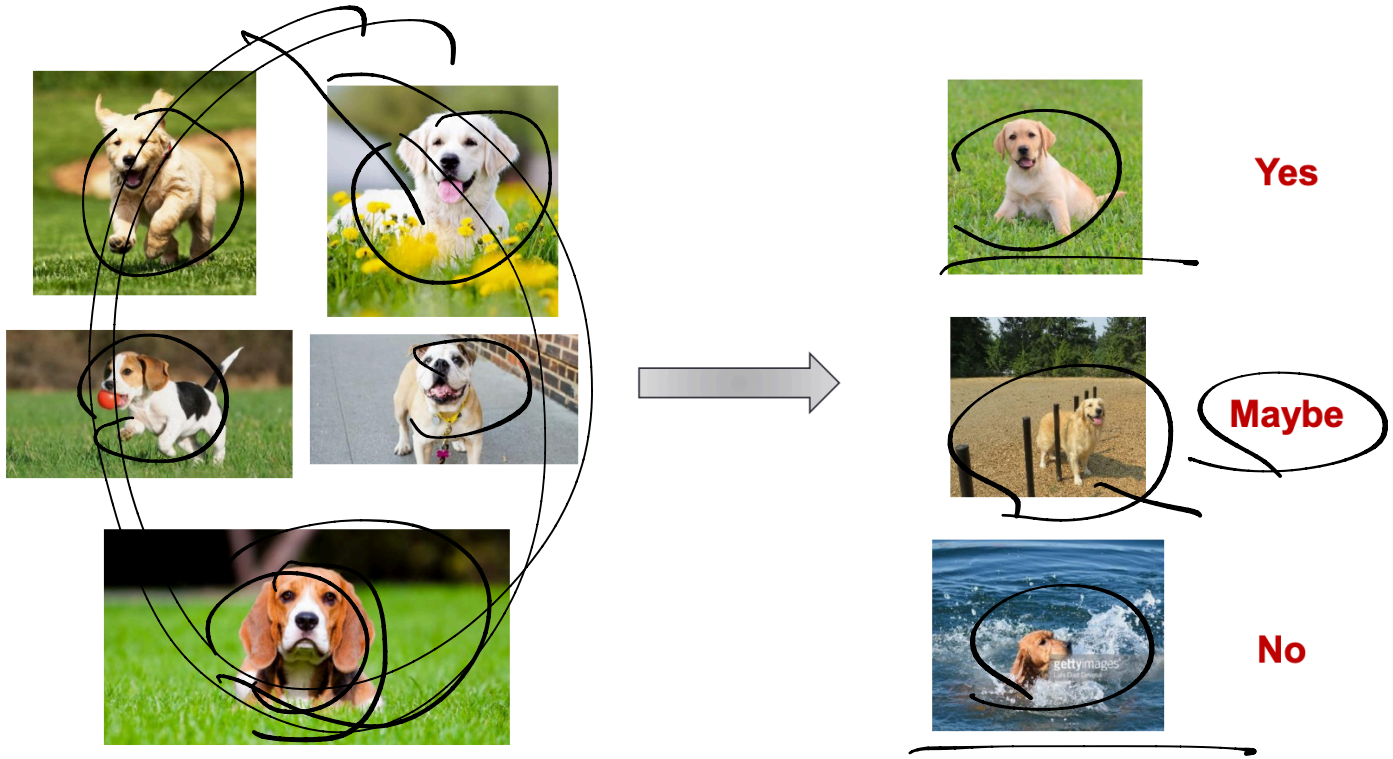
What do we learn from the simpson's paradox?

Correlation does not imply causation

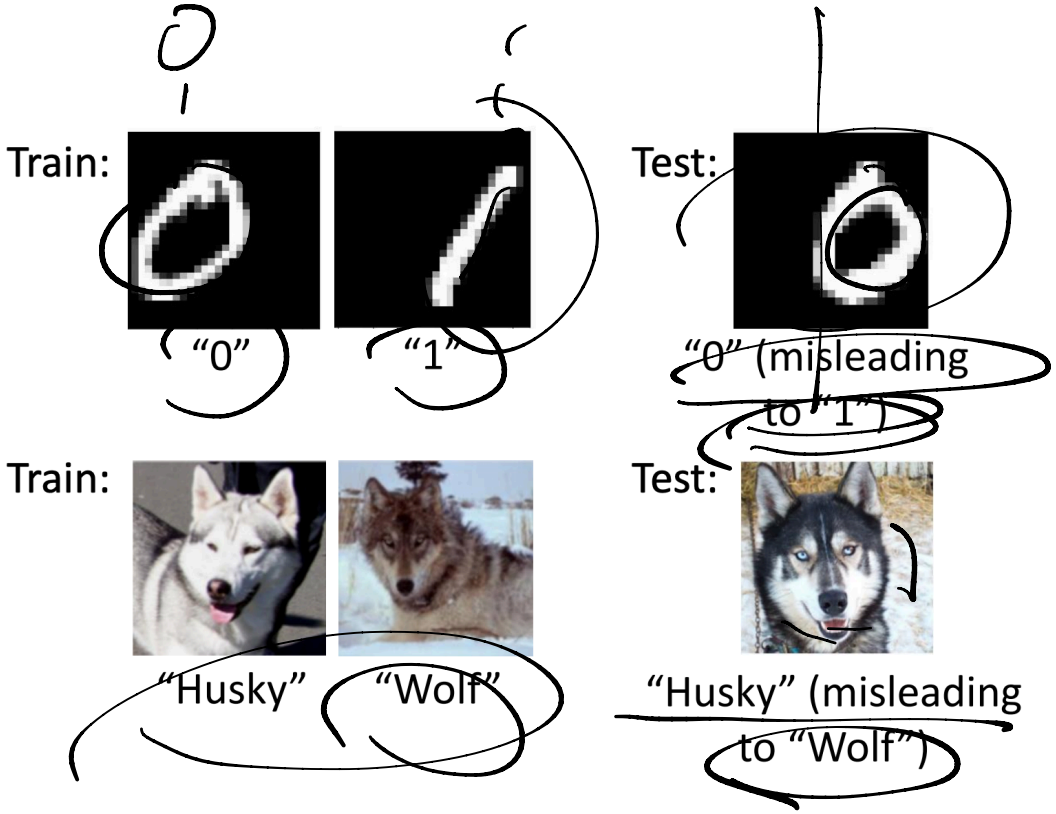
Correlation is not enough

Statistical learning vs Causal learning

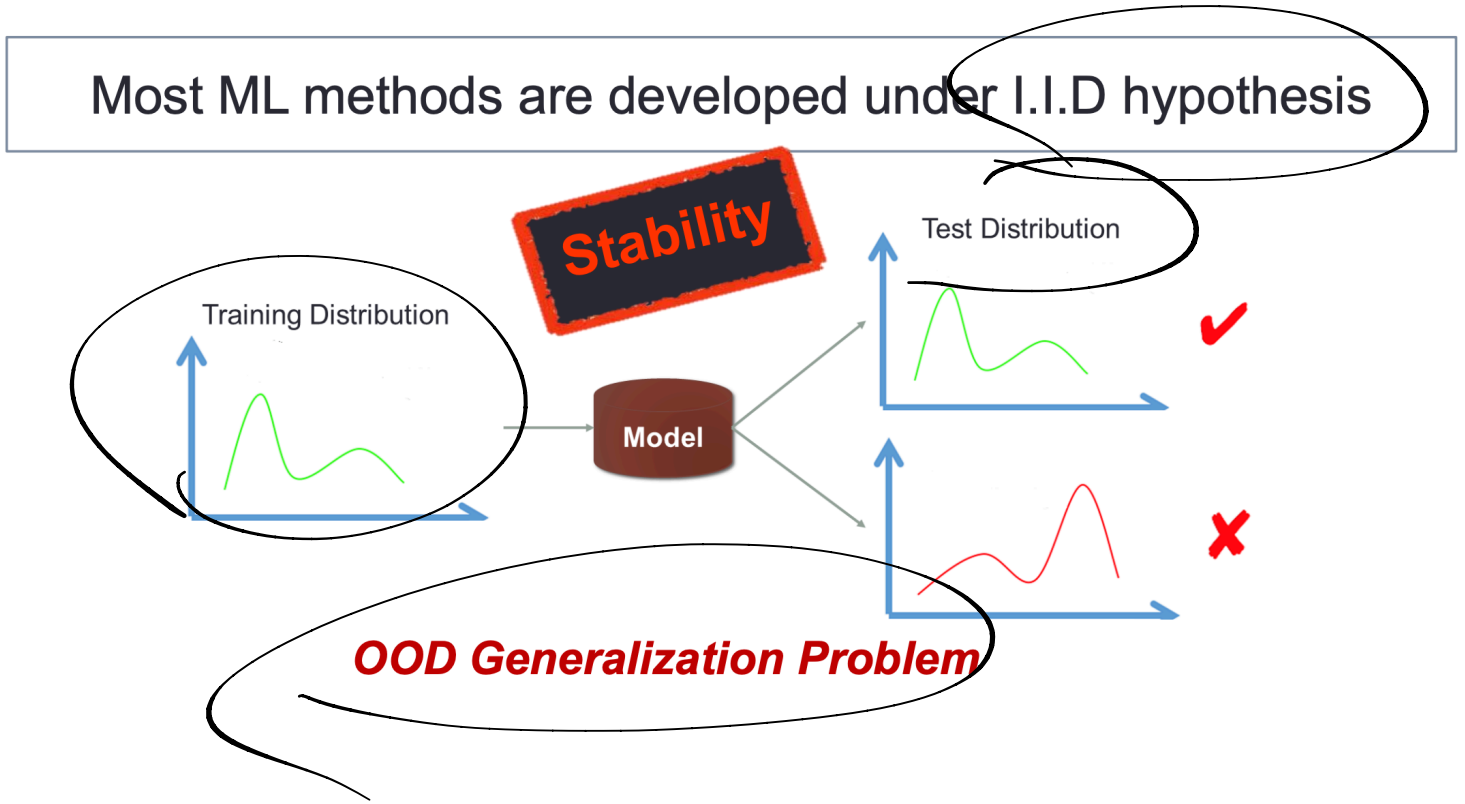
Why causality matters in machine learning?



