

- ► Introduction
- ► Motivation
- ► Causality
- ► Methods

Introduction

► Conclusion

The Plan for Week 4

► Today

INTRODUCTION

•0000

- ► Lecture
- ► Labs
 - ► Quiz (Moodle)
 - ► Modelling (Colab)

Do the quiz before starting the lab exercises.

RESOURCES

INTRODUCTION 00000

- ► Textbooks
 - ▶ J. Pearl and D. Mackenzie, The Book of Why: The New Science of Cause and Effect, 1st ed. USA: Basic Books. Inc., 2018. 1
 - ▶ J. Pearl, M. Glymour, and N. P. Jewell, Causal Inference in Statistics: A Primer. John Wiley & Sons, 2016.²
 - ▶ J. Peters, D. Janzing, and B. Scholkopf, Elements of Causal Inference: Foundations and Learning Algorithms. The MIT Press, 2017.³
- ▶ Online
 - ► Introduction to Causal Inference⁴

See Moodle page for a more extensive list of additional resources.

¹http://bayes.cs.ucla.edu/WHY/

²http://bayes.cs.ucla.edu/PRIMER/

³https://mitpress.mit.edu/books/elements-causal-inference

⁴https://www.bradyneal.com/causal-inference-course

Tools

INTRODUCTION

00000

We are going to use the following:

- ► Python 3
- ► scikit-learn (ML methods)
- ► EconML⁵ (CI estimators)
- ▶ the usual stack (numpy, pandas, matplotlib)
- ► Google Colab

⁵https://github.com/microsoft/EconML

A MACHINE LEARNING PERSPECTIVE

We will need the following:

Introduction ooo•o

- ightharpoonup Supervised learning predict y given (X, y) samples
 - ► Regression (continuous outcome)
 - ► Classification (binary outcome)
- ► Basic data exploration
- ► Data pre-processing
- ► Training and testing
- ► Using metrics

We know all this by now -> we can do causal inference!

WHY DO I NEED THIS?

Introduction oooo

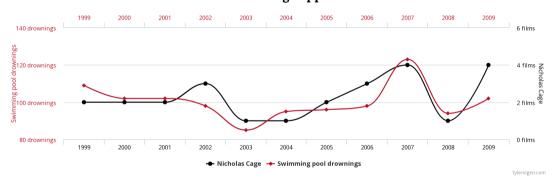
- ▶ Data science is more than just ML
- ► It's about decision making
- ► Associations vs. causal relations
- ► Correlation does not imply causation
- ▶ Also: biases and shifts within the data that skew the results
- ► Wrong conclusions -> bad decisions

Spurious Correlations

INTRODUCTION

Number of people who drowned by falling into a pool correlates with

Films Nicolas Cage appeared in



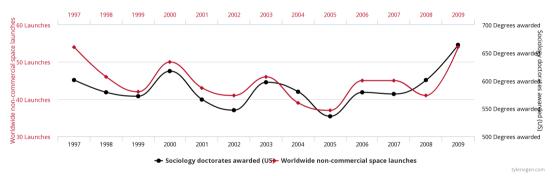
Credit: https://www.tylervigen.com/spurious-correlations

INTRODUCTION

Worldwide non-commercial space launches

correlates with

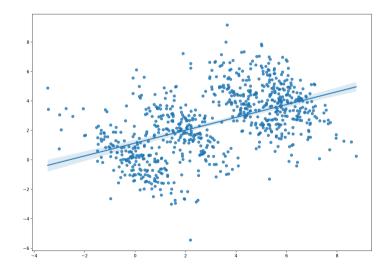
Sociology doctorates awarded (US)



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

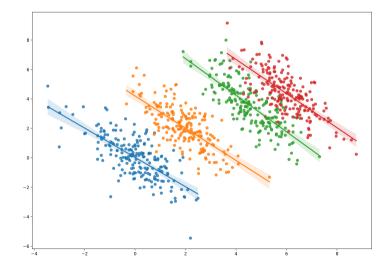
SIMPSON'S PARADOX

Introduction



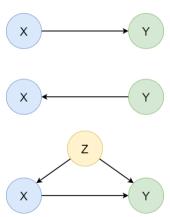
SIMPSON'S PARADOX

Introduction



TAKEAWAY

- ► We need to think about the causal links within the data (causal graphs).
- ► Cause and effect
- ▶ Question: As we *change* the cause, how does the effect *change*?