Why causality matters in machine learning?

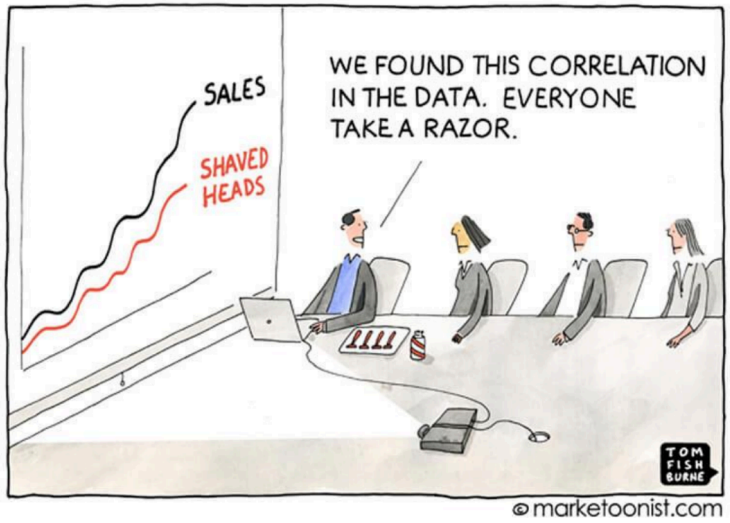


Why causality matters in machine learning?



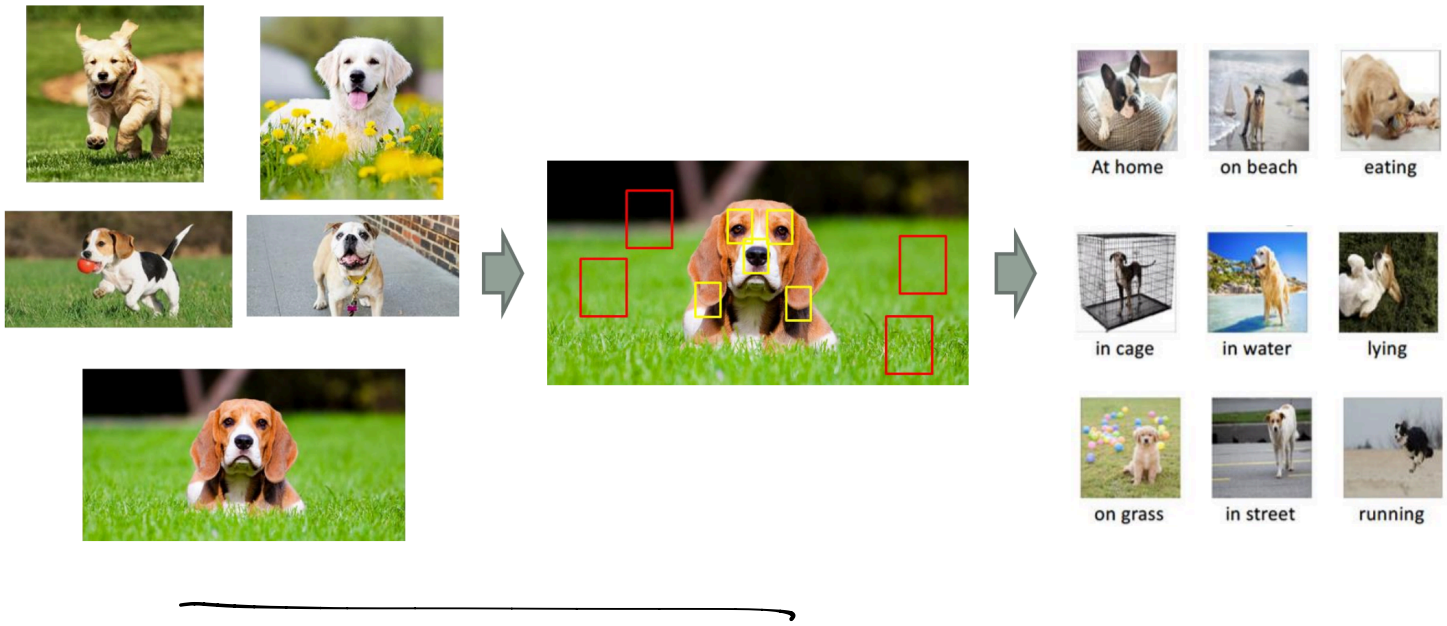
Why causality matters in machine learning?

Correlation is the very basics of machine learning.



Why causality matters in machine learning?

Relying solely on correlation can cause problems



Part I.2

Simpson's paradox and Examples

What is causal inference?

Inferring the effects of any treatment/policy/intervention/etc.

Examples:

- Effect of treatment on a disease
- Effect of climate change policy on emissions
- Effect of social media on mental health
- Many more (effect of X on Y)

What is causal inference?

Inferring the effects of any treatment/policy/intervention/etc.

Examples:

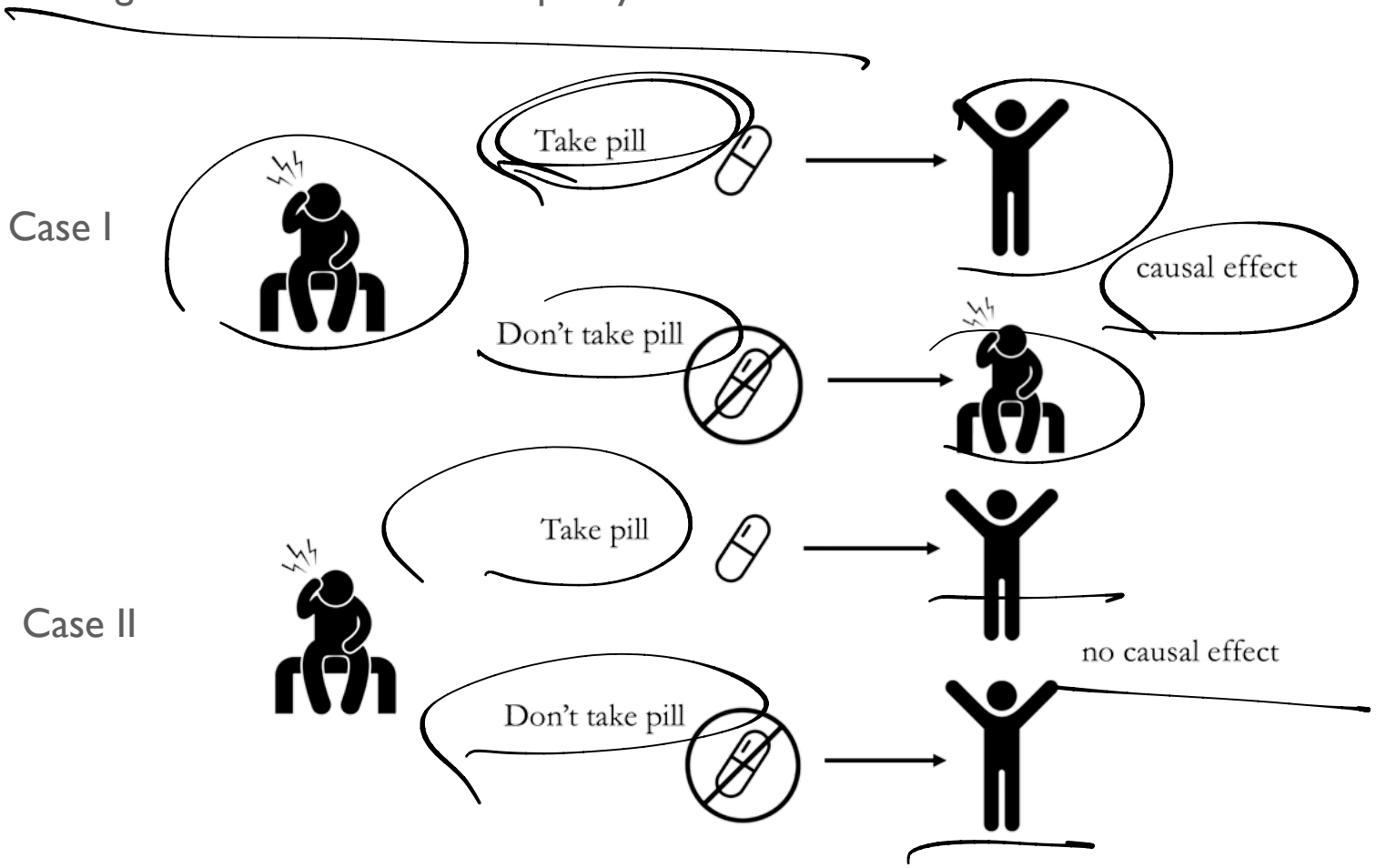
- Effect of treatment on a disease
- Effect of climate change policy on emissions
- Effect of social media on mental health
- Many more (effect of X on Y)

How do we measure causal effects with interventions?

How do we measure causal effects in observational studies?

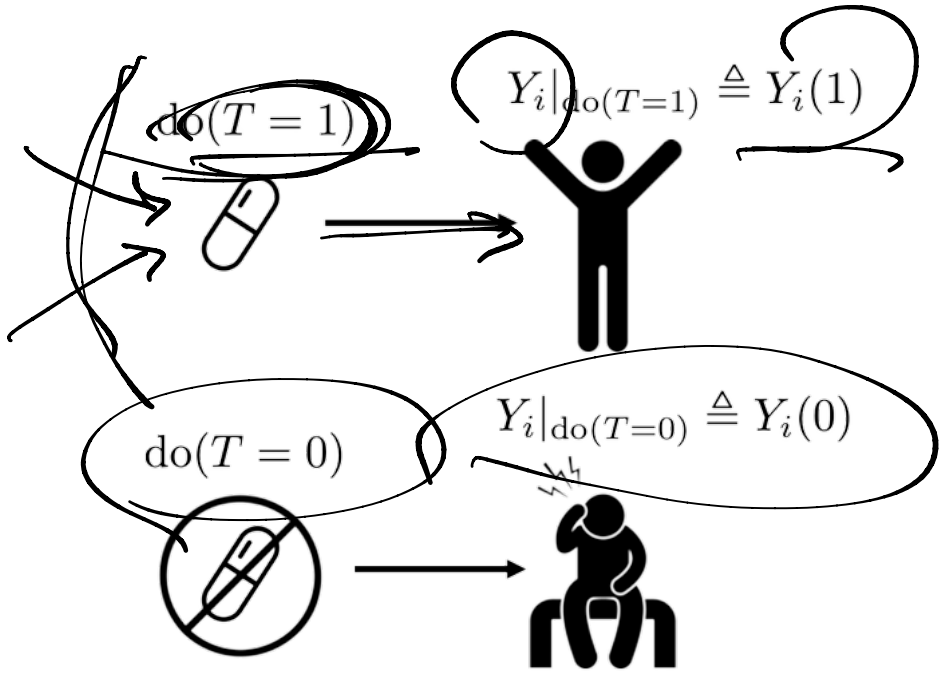
Potential outcomes

Inferring the effect of treatment/policy on some outcome



Do Operator

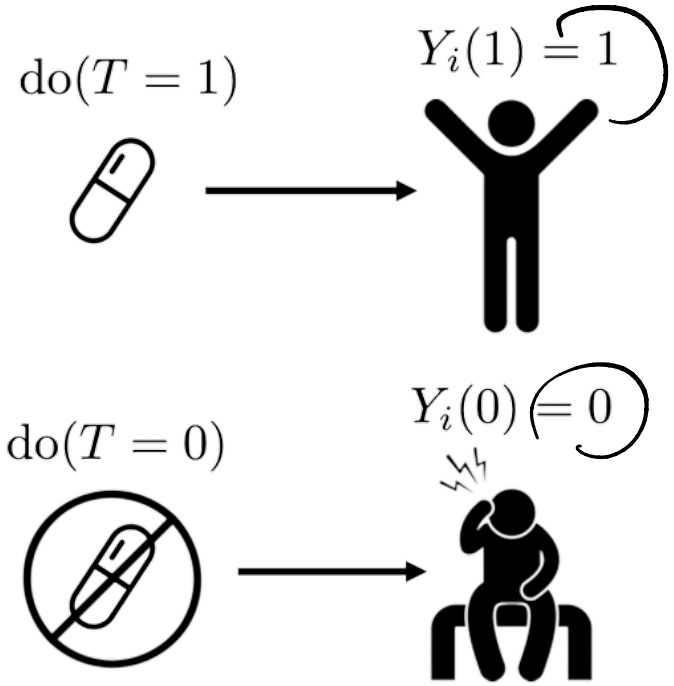
Inferring the effect of treatment/policy on some outcome



T : observed treatment
Y : observed outcome
i : used in subscript to denote a specific unit/individual
$Y_i(1)$: potential outcome under treatment
$Y_i(0)$: potential outcome under no treatment

Do Operator

Inferring the effect of treatment/policy on some outcome

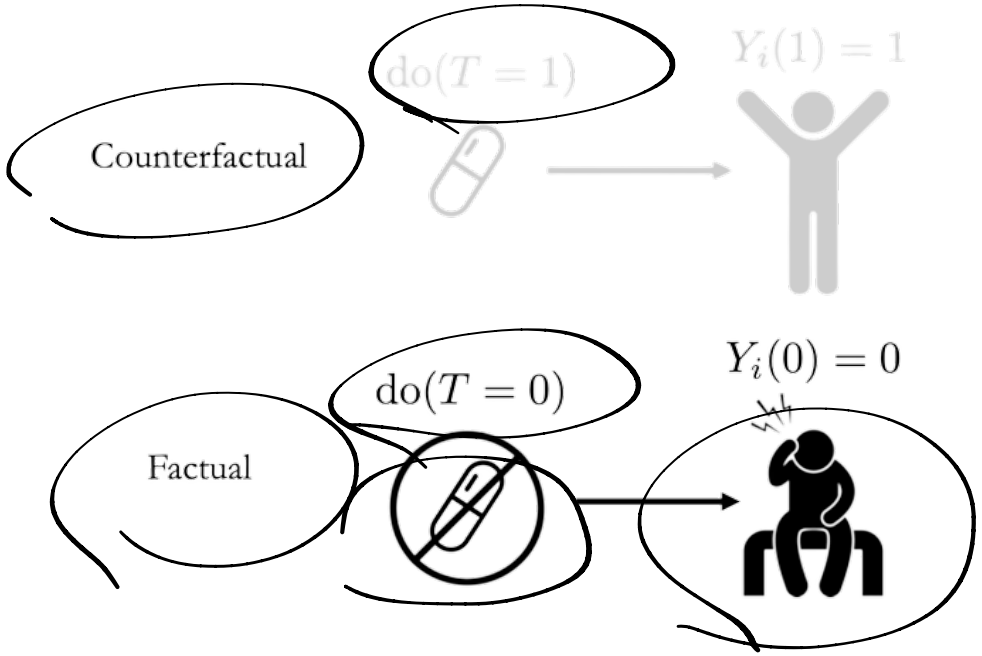


T : observed treatment
Y : observed outcome
i : used in subscript to denote a specific unit/individual
$Y_i(1)$: potential outcome under treatment
$Y_i(0)$: potential outcome under no treatment

Causal effect

$$Y_i(1) - Y_i(0) = 1$$

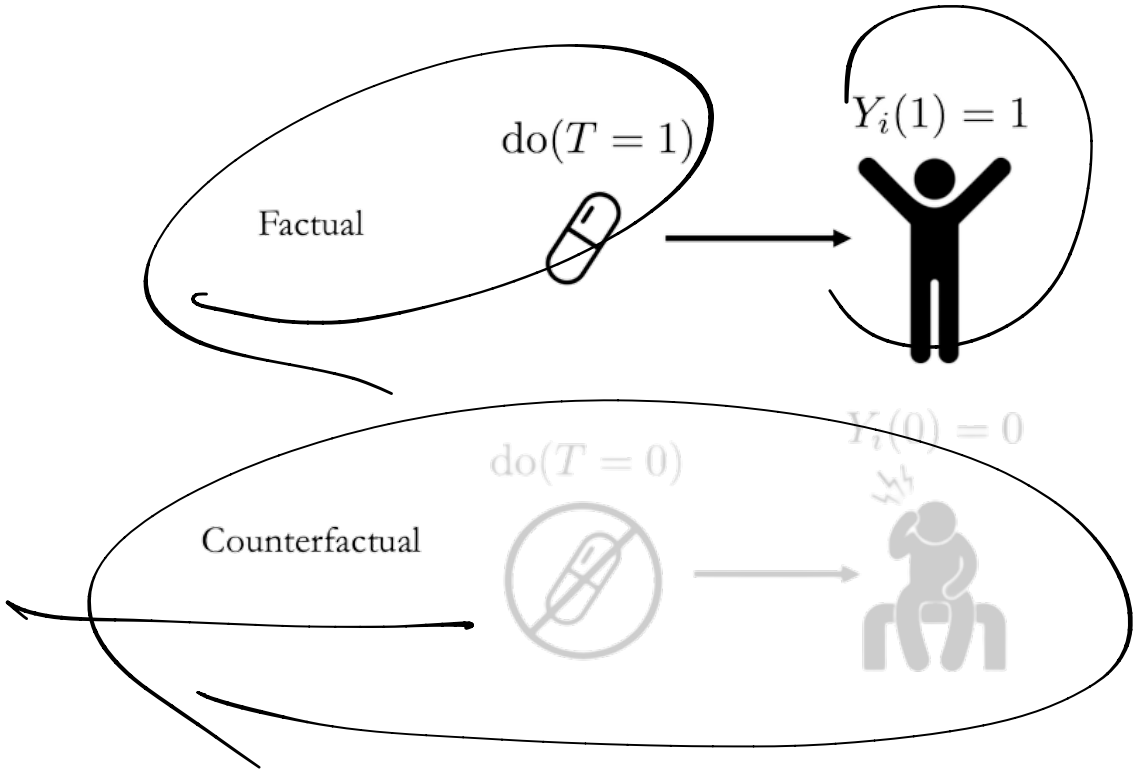
A Fundamental Problem of Causal Inference



Causal effect

$$Y_i(1) - Y_i(0) = 1$$

A Fundamental Problem of Causal Inference



Causal effect

$Y_i(1) - Y_i(0) = 1$

Causal inference with observations (Optional)

Inferring the effects of any treatment/policy/intervention/etc.