PROBLEM SETTING

We want to estimate the causal effect of treatment T on outcome Y

- \blacktriangleright What benefits accrue if we intervene to change T?
- ► Treatment must be modifiable
- ► We observe only one outcome per each individual

Ideal scenario:

- 1. Assume state S_0
- 2. Apply the treatment (t=1)
- 3. Observe the outcome (Y_1)
- 4. Reset the state to S_0
- 5. Do not apply the treatment (t=0)
- 6. Observe the outcome (Y_0)
- 7. Compare the outcomes Y_1 and Y_0 to get the causal effect

REAL-LIFE EXAMPLE

- \blacktriangleright My headache went away after I had taken the aspirin (Y_1)
- ▶ Would the headache have gone away without taking the aspirin? $(Y_0 =?)$
- ▶ We cannot go back in time and test the alternative!
- ► Cannot reset the state -> cannot compare the outcomes -> no effect
- ► Test more people and measure the average outcome?

More Examples

INTRODUCTION

- ► Developing a new vaccine
- ► Government policy
- ▶ Recommending the best treatment for a specific patient

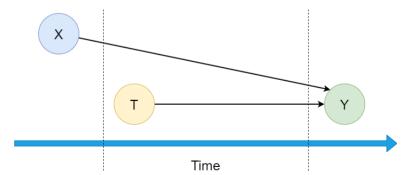
It's about finding out how a specific action affects a system of interest.

- ► Action == intervention (something we change)
- ► System == the very thing we study (group of people, physical objects, etc.)
- ► Outcome == system's characteristic of interest (response)
- ► Effect == difference between outcomes

INTRODUCTION

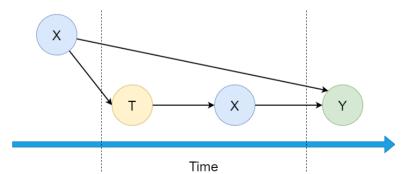
RANDOMISED CONTROLLED TRIALS

- ▶ Data from controlled experiments
- ightharpoonup Randomised T people assigned T=0 (control) or T=1 (treated)
- ► This mimicks observing alternative reality
- ightharpoonup Record background characteristics as $X = [X_1, X_2, ..., X_n]$
- ► Can be expensive or even unfeasible (e.g. smoking)



Observational Data

- ► Passively collected data (non-experimental)
- ► Abundant nowadays
- ► Quasi-experimental study
- \blacktriangleright Keep only X recorded before Y (discard other)
- ► Lack of randomisation and control (imbalances)



ML PERSPECTIVE

- ► Correlation vs. causation
- ► Outliers different meaning
- ► Imbalanced data (not just Y)
- ► Out-of-distribution (OOD) generalisation
- ► ML vs. CI:
 - ► ML: predict Y given (X, Y) samples
 - ► CI: predict effects given (X, Y) samples

MORE ON ML VS. CI

ML

INTRODUCTION

- ► Train on (X, Y) samples
- ► Predict Y given X test samples
- ► Assumes the same distribution of training and testing samples

CI

- ► Train on (X, T, Y) samples
- ightharpoonup Predict Y for (X, T) and (X, 1-T)
- ► (X, 1-T): predict the outcomes we haven't observed
- ► Treated (t = 1) and control (t = 0) groups often have different distributions
- ► We learn from one distribution, but make predictions for a different one!
- ► The usual IID assumption no longer applies here

FUNDAMENTALS

INTRODUCTION

$$Effect = Y_1 - Y_0$$

•00000000000000

Causality

#	X_1	X_2	X_3	Τ	Y_0	Y_1
1	1.397	0.996	0	1	?	4.771
2	0.269	0.196	1	0	2.956	?
3	1.051	1.795	1	1	?	4.164
4	0.662	0.196	0	1	?	6.172
5	0.856	1.795	1	0	7.834	?