Examples:

- Effect of treatment on a disease
- Effect of climate change policy on emissions
- Effect of social media on mental health
- Many more (effect of X on Y)

How do we measure causal effects with interventions?

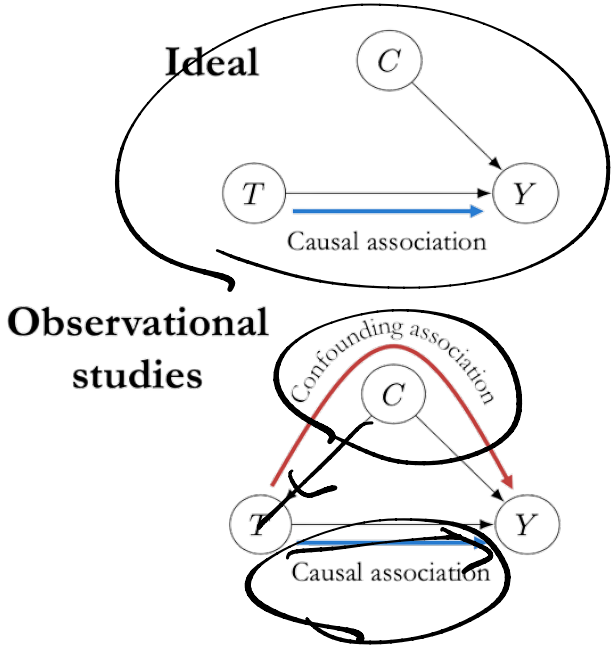
How do we measure causal effects in observational studies?

Causal inference with observations (Optional)

How do we measure causal effects in observational studies?

Can't always randomize treatment

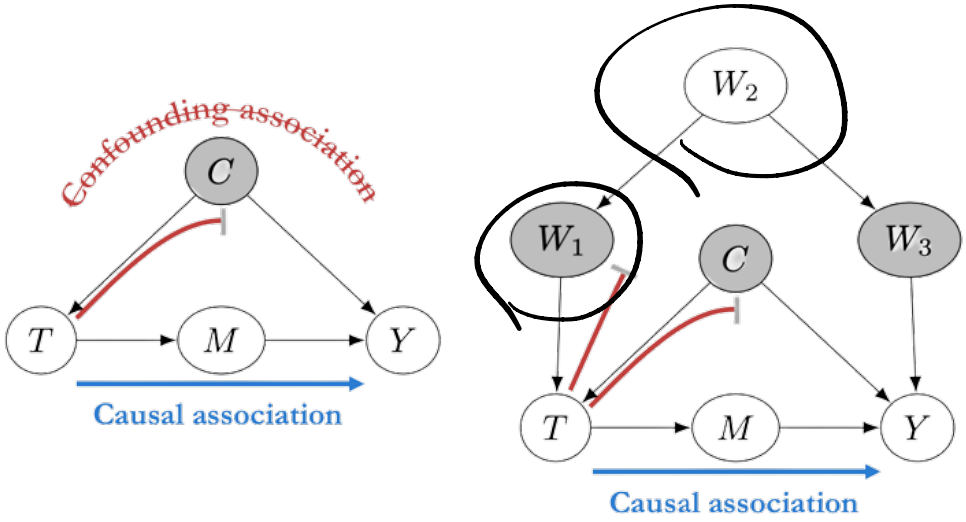
- **Ethical reasons** (e.g. unethical to randomize people to smoke for measuring effect on lung cancer)
- **Infeasibility** (e.g. can't randomize countries into communist/capitalist systems to measure effect on GDP)
- **Impossibility** (e.g. can't change a living person's DNA at birth for measuring effect on breast cancer)



Causal inference with observations (Optional)

Solution: backdoor adjustment

Formal assumptions are needed (omitted)



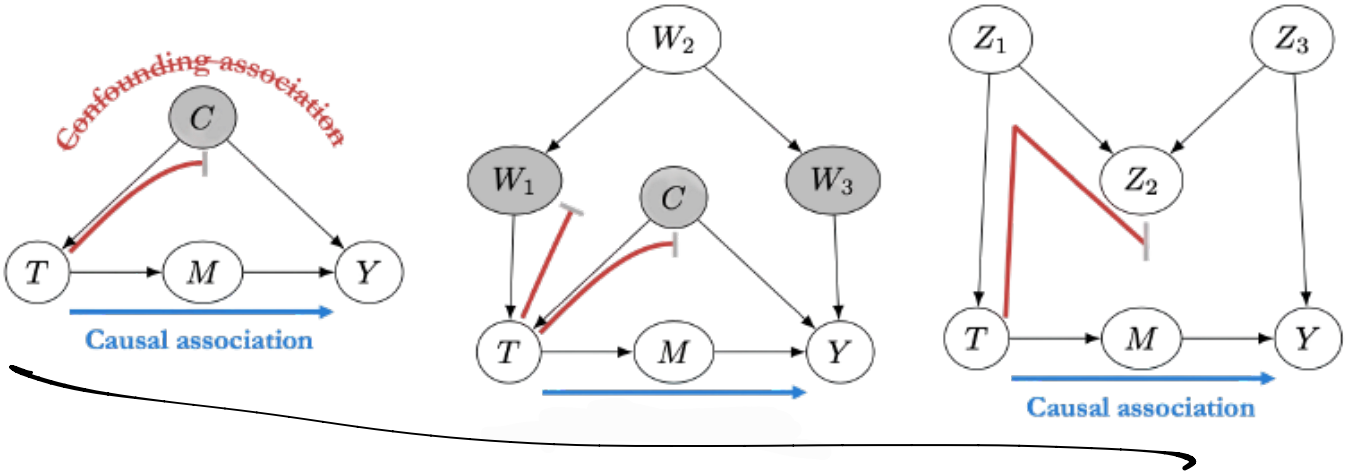
Causal inference with observations (optional)

Solution: backdoor adjustment

Formal assumptions are needed (omitted)

$$\mathbb{E}[Y|\mathrm{do}(T=t)] = \mathbb{E}_W \mathbb{E}[Y|t, W]$$

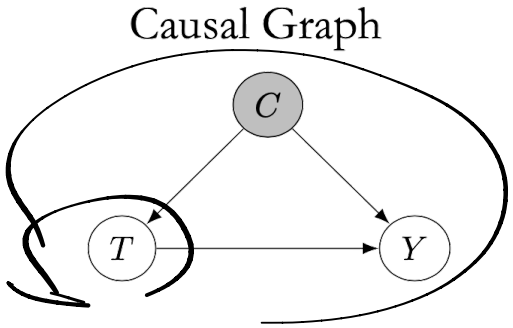
Shaded nodes are examples of sufficient adjustment sets W



Application to the COVID-29 example

Treatment	Mild	Severe	Total	Causal
	Condition			
A	15% (210/1400)	30% (30/100)	**16%** (240/1500)	19.4%
B	**10%** (5/50)	**20%** (100/500)	19% (105/550)	**12.9%**
	$\mathbb{E}[Y\|t, C=0]$	$\mathbb{E}[Y\|t, C=1]$	$\mathbb{E}[Y\|t]$	$\mathbb{E}[Y\|\text{do}(t)]$

Assume this causal graph:



$$\mathbb{E}[Y|\text{do}(T=t)] = \mathbb{E}_C\mathbb{E}[Y|t,C] = \sum \mathbb{E}[Y|t,c]P(c)$$

$P(C=\text{mild})$ $P(C=\text{severe})$

$t=A$ $\quad \frac{1450}{2050}(0.15) + \frac{600}{2050}(0.30) \approx 0.194$

$t=B$ $\quad \frac{1450}{2050}(0.10) + \frac{600}{2050}(0.20) \approx 0.129$

Part II

Causal Discovery

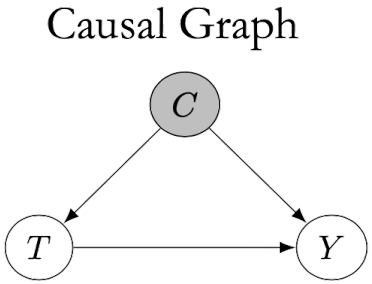
Part II

Causal Discovery

I. Linear Case

What is causal discovery?

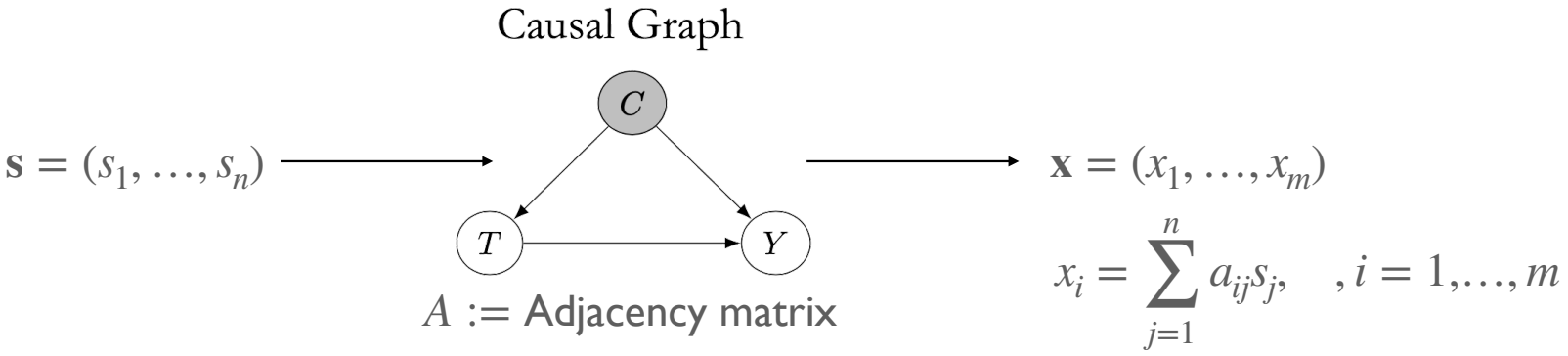
How do we know this relation for the COVID-29 example?



A key problem: identifiability

What is causal discovery?

How do we know this relation for the COVID-29 example?



A key problem: identifiability

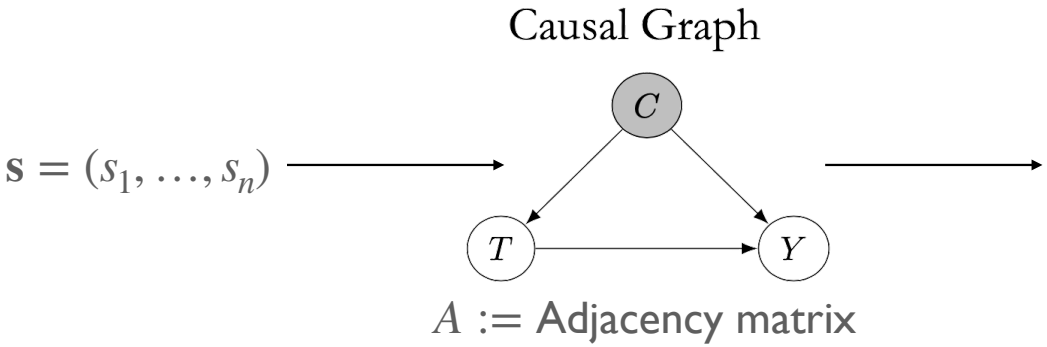
Many methods …

We focus on ICA in this lecture

Suppose the underlying mechanism is linear

What is causal discovery?

How do we know this relation for the COVID-29 example?



structural equation model (SEM)

$$\mathbf{x} = (x_1, \ldots, x_m)$$

$$x_i = \sum_{j=1}^{n} a_{ij} s_j, \quad , i = 1, \ldots, m$$

Identifiability: Observe $\mathbf{x}$, want A and $\mathbf{s}$

Many methods …

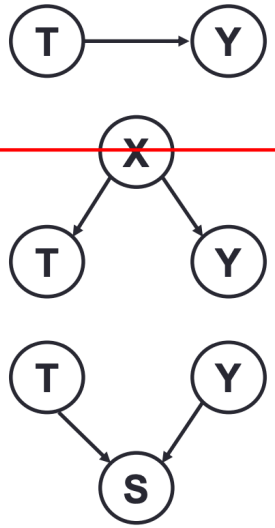
We focus on ICA in this lecture

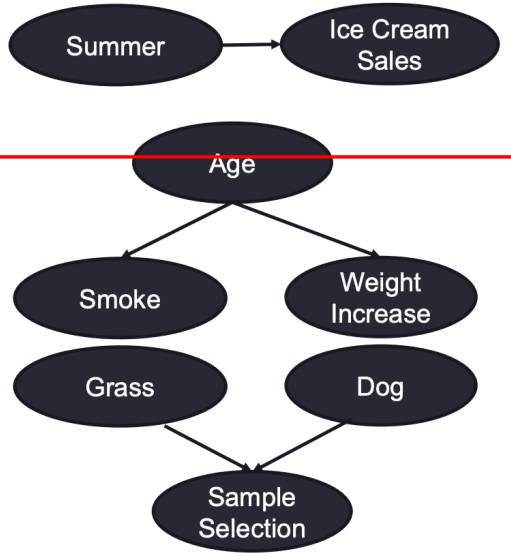
Suppose the underlying mechanism is linear

Why causality matters in machine learning?

Three sources of correlation:

- Causation
  - Causal mechanism
  - Stable and explainable
- Confounding
  - Ignoring X
  - Spurious Correlation
- Sample Selection Bias
  - Conditional on S
  - Spurious Correlation





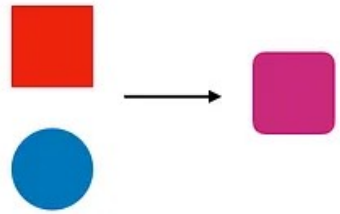
How do identify them, as a graph?

Independent Component Analysis

ICA as principled unsupervised learning

PCA

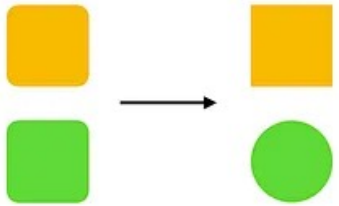
Compresses information



Requires preprocessing: autoscaling

ICA

Separates information



Requires preprocessing: autoscaling

Often benefits from first applying PCA

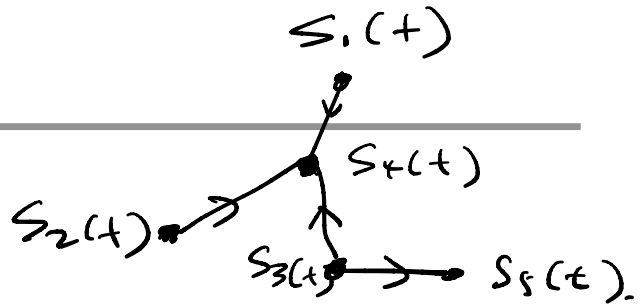
Independent Component Analysis

ICA as principled unsupervised learning

Unsupervised learning can have different goals

1) Accurate model of data distribution?
   - E.g. Variational Autoencoders are good
2) Sampling points from data distribution?
   - E.g. Generative Adversarial Networks are good
3) Useful features for supervised learning?
   - Many methods, "Representation learning"
4) Reveal underlying structure in data, disentangle latent quantities?
   - Independent Component Analysis

Independent Component Analysis



ICA as principled unsupervised learning

Linear independent component analysis (ICA)

$$x_i(t) = \sum_{j=1}^{n} a_{ij} s_j(t) \quad \text{for all } i, j = 1 \ldots n$$

$A = (a_{ij})$

(2) $x(t) = A \cdot s(t)$

mixing matrix

- $x_i(t)$ is i-th observed signal at sample point t (possibly time)
- a_{ij} constant parameters describing "mixing"
- Assuming independent, non-Gaussian latent "sources" s_j

Identifiability: Find Independent Components (Sources)

Independent Component Analysis

ICA as principled unsupervised learning

Linear independent component analysis (ICA)

$$x_i(t) = \sum_{j=1}^{n} a_{ij} s_j(t) \quad \text{for all } i, j = 1 \ldots n \qquad (2)$$

- $x_i(t)$ is i-th observed signal at sample point t (possibly time)
- a_{ij} constant parameters describing "mixing"
- Assuming independent, non-Gaussian latent "sources" s_j

The independent components are identifiable (up to permutation and scaling of the sources)

Assumptions: At most one of the sources s_j is Gaussian

$A = (a_{ij})$ is full-rank

Independent Component Analysis

ICA as principled unsupervised learning

Linear independent component analysis (ICA)

$$x_i(t) = \sum_{j=1}^{n} a_{ij} s_j(t) \quad \text{for all } i, j = 1 \ldots n \tag{2}$$

- $x_i(t)$ is i-th observed signal at sample point t (possibly time)
- a_{ij} constant parameters describing "mixing"
- Assuming independent, non-Gaussian latent "sources" s_j

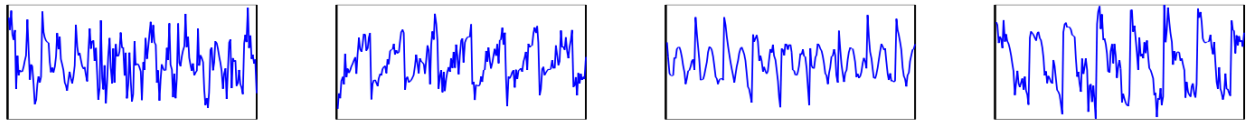
ICA is identifiable, i.e. well-defined: (Darmois-Skitovich ∼1950; Comon, 1994)

- Observing only x_i we can recover both a_{ij} and s_j
- I.e. original sources can be recovered