Observed and unobserved outcomes are factuals and counterfactuals respectively.

Missing counterfactuals: This is known as the fundamental problem of causal inference. We cannot *observe* the difference, but we can **approximate** it.

TREATMENT EFFECT

INTRODUCTION

Let us define the **true** outcome $\mathcal{Y}_t^{(i)}$ of individual (i) that received treatment $t \in \{0, 1\}$. The Individual Treatment Effect (ITE) is then defined as follows:

$$ITE^{(i)} = \mathcal{Y}_1^{(i)} - \mathcal{Y}_0^{(i)}$$

The Average Treatment Effect (ATE) builds on ITE:

$$ATE = \mathbb{E}[ITE]$$

Note: empirical (sample) ATE is the mean of ITEs.

TREATMENT EFFECT - ITE EXAMPLE

We are given the outcomes Y for both the treated (t=1) and control (t=0) case, where $Y_1 = 3$ and $Y_0 = 2$.

What is the value of ITE?

TREATMENT EFFECT - ITE EXAMPLE (2)

We are given the outcomes Y for both the treated (t = 1) and control (t = 0) case, where $Y_1 = 3$ and $Y_0 = 2$.

What is the value of ITE?

$$ITE^{(i)} = \mathcal{Y}_1^{(i)} - \mathcal{Y}_0^{(i)}$$

$$ITE = 3 - 2 = 1$$

TREATMENT EFFECT - ATE EXAMPLE

We are given the following data:

 $ightharpoonup Y_0 \in \{2, 3, 1\}$

INTRODUCTION

 $ightharpoonup Y_1 \in \{3,4,2\}$

What is the value of ATE?

Treatment Effect - ATE Example (2)

We are given the following data:

 $ightharpoonup Y_0 \in \{2, 3, 1\}$

INTRODUCTION

► $Y_1 \in \{3, 4, 2\}$

What is the value of ATE?

$$ATE = \mathbb{E}[ITE]$$
 $ITE^{(0)} = 3 - 2 = 1$
 $ITE^{(1)} = 4 - 3 = 1$
 $ITE^{(2)} = 2 - 1 = 1$

$$ATE = \frac{ITE^{(0)} + ITE^{(1)} + ITE^{(2)}}{3} = \frac{1+1+1}{3} = \frac{3}{3} = 1$$

Metrics

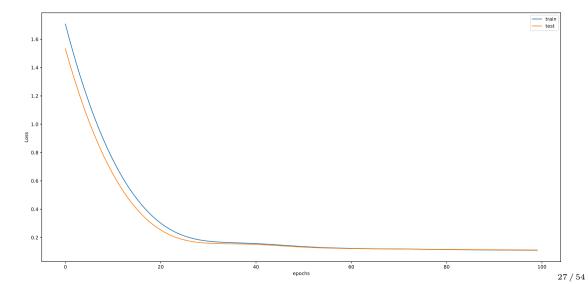
INTRODUCTION

- ▶ In practice, we want to measure how accurate our inference model is
- ▶ This is often done by measuring the amount of error (ϵ) or risk (\mathcal{R}) introduced by a model

Examples:

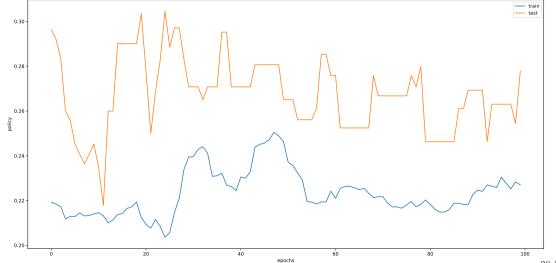
- ightharpoonup ϵ_{ATE}
- ightharpoonup ϵ_{PEHE}
- ightharpoonup ϵ_{ATT}
- ightharpoons \mathcal{R}_{pol}

METRICS - MOTIVATION



METRICS - MOTIVATION (2)