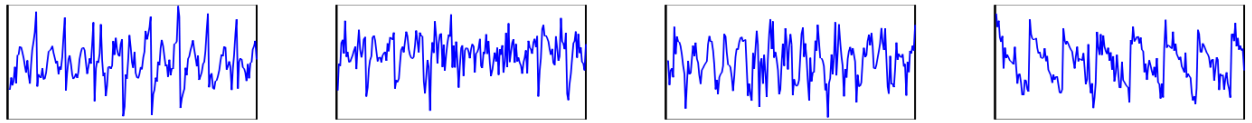
Independent Component Analysis

Identifiability means ICA does blind source separation

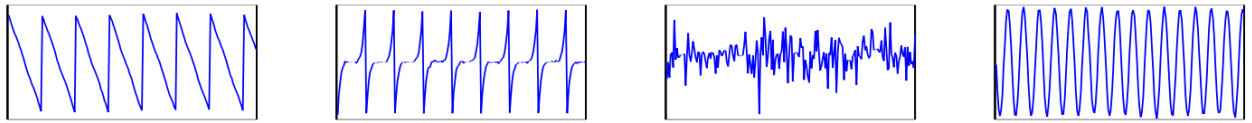
Observed signals:



Principal components:

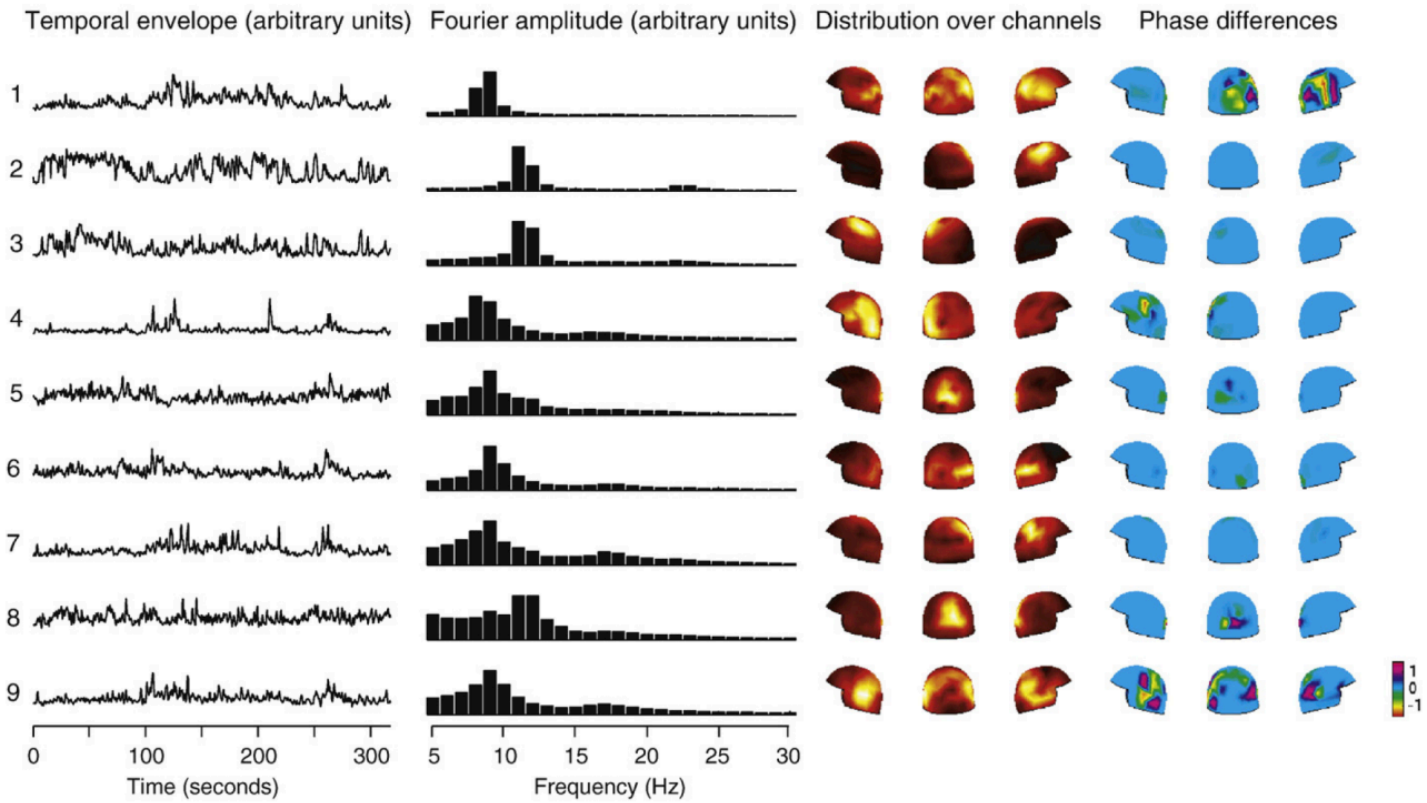


Independent components are original sources:



credits: Aapo Hyvarinen

Independent Component Analysis



(Hyvärinen, Ramkumar, Parkkonen, Hari, 2010)

credits: Aapo Hyvarinen

Part II

Causal Discovery and Disentanglement

2. General Case

Nonlinear Independent Component Analysis (optional)

What if we consider the nonlinear setting?

Linear ICA: $\mathbf{x} = A\mathbf{s}$

Deep generative models: $\mathbf{x} = f(\mathbf{s})$ What is f^{-1}?

Identifiability of the deep latent-variable models.

$$p_\theta(x) = p_{\theta*}(x) \longrightarrow \theta* = \theta \longrightarrow p_{\theta*}(x, z) = p_\theta(x, z)$$

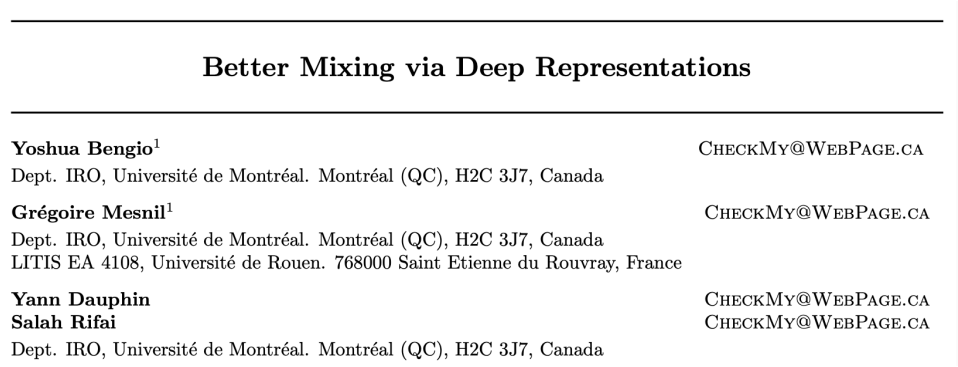
$$\Longrightarrow \quad p_{\theta*}(z) = p_\theta(z)$$

$$p_{\theta*}(x \mid z) = p_\theta(x \mid z)$$

Disentanglement

Nonlinear Independent Component Analysis (optional)

Disentanglement



Better Mixing via Deep Representations

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Find disentangled representations in unsupervised data.

An important topic in causal learning

A problem in deep generative models

Identifiability of Nonlinear Independent Component Analysis (optional)

Identifiability

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = p_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) \implies \boldsymbol{\theta} = \hat{\boldsymbol{\theta}} \ \forall(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}})$$

Deep generative models: $\mathbf{x} = f(\mathbf{s})$ What is f^{-1}?

Deep generative models are are **not identifiable in general**

(Hyvärinen and Pajunen, 1999; Khemakhem et al., 2020; Locatello et al., 2019)

$\implies$ basic VAEs, GANs, Nonlinear ICA etc. are unidentifiable:

Identifiability problem

$$p_{\mathbf{f}}(\mathbf{x}) = p_{\hat{\mathbf{f}}}(\mathbf{x}) \not\implies \mathbf{f} = \hat{\mathbf{f}}$$

Identifiability of Nonlinear Independent Component Analysis (optional)

Identifiability

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = p_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) \implies \boldsymbol{\theta} = \hat{\boldsymbol{\theta}} \ \forall(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}})$$

Deep generative models: $\mathbf{x} = f(\mathbf{s})$ What is f^{-1}?

Deep generative models are are **not identifiable in general**

(Hyvärinen and Pajunen, 1999; Khemakhem et al., 2020; Locatello et al., 2019)

$\implies$ basic VAEs, GANs, Nonlinear ICA etc. are unidentifiable:

We can add structures/assumptions on the distribution of $\mathbf{s}$ to ensure identifiability

Identifiability of Nonlinear Independent Component Analysis (optional)

Identifiability

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = p_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) \implies \boldsymbol{\theta} = \hat{\boldsymbol{\theta}} \ \forall(\boldsymbol{\theta}, \hat{\boldsymbol{\theta}})$$

Deep generative models: $\mathbf{x} = f(\mathbf{s})$

Deep generative models are are **not identifiable in general**

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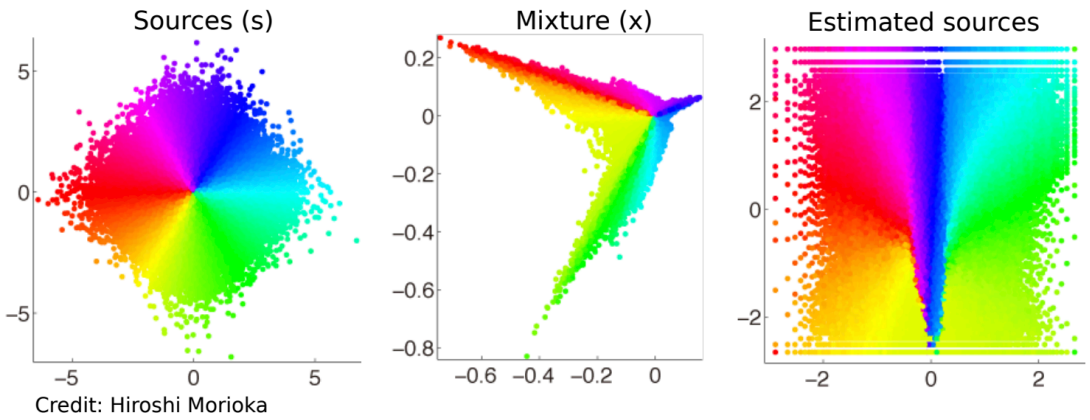
$\implies$ basic VAEs, GANs, Nonlinear ICA etc. are unidentifiable:

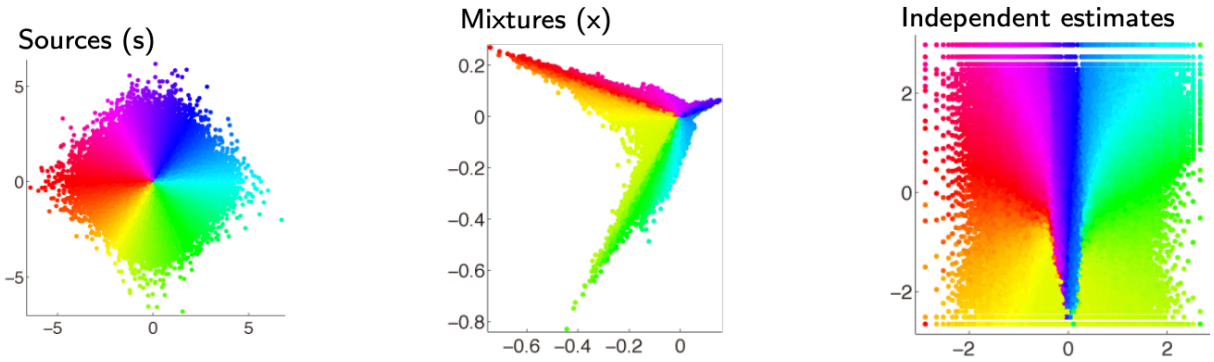


Identifiability of Nonlinear Independent Component Analysis (optional)

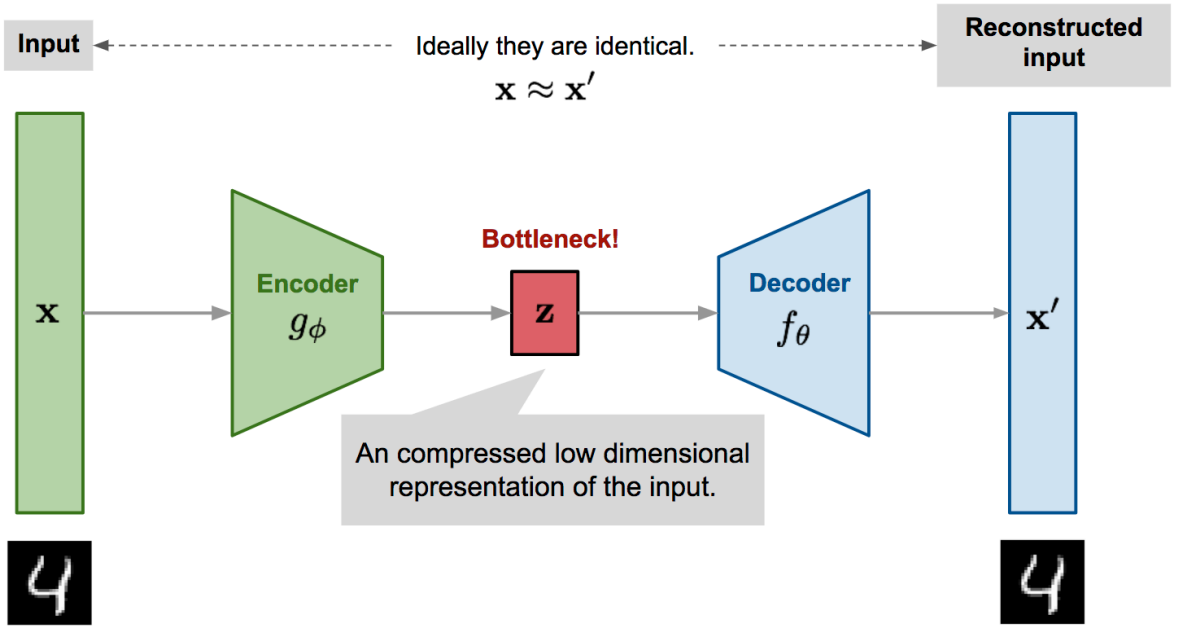
Extend ICA to nonlinear case to get deep learning?
Unfortunately, "basic" nonlinear ICA is not identifiable:
If we define nonlinear ICA model simply as

$$x_i(t) = f_i(s_1(t), \ldots, s_n(t)) \quad \text{for all } i, j = 1 \ldots n$$

we cannot recover original sources (Darmois, 1952; Hyvärinen & Pajunen, 1999)



β-VAE



Why?

$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x} \mid \mathbf{z})] - \beta D_{KL}(\log q_\theta(\mathbf{z} \mid \mathbf{x}) || p(\mathbf{z}))$ Increase β can encourage disentanglement

Higgins, Irina, et al. "beta-vae: Learning basic visual concepts with a constrained variational framework." International conference on learning representations. 2017.

β-VAE

From the last lecture:

$$\max_{\phi,\theta} \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

- maximize $\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})]$: reconstruct $\mathbf{x}$
- minimize $D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$: approximate prior

$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x} \mid \mathbf{z})] - \beta D_{KL}(\log q_\theta(\mathbf{z} \mid \mathbf{x})||p(\mathbf{z}))$ Increase β can encourage disentanglement

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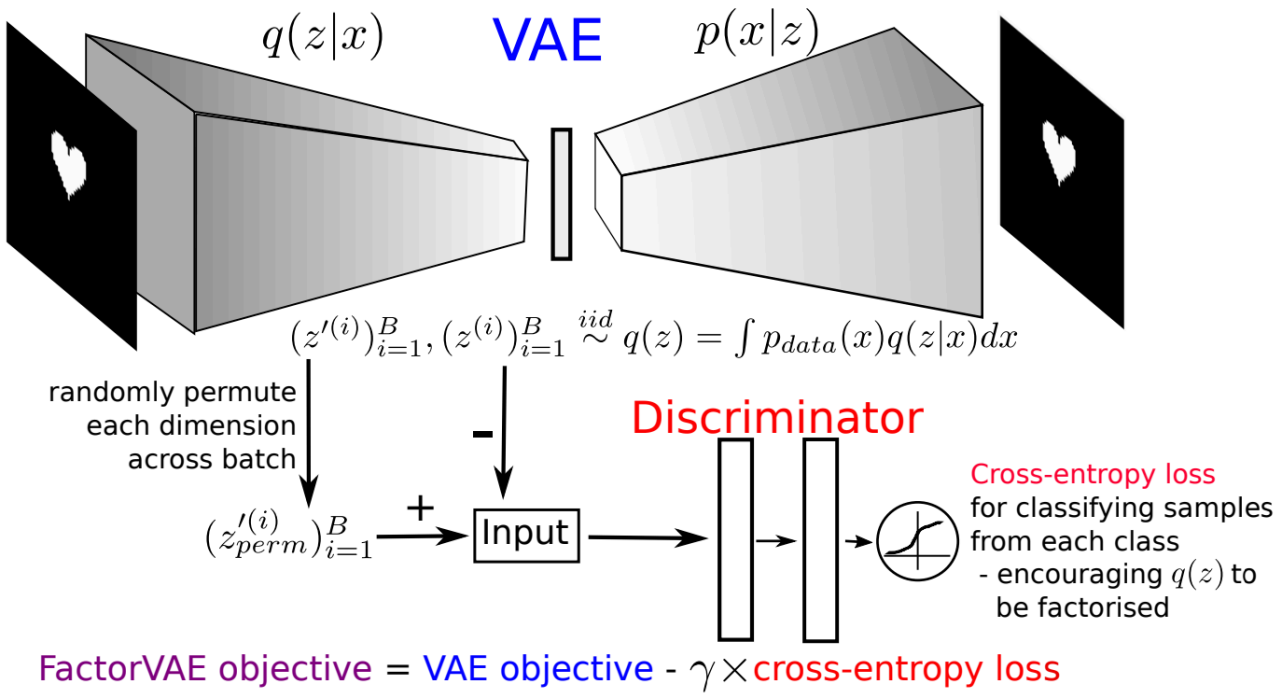
FactorVAE