Introduction



METRICS - PREDICTIONS

INTRODUCTION

Let us denote $\hat{u}_{t}^{(i)}$ as **predicted** outcome for individual (i) that received treatment t. Then, our predicted ITE and ATE can be written as:

Causality

0000000000000000

$$\widehat{ITE}^{(i)} = \hat{y}_1^{(i)} - \hat{y}_0^{(i)}$$

$$\widehat{ATE} = \frac{1}{n} \sum_{i=1}^{n} \widehat{ITE}^{(i)}$$

Metrics - Measuring Errors

This allows us to define the following measurement errors:

$$\epsilon_{PEHE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\widehat{ITE}^{(i)} - ITE^{(i)})^2}$$

$$\epsilon_{ATE} = \left| \widehat{ATE} - ATE \right|$$

Where PEHE stands for Precision in Estimation of Heterogeneous Effect, and which essentially is a Root Mean Squared Error (RMSE) between predicted and true ITEs.

BENCHMARK DATASETS

Semi-simulated data or combinations of experimental and observational datasets. We use metrics depending on what kind of information we have access to (true effects/counterfactuals).

Some well-established causal inference datasets:

► IHDP

- ► Jobs
- ► News
- ► Twins
- ► ACIC challenges

Metrics - Types

With effect/counterfactuals

 $ightharpoonup \epsilon_{ATE}$

INTRODUCTION

- ightharpoonup ϵ_{PEHE}
- ► Datasets with simulated outcomes
- ► (it's unnatural to observe both outcomes!)

Without effect/counterfactuals

- $ightharpoonup \epsilon_{ATT}$ (ATE on the Treated)
- $ightharpoonup \mathcal{R}_{pol}$ (Policy Risk)
- ► Datasets closer to reality
- ► Either purely observational or mixed with RCTs

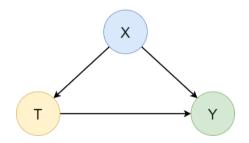
ASSUMPTIONS

- ► Ignorability:
 - ► No hidden confounders (we observe everything)
- \blacktriangleright All background covariates X happened before the outcome Y
- ightharpoonup Modifiable treatment T
- ► Stable Unit Treatment Value Assumption (SUTVA):
 - ► No interference between units
 - ► Consistent treatment (different versions disallowed)

Assumptions (2)

INTRODUCTION

► Most CI estimators assume the *triangle* graph

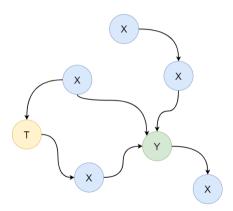


- ► This is a very simplistic view of the world
- ► Actual reality can be much more complex

Assumptions (3)

Introduction

- ► Can we infer graphs from data?
- ► Causal discovery



Modern Approaches

Introduction

Mosty regression and classification (classic ML), but combined in a smart way.

- ► Recent surveys on modern causal inference methods ⁶ ⁷
- ► Most popular:
 - ► Inverse Propensity Weighting (IPW)
 - ► Doubly-Robust
 - ► Double/Debiased Machine Learning
 - ► Causal Forests
 - ► Meta-Learners
 - ► Multiple based on neural networks (very advanced)

We will start with a simple regression, enhance it with IPW, and conclude with Meta-Learners.

⁶https://dl.acm.org/doi/10.1145/3397269

⁷https://arxiv.org/abs/2002.02770

S-Learner

INTRODUCTION

We want to estimate

$$\mu(t, x) = \mathbb{E}[\mathcal{Y}|X = x, T = t]$$

- 1. Obtain $\hat{\mu}(t,x)$ estimator.
- 2. Predict ITE as

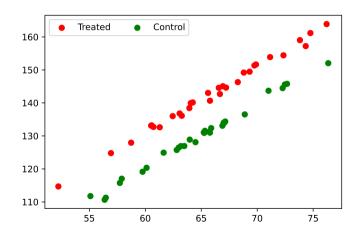
$$\widehat{ITE}(x) = \hat{\mu}(1, x) - \hat{\mu}(0, x)$$