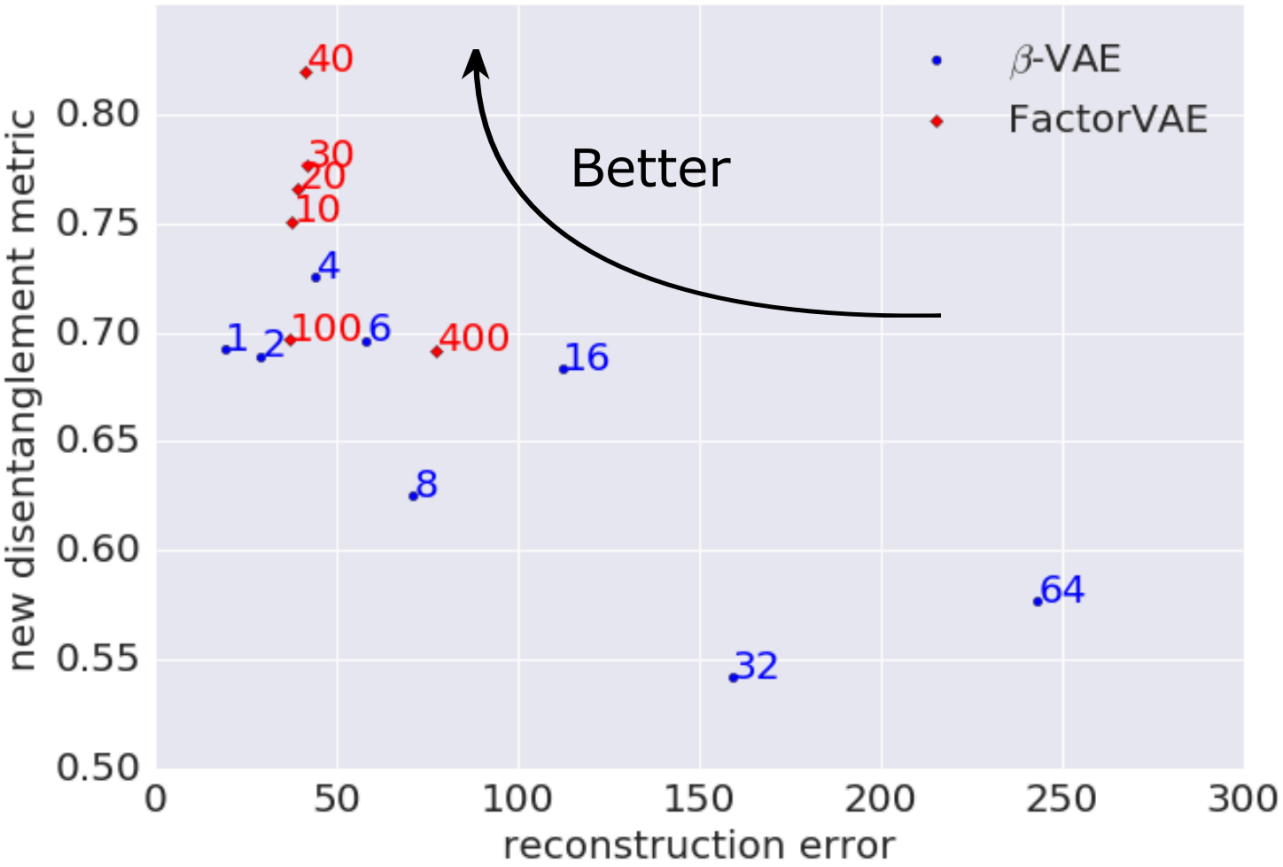
Idea: β-VAE optimizes the two terms together, FactorVAE separates them



Kim, H. and Mnih, A., 2018, July. Disentangling by factorising. In International Conference on Machine Learning (pp. 2649-2658). PMLR.

FactorVAE

Idea: β-VAE optimizes the two terms together, FactorVAE separates them



Identifiable VAE (i-VAE)

VAE $p(z) \longrightarrow p(z \mid u)$ i-VAE

Main Assumption: A conditionally factorized prior distribution over the latent variables $p_\theta(z|u)$, where u is an additionally observed variable
And the data generation stage is a additive noise model $x = f(z) + \epsilon$

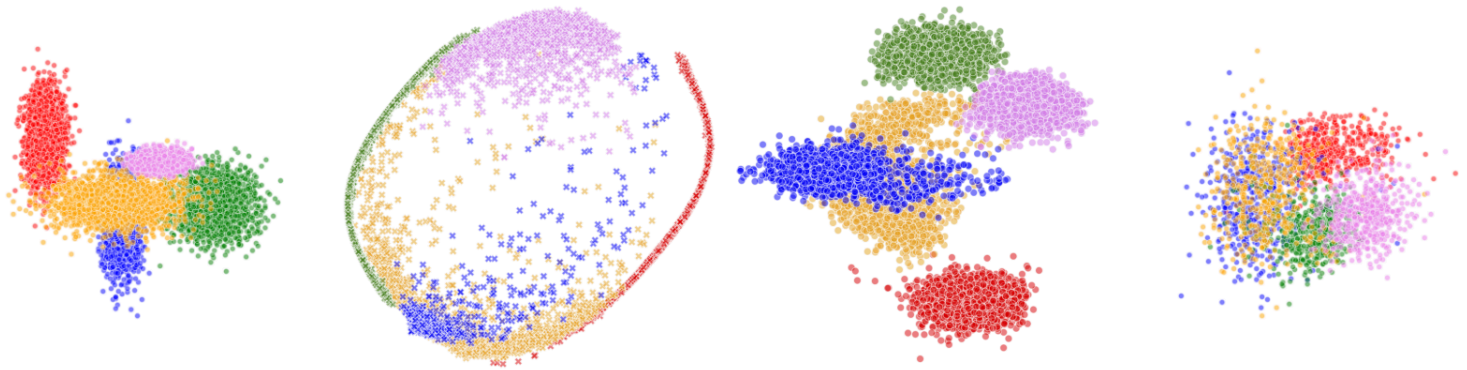
$p(z|u)$ is conditionally factorial

$$p(z|u) = \prod_{i=1}^{n} p(z_i|u),$$

Maximize $ELBO = E_D(E_{q_\phi(z|x,u)} \log p_\theta(x|z,u) - KL(q_\phi(z|x,u)||p(z|u))$

Khemakhem, Ilyes, et al. "Variational autoencoders and nonlinear ica: A unifying framework." International Conference on Artificial Intelligence and Statistics. PMLR, 2020.

Identifiable VAE (i-VAE)



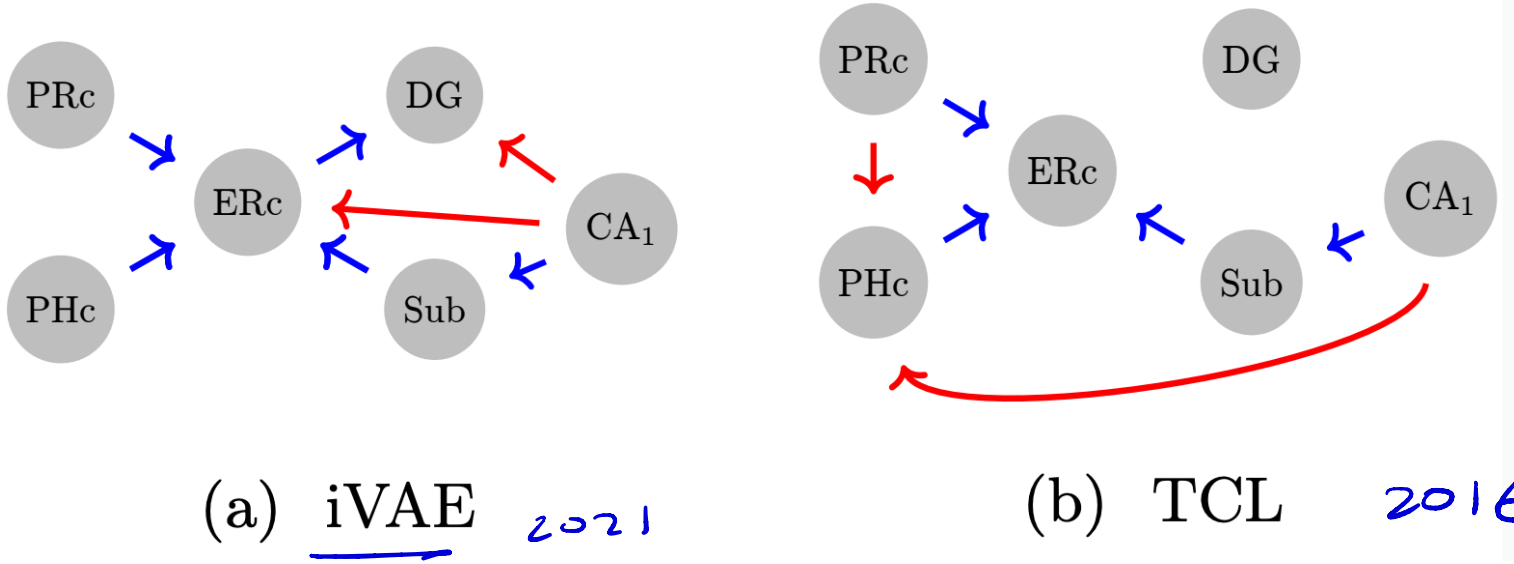
(a) $p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{u})$ (b) $p_{\boldsymbol{\theta}^*}(\mathbf{x}|\mathbf{u})$ (c) $p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x},\mathbf{u})$ (d) $p_{\mathrm{VAE}}(\mathbf{z}|\mathbf{x})$

i-VAE for Causal Discovery

hippocampal fMRI data

Blue: Correct (feasible given anatomical connectivity)

Red: Incorrect (incompatible with anatomical structure)



(a) iVAE 2021 (b) TCL 2016.

Q: Which method is better?

Part III

Summary

Learning Outcomes

- Appreciate how causal learning differs from statistical learning
- Understand the tasks of causal inference and causal discovery
- Be able to describe ICA and its identifiability
- Be able to connect nonlinear ICA and the disentanglement problem in generative models
- Know what β-VAE, FactorVAE, I-VAE are

Motivation

Trustworthy ML