- ► Single model approach
- ► Allows heterogenous treatment effects
- ► Can be biased (next slide)

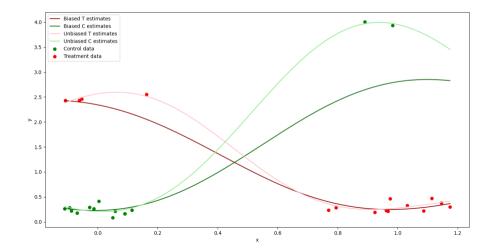
S-Learner - Code

```
lr = LinearRegression()
# input: [X, T], target: Y
lr.fit(np.concatenate([x train, t train], axis=1), y train)
# predict Y0 given [X, 0] - set T=0
y0 pred = lr.predict(np.concatenate([x test, np.zeros like(t test)], axis=1))
# predict Y1 given [X, 1] - set T=1
y1 pred = lr.predict(np.concatenate([x test, np.ones like(t test)], axis=1))
# effect = v1 - v0
effect pred = y1 pred - y0 pred
```

WHEN IT WORKS



BIASED ESTIMATORS



Propensity Score

$$e(x) = P(t_i = 1 | x_i = x)$$

- ▶ Probability of a unit i receiving the treatment (T=1)
- ► For discrete treatments, this is a classification problem
- ▶ Binary classification in most cases as $t \in \{0, 1\}$
- \blacktriangleright We denote $\hat{e}(x)$ as our estimation

IPW ESTIMATOR

Using the propensity score $\hat{e}(x)$, we can obtain the following weights

$$w_i = \frac{t_i}{\hat{e}(x_i)} + \frac{1 - t_i}{1 - \hat{e}(x_i)}$$

- ► These are called Inverse Propensity Weights (IPW)
- ▶ Use the weights to perform **weighted** regression
- ► Similar to S-Learner, but combines regression and classification
- ► Sample importance (pay attention to scarce data points)
- \blacktriangleright Either $\hat{e}(x)$ or $\hat{\mu}(x)$ can still have bias (misspecification)
- ▶ Doubly-Robust method attempts to address that

IPW ESTIMATOR - CODE

```
clf = LogisticRegression()
weights = get_ps_weights(clf, x_train, t_train)
lr = LinearRegression()
# input: [X, T], target: Y
lr.fit(np.concatenate([x_train, t_train], axis=1), y_train, sample_weight=weights)
...
```

T-LEARNER

- ▶ Treated and control distributions are often different
- \triangleright Solution: fit two separate regressors

$$\mu_1(x) = \mathbb{E}[\mathcal{Y}|X=x,T=1]$$

$$\mu_0(x) = \mathbb{E}[\mathcal{Y}|X=x, T=0]$$

- 1. Learn $\mu_1(x)$ from treated units, obtain $\hat{\mu}_1(x)$.
- 2. Learn $\mu_0(x)$ from control units, obtain $\hat{\mu}_0(x)$.
- 3. Predict ITE as

$$\widehat{ITE}(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x)$$

T-Learner - Code

```
m0 = LinearRegression()
m1 = LinearRegression()
t0 idx = (t train == 0).flatten()
t1 idx = (t train == 1).flatten()
# train on control units
m0.fit(x train[t0 idx], y train[t0 idx])
# train on treated units
m1.fit(x train[t1 idx], y train[t1 idx])
y0 pred = m0.predict(x test)
v1 pred = m1.predict(x test)
effect pred = v1 pred - v0 pred
```

T-Learner - Code (2)

```
tl = TLearner(models=LinearRegression())
tl.fit(y_train, t_train, X=x_train)
effect_pred = tl.effect(x_test)
```

X-Learner

A hybrid of the previous approaches (details here⁸). There are three main stages.

- 1. Learn treated and control separately (same as T-Learner).
- 2. Predict and learn *imputed* effects (mix of Y_f and Y_{cf}).
- 3. Learn a propensity score function.

The final treatment effect estimate is a weighted average of the two estimates from Stage 2:

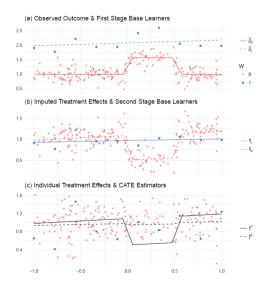
$$\hat{\tau}(x) = \hat{e}(x)\hat{\tau}_0(x) + (1 - \hat{e}(x))\hat{\tau}_1(x)$$

⁸http://arxiv.org/abs/1706.03461

X-Learner - Code

```
xl = XLearner(models=LinearRegression(), propensity_model=LogisticRegression())
xl.fit(y_train, t_train, X=x_train)
effect_pred = xl.effect(x_test)
```

X-Learner - Intuition



SUMMARY

- ► We just scratched the surface here
- ► Causal discovery (inferring graphs from data) big topic on its own
- Estimating causal effects vs. recommending treatments⁹
- ▶ Other methods
 - ► Instrumental variables
 - ► Relaxing the common assuptions
 - ► Trees, neural networks, policy learners

⁹http://arxiv.org/abs/2104.04103

MAIN TAKEAWAYS

- ► Causal inference is about estimating causal effects
 - ► For instance, measure the effectiveness of a treatment
- ▶ RCTs are the most reliable source of data, but can be unfeasible to obtain
- ▶ Non-experimental data are a great alternative, but can be biased
- ▶ Most methods are about finding *unbiased* estimators
- ▶ Machine Learning and Causal Inference can be both mutually beneficial
 - ► ML delivers better CI estimators
 - ► CI helps ML with OOD generalisation
- ▶ Assumptions and graphs are important and must be considered in applications

ACKNOWLEDGEMENTS

INTRODUCTION

This lecture builds heavily on the materials from Introduction to Machine Learning for Causal Analysis Using Observational Data online course, delivered on June 22-23 2021 by Damian Machlanski, Dr Spyros Samothrakis and Professor Paul Clarke.

References

- ▶ J. M. Robins, A. Rotnitzky, and L. P. Zhao, 'Estimation of Regression Coefficients When Some Regressors are not Always Observed', Journal of the American Statistical Association, vol. 89, no. 427, pp. 846–866, Sep. 1994.
- ▶ U. Shalit, F. D. Johansson, and D. Sontag, 'Estimating individual treatment effect: generalization bounds and algorithms', in International Conference on Machine Learning, Jul. 2017, рр. 3076–3085.
- ▶ V. Chernozhukov et al., 'Double/debiased machine learning for treatment and structural parameters', The Econometrics Journal, vol. 21, no. 1, pp. C1–C68, Feb. 2018.
- ▶ S. Wager and S. Athey, 'Estimation and Inference of Heterogeneous Treatment Effects using Random Forests', Journal of the American Statistical Association, vol. 113, no. 523, pp. 1228–1242, Jul. 2018.
- ▶ S. R. Künzel, J. S. Sekhon, P. J. Bickel, and B. Yu. 'Meta-learners for Estimating Heterogeneous Treatment Effects using Machine Learning', Proc Natl Acad Sci USA, vol. 116, no. 10, pp. 4156-4165, Mar. 2019.
- ▶ R. Guo, L. Cheng, J. Li, P. R. Hahn, and H. Liu, 'A Survey of Learning Causality with Data: Problems and Methods', ACM Comput. Surv., vol. 53, no. 4, p. 75:1-75:37, Jul. 2020.
- ▶ L. Yao, Z. Chu, S. Li, Y. Li, J. Gao, and A. Zhang, 'A Survey on Causal Inference', arXiv:2002.02770 [cs. stat], Feb. 2020.

WHAT'S NEXT?

INTRODUCTION

- ► Moodle quiz
 - ► A few theoretical Qs
 - ► Calculating effects and some metrics
- ► Modelling
 - ► Two datasets
 - ► S-Learner, IPW, X-Learner
 - ► Follow the instructions within the notebook

Important: Do the quiz **first** before moving to the modelling part (you will need to know how to calulate effects and metrics